

PARTICLES AND QUANTUM FIELDS

Particles and Quantum Fields

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*To my wife Annemarie
and our son Hagen Michael II*

Preface

This book arose from lectures I gave at the Freie Universität Berlin over the past five decades. They were intended to prepare graduate students for their research in elementary-particle physics or in many-body theory of condensed matter. They should serve as a general introduction and a basis for understanding more advanced work on the subject.

The theory of quantum fields presented in this book is mainly based on the perturbative approach. Elementary particles are introduced initially without any interactions. These are added later, and their strength is parametrized by some coupling constant g . The consequences are studied order by order in g , with the particles propagating forward from interaction to interaction. Such a treatment is clearly a gross simplification of what happens in nature, where even the existence of a free particle involves the full interaction from the very beginning. Nevertheless, this kind of procedure has been the basis of many successful theories. In all of them, there exist dominant freely propagating excitations or elementary particles at least in some experimentally accessible limit. The most prominent example is the theory of strongly interacting particles. There they are described as being composed of quarks held together by gluons which interact via a nonabelian gauge theory called quantum chromodynamics (QCD). In the limit of large energies, the particles behave like free point-like particles. This behavior was named *parton-like* by Richard Feynman. The existence of such a limiting behavior in QCD was called *asymptotic freedom*. It was the main reason for the possibility of developing a theory for these particles, which gave good explanations of many interaction processes between elementary particles. The initial *creation* of the particles, however, remained far from being understood. It involves a regime of strong interactions where perturbation theory fails.

A field-theoretic method to reach into this regime has been developed in quantum field theory of many-body physics. There a separation of the two regimes, the formation of particle-like excitation and their scattering, is much clearer to observe experimentally than in particle physics. For this reason, many-body theory has been a major source of inspiration for the development of theoretical methods to describe strongly interacting phenomena. An extension of perturbation theory into the strongly interacting regime has so far been possible mainly by employing resummation techniques. Initially, theorists have summed certain classes of Feynman diagrams by repeating infinitely many times the same interaction leading to a geometric series whose sum can be evaluated. This has allowed the understanding of many pronounced observable phenomena as consequences of a sum of infinitely

many bubbles and ladders of diagrams. The methods for this were developed by Hartree, Fock, and Bogoliubov in many-body theory, and by Bethe and Salpeter in quantum electrodynamics.

The development of renormalization group theory has led to a generalization of this method. It permits to extend the sum of bubbles and ladders to sums of diagrams of many different topologies. This makes them applicable in the regime of strong couplings, where they can be used to study various many-body phenomena even in the so-called *critical regime*. There the interactions become so strong that they are much more important than the free-particle propagation.

In many-body theory, one can parametrize the separation of the two regimes quite clearly by formulating the theory on a lattice. The propagation is characterized by a so-called hopping amplitude from lattice point to lattice point. The critical regime is reached when the masses of some of the participating excitations go to zero. In this limit, the range of their propagation tends to infinity, and their interaction becomes increasingly important.

An efficient alternative to the summation of infinitely many perturbation-theoretic diagrams is based on a variational approach. Its power was discovered in 1877 by John Rayleigh and formalized by Walter Ritz in 1908. Some time ago, the theory was revived by Feynman and Kleinert.¹ They set up a first-order variational approximation to path integrals, which led to reasonable approximations for a variety of quantum mechanical problems. The approximations were later expanded to all orders, and have finally led to the powerful *field-theoretic variational perturbation theory* (VPT). In that form, the theory is able to simplify and replace the popular renormalization group approach of critical phenomena. It has been successfully applied to many phase transitions, and is published in a monograph.²

An important aspect of a theory of critical phenomena is the fact that the free-field propagators play no longer the important role they have in perturbation expansions. The underlying free-particle behavior is based on a Gaussian approximation to field fluctuations. In the critical regime, this approximation of the distributions has tails which follow power-like distributions. Such tails are observed in the statistics of very rare events, which are called “black-swan events”.³ These occur in nature in many different circumstances, ranging from oceanic monster waves over earthquakes and wind gusts, to catastrophic crashes of financial markets.⁴

I want to thank my friend Remo Ruffini for creating an extremely lively and inspiring environment for scientific work in particle and astrophysics at many exciting places of the globe, where I was invited for lectures and discussions of topics of this

¹R.P. Feynman and H. Kleinert, Phys. Rev. A *34*, 5080 (1986).

²H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of Φ^4 -Theories*, World Scientific, Singapore 2001, pp. 1–489 (<http://klnrt.de/b8>). See Chapter 20 for the variational approach.

³H. Kleinert, *Quantum Field Theory of Black-Swan Events*, EPL *100*, 10001 (2013) (www.ejtp.com/articles/ejtpv11i31p1.pdf); *Effective Action and Field Equation for BEC from Weak to Strong Couplings*, J. Phys. B *46*, 175401 (2013) (<http://klnrt.de/403>).

⁴H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, World Scientific, Singapore, 2009 (<http://klnrt.de/b5>). See Chapter 20.

book. Ruffini, who holds a chair in theoretical physics at the university of Rome “La Sapienza”, founded an international center which I am part of, where scientists from all over the world do research, and where students can prepare their Ph.D. degree (for details see ICRANet.org).

I am also very grateful to my colleague Axel Pelster who, for many years, has shared with me the burden and joy of bringing students of the Freie Universität Berlin to their master’s and doctor’s degrees. His careful reading of large parts of the manuscript has produced useful insights and corrections.

Another person who greatly helped me to spot errors in Chapters 23 and 24 is my former CERN colleague and friend Franco Buccella, professor of theoretical physics in beautiful Naples. These chapters were also proofread by Harald Fritzsch. In Chapter 30 several corrections came from Claus Kiefer, Hans Ohanian, Kellogg Stelle, Pisin Chen, She-Sheng Xue, and Václav Zatloukal.

Finally I want to thank Dr. Annemarie Kleinert for her patience and sacrifice of a lot of time, in which she set aside her own research projects to help me spot and correct many errors. Without her repeated reading the manuscript and her persistent encouragement, the book would certainly never have been finished.

The reader who detects errors, is kindly asked to report them by email to h@klmrt.de.

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Berlin, April 2016

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*Any wide piece of ground is the potential site of a palace,
but there's no palace till it's built.*
FERNANDO PESSOA (1888-1935), The Book of Disquiet

1

Fundamentals

Before turning to the actual subject of this book it is useful to recall some basic theoretical background underlying the theory to be developed.

1.1 Classical Mechanics

The orbits of a classical-mechanical system are described by a set of time-dependent generalized coordinates $q_1(t), \dots, q_N(t)$. A Lagrangian

$$L(q_i, \dot{q}_i, t) \tag{1.1}$$

depending on $q_1, \dots, q_N$ and the associated velocities $\dot{q}_1, \dots, \dot{q}_N$ governs the dynamics of the system. The dots denote the time derivative d/dt . The Lagrangian is at most a quadratic function of $\dot{q}_i$. The time integral

$$\mathcal{A}[q_i] = \int_{t_a}^{t_b} dt L(q_i(t), \dot{q}_i(t), t) \tag{1.2}$$

of the Lagrangian along an arbitrary path $q_i(t)$ is called the *action* of this path. The path being actually chosen by the system as a function of time is called the *classical path* or the *classical orbit* $q_i^{\text{cl}}(t)$. It has the property of extremizing the action in comparison with all neighboring paths

$$q_i(t) = q_i^{\text{cl}}(t) + \delta q_i(t) \tag{1.3}$$

having the same endpoints $q(t_b), q(t_a)$, i.e.

$$\delta q_i(t_a) = \delta q_i(t_b) = 0. \tag{1.4}$$

To express this property formally, one introduces the *variation* of the action as the linear term in the Taylor expansion of $\mathcal{A}[q_i]$ in powers of $\delta q_i(t)$:

$$\delta \mathcal{A}[q_i] \equiv \{\mathcal{A}[q_i + \delta q_i] - \mathcal{A}[q_i]\}_{\text{lin term in } \delta q_i}. \tag{1.5}$$

The extremal principle for the classical path is then

$$\delta\mathcal{A}[q_i]\Big|_{q_i(t)=q_i^{\text{cl}}(t)} = 0, \quad (1.6)$$

for all variations with the property (1.4).

Since the action is a temporal integral of a Lagrangian, the extremality property can be phrased in terms of differential equations. Let us calculate $\delta\mathcal{A}[q_i]$ explicitly:

$$\begin{aligned} \delta\mathcal{A}[q_i] &= \{\mathcal{A}[q_i + \delta q_i] - \mathcal{A}[q_i]\}_{\text{lin}} \\ &= \int_{t_a}^{t_b} dt \{L(q_i(t) + \delta q_i(t), \dot{q}_i(t) + \delta \dot{q}_i(t), t) - L(q_i(t), \dot{q}_i(t), t)\}_{\text{lin}} \\ &= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i(t) \right\} \\ &= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right\} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta q_i(t) \Big|_{t_a}^{t_b}. \end{aligned} \quad (1.7)$$

The last expression arises from the previous one by a partial integration of the $\delta \dot{q}_i$ -term. Here, as in the entire book, repeated indices are understood to be summed (*Einstein's summation convention*). The endpoint terms (also referred to as *surface* or *boundary terms*), where the time t is equal to t_a or t_b may be dropped due to (1.4). Thus we find that the classical orbit $q_i^{\text{cl}}(t)$ satisfies the *Euler-Lagrange equations*:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}. \quad (1.8)$$

There exists an alternative formulation of classical dynamics. It is based on a Legendre-transformed function of the Lagrangian called the *Hamiltonian*:

$$H \equiv \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i - L(q_i, \dot{q}_i, t). \quad (1.9)$$

Its value at any time is equal to the energy of the system. According to the general theory of Legendre transformations [2], the natural variables on which H depends are no longer q_i and $\dot{q}_i$, but q_i and the generalized momenta p_i . The latter are defined by the equations

$$p_i \equiv \frac{\partial}{\partial \dot{q}_i} L(q_i, \dot{q}_i, t), \quad (i = 1, \dots, N). \quad (1.10)$$

In order to express the Hamiltonian $H(p_i, q_i, t)$ in terms of its proper variables p_i, q_i , the equations (1.10) have to be solved for $\dot{q}_i$ by a velocity function

$$\dot{q}_i = v_i(p_i, q_i, t). \quad (1.11)$$

This is possible provided the *Hessian metric*

$$h_{ij}(q_i, \dot{q}_i, t) \equiv \frac{\partial^2}{\partial \dot{q}_i \partial \dot{q}_j} L(q_i, \dot{q}_i, t) \quad (1.12)$$

is nonsingular. The result is inserted into (1.9), leading to the Hamiltonian as a function of p_i and q_i :

$$H(p_i, q_i, t) = p_i v_i(p_i, q_i, t) - L(q_i, v_i(p_i, q_i, t), t). \quad (1.13)$$

In terms of this Hamiltonian, the action is the following functional of $p_i(t)$ and $q_i(t)$:

$$\mathcal{A}[p_i, q_i] = \int_{t_a}^{t_b} dt [p_i(t) \dot{q}_i(t) - H(p_i(t), q_i(t), t)]. \quad (1.14)$$

This is the so-called *canonical form* of the action. The classical orbits are now specified by $p_i^{\text{cl}}(t)$, $q_i^{\text{cl}}(t)$. They extremize the action in comparison with all neighboring orbits in which the coordinates $q_i(t)$ are varied at fixed endpoints [see (29.5), (1.4)], whereas the momenta $p_i(t)$ are varied without restriction:

$$\begin{aligned} q_i(t) &= q_i^{\text{cl}}(t) + \delta q_i(t), & \delta q_i(t_a) = \delta q_i(t_b) = 0, \\ p_i(t) &= p_i^{\text{cl}}(t) + \delta p_i(t). \end{aligned} \quad (1.15)$$

In general, the variation is

$$\begin{aligned} \delta \mathcal{A}[p_i, q_i] &= \int_{t_a}^{t_b} dt \left[\delta p_i(t) \dot{q}_i(t) + p_i(t) \delta \dot{q}_i(t) - \frac{\partial H}{\partial p_i} \delta p_i - \frac{\partial H}{\partial q_i} \delta q_i \right] \\ &= \int_{t_a}^{t_b} dt \left\{ \left[\dot{q}_i(t) - \frac{\partial H}{\partial p_i} \right] \delta p_i - \left[\dot{p}_i(t) + \frac{\partial H}{\partial q_i} \right] \delta q_i \right\} + p_i(t) \delta q_i(t) \Big|_{t_a}^{t_b}. \end{aligned} \quad (1.16)$$

Since this variation has to vanish for classical orbits, we find that $p_i^{\text{cl}}(t)$, $q_i^{\text{cl}}(t)$ must be solutions of the *Hamilton equations* of motion

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i}, \\ \dot{q}_i &= \frac{\partial H}{\partial p_i}. \end{aligned} \quad (1.17)$$

These agree with the Euler-Lagrange equations (1.8) via (1.9) and (1.10), as can easily be verified. The $2N$ -dimensional space of all p_i and q_i is called the *phase space*.

An arbitrary function $O(p_i(t), q_i(t), t)$ changes along an arbitrary path as follows:

$$\frac{d}{dt} O(p_i(t), q_i(t), t) = \frac{\partial O}{\partial p_i} \dot{p}_i + \frac{\partial O}{\partial q_i} \dot{q}_i + \frac{\partial O}{\partial t}. \quad (1.18)$$

If the path coincides with a classical orbit, we may insert (1.17) and find

$$\begin{aligned} \frac{dO}{dt} &= \frac{\partial H}{\partial p_i} \frac{\partial O}{\partial q_i} - \frac{\partial O}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial O}{\partial t} \\ &\equiv \{H, O\} + \frac{\partial O}{\partial t}. \end{aligned} \quad (1.19)$$

Here we have introduced the symbol $\{A, B\}$ called *Poisson brackets*:

$$\{A, B\} \equiv \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} - \frac{\partial B}{\partial p_i} \frac{\partial A}{\partial q_i}, \quad (1.20)$$

again with the Einstein summation convention for the repeated index i . The Poisson brackets have the obvious properties

$$\{A, B\} = -\{B, A\} \quad \text{antisymmetry}, \quad (1.21)$$

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \quad \text{Jacobi identity.} \quad (1.22)$$

If two quantities have vanishing Poisson brackets, they are said to *commute*.

The original Hamilton equations are a special case of (1.19):

$$\begin{aligned} \frac{d}{dt} p_i &= \{H, p_i\} = \frac{\partial H}{\partial p_j} \frac{\partial p_i}{\partial q_j} - \frac{\partial p_i}{\partial p_j} \frac{\partial H}{\partial q_j} = -\frac{\partial H}{\partial q_i}, \\ \frac{d}{dt} q_i &= \{H, q_i\} = \frac{\partial H}{\partial p_j} \frac{\partial q_i}{\partial q_j} - \frac{\partial q_i}{\partial p_j} \frac{\partial H}{\partial q_j} = \frac{\partial H}{\partial p_i}. \end{aligned} \quad (1.23)$$

By definition, the phase space variables p_i, q_i satisfy the Poisson brackets

$$\begin{aligned} \{p_i, q_j\} &= \delta_{ij}, \\ \{p_i, p_j\} &= 0, \\ \{q_i, q_j\} &= 0, \end{aligned} \quad (1.24)$$

and because of (1.23) this remains true for all times:

$$\begin{aligned} \{p_i(t), q_j(t)\} &= \delta_{ij}, \\ \{p_i(t), p_j(t)\} &= 0, \\ \{q_i(t), q_j(t)\} &= 0. \end{aligned} \quad (1.25)$$

A function $O(p_i, q_i)$ which has no *explicit* dependence on time and which, moreover, commutes with H (i.e., $\{O, H\} = 0$), is a *constant of motion* along the classical path, due to (1.19). In particular, H itself is often time-independent, i.e., of the form

$$H = H(p_i, q_i). \quad (1.26)$$

Then, since H commutes with itself, the energy is a constant of motion.

The Lagrangian formalism has the virtue of being independent of the particular choice of the coordinates q_i . Let Q_i be any other set of coordinates describing the system. If it is connected with q_i by what is called a *local*¹ or *point transformation*

$$q_i = f_i(Q_j, t). \quad (1.27)$$

¹Here the property *local* refers to a *specific time*. This terminology is of common use in field theory where *local* refers, more generally, to a *specific spacetime point*.

Certainly, to be useful, this relation must be invertible, at least in some neighborhood of the classical path

$$Q_i = f^{-1}_i(q_j, t). \quad (1.28)$$

Otherwise Q_i and q_i could not both parametrize the same system. Therefore, f_i must have a nonvanishing Jacobi determinant:

$$\det \left(\frac{\partial f_i}{\partial Q_j} \right) \neq 0. \quad (1.29)$$

In terms of Q_i , the initial Lagrangian takes the form

$$L' (Q_j, \dot{Q}_j, t) \equiv L (f_i (Q_j, t), \dot{f}_i (Q_j, t), t) \quad (1.30)$$

and the action reads

$$\begin{aligned} \mathcal{A} &= \int_{t_a}^{t_b} dt L' (Q_j(t), \dot{Q}_j(t), t) \\ &= \int_{t_a}^{t_b} dt L (f_i (Q_j(t), t), \dot{f}_i (Q_j(t), t), t). \end{aligned} \quad (1.31)$$

By performing variations $\delta Q_j(t)$, $\delta \dot{Q}_j(t)$ in the first expression while keeping $\delta Q_j(t_a) = \delta Q_j(t_b) = 0$, we find the equations of motion

$$\frac{d}{dt} \frac{\partial L'}{\partial \dot{Q}_j} - \frac{\partial L'}{\partial Q_j} = 0. \quad (1.32)$$

The variation of the lower expression, on the other hand, gives

$$\begin{aligned} \delta \mathcal{A} &= \int_{t_a}^{t_b} dt \left(\frac{\partial L}{\partial q_i} \delta f_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{f}_i \right) \\ &= \int_{t_a}^{t_b} dt \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) \delta f_i + \frac{\partial L}{\partial \dot{q}_i} \delta f_i \Big|_{t_a}^{t_b}. \end{aligned} \quad (1.33)$$

If δq_i is arbitrary, then so is δf_i . Moreover, with $\delta q_i(t_a) = \delta q_i(t_b) = 0$, also δf_i vanishes at the endpoints. Hence the extremum of the action is determined equally well by the Euler-Lagrange equations for $Q_j(t)$ [as it was by those for $q_i(t)$].

Note that the locality property is quite restrictive for the transformation of the generalized velocities $\dot{q}_i(t)$. They will necessarily be linear in $\dot{Q}_j$:

$$\dot{q}_i = \dot{f}_i(Q_j, t) = \frac{\partial f_i}{\partial Q_j} \dot{Q}_j + \frac{\partial f_i}{\partial t}. \quad (1.34)$$

In phase space, there exists also the possibility of performing local changes of the canonical coordinates p_i, q_i to new ones P_j, Q_j . Let them be related by

$$\begin{aligned} p_i &= p_i(P_j, Q_j, t), \\ q_i &= q_i(P_j, Q_j, t), \end{aligned} \quad (1.35)$$

whose inverse relations are

$$\begin{aligned} P_j &= P_j(p_i, q_i, t), \\ Q_j &= Q_j(p_i, q_i, t). \end{aligned} \quad (1.36)$$

Now, while the Euler-Lagrange equations maintain their form under *any* local change of coordinates, the Hamilton equations do not hold, in general, for any transformed coordinates $P_j(t), Q_j(t)$. The local transformations $p_i(t), q_i(t) \rightarrow P_j(t), Q_j(t)$ for which they hold, are referred to as *canonical*. They are characterized by the form invariance of the action, up to an arbitrary surface term,

$$\begin{aligned} \int_{t_a}^{t_b} dt [p_i \dot{q}_i - H(p_i, q_i, t)] &= \int_{t_a}^{t_b} dt [P_j \dot{Q}_j - H'(P_j, Q_j, t)] \\ &\quad + F(P_j, Q_j, t) \Big|_{t_a}^{t_b}, \end{aligned} \quad (1.37)$$

where $H'(P_j, Q_j, t)$ is some new Hamiltonian. Its relation with $H(p_i, q_i, t)$ must be chosen in such a way that the equality of the action holds for *any* path $p_i(t), q_i(t)$ connecting the same endpoints (at least any in some neighborhood of the classical orbits). If such an invariance exists then a variation of this action yields for $P_j(t)$ and $Q_j(t)$ the Hamilton equations of motion governed by H' :

$$\begin{aligned} \dot{P}_i &= -\frac{\partial H'}{\partial Q_i}, \\ \dot{Q}_i &= \frac{\partial H'}{\partial P_i}. \end{aligned} \quad (1.38)$$

The invariance (1.37) can be expressed differently by rewriting the integral on the left-hand side in terms of the new variables $P_j(t), Q_j(t)$,

$$\int_{t_a}^{t_b} dt \left\{ p_i \left(\frac{\partial q_i}{\partial P_j} \dot{P}_j + \frac{\partial q_i}{\partial Q_j} \dot{Q}_j + \frac{\partial q_i}{\partial t} \right) - H(p_i(P_j, Q_j, t), q_i(P_j, Q_j, t), t) \right\}, \quad (1.39)$$

and subtracting it from the right-hand side, leading to

$$\int_{t_a}^{t_b} \left\{ \left(P_j - p_i \frac{\partial q_i}{\partial Q_j} \right) dQ_j - p_i \frac{\partial q_i}{\partial P_j} dP_j - \left(H' + p_i \frac{\partial q_i}{\partial t} - H \right) dt \right\} = -F(P_j, Q_j, t) \Big|_{t_a}^{t_b}. \quad (1.40)$$

The integral is now a line integral along a curve in the $(2N + 1)$ -dimensional space, consisting of the $2N$ -dimensional phase space variables p_i, q_i and of the time t . The right-hand side depends only on the endpoints. Thus we conclude that the integrand on the left-hand side must be a total differential. As such it has to satisfy the standard Schwarz integrability conditions [3], according to which all second

derivatives have to be independent of the sequence of differentiation. Explicitly, these conditions are

$$\begin{aligned}\frac{\partial p_i}{\partial P_k} \frac{\partial q_i}{\partial Q_l} - \frac{\partial q_i}{\partial P_k} \frac{\partial p_i}{\partial Q_l} &= \delta_{kl}, \\ \frac{\partial p_i}{\partial P_k} \frac{\partial q_i}{\partial P_l} - \frac{\partial q_i}{\partial P_k} \frac{\partial p_i}{\partial P_l} &= 0, \\ \frac{\partial p_i}{\partial Q_k} \frac{\partial q_i}{\partial Q_l} - \frac{\partial q_i}{\partial Q_k} \frac{\partial p_i}{\partial Q_l} &= 0,\end{aligned}\tag{1.41}$$

and

$$\begin{aligned}\frac{\partial p_i}{\partial t} \frac{\partial q_i}{\partial P_l} - \frac{\partial q_i}{\partial t} \frac{\partial p_i}{\partial P_l} &= \frac{\partial(H' - H)}{\partial P_l}, \\ \frac{\partial p_i}{\partial t} \frac{\partial q_i}{\partial Q_l} - \frac{\partial q_i}{\partial t} \frac{\partial p_i}{\partial Q_l} &= \frac{\partial(H' - H)}{\partial Q_l}.\end{aligned}\tag{1.42}$$

The first three equations define the so-called *Lagrange brackets* in terms of which they are written as

$$\begin{aligned}(P_k, Q_l) &= \delta_{kl}, \\ (P_k, P_l) &= 0, \\ (Q_k, Q_l) &= 0.\end{aligned}\tag{1.43}$$

Time-dependent coordinate transformations satisfying these equations are called *symplectic*. After a little algebra involving the matrix of derivatives

$$J = \begin{pmatrix} \partial P_i / \partial p_j & \partial P_i / \partial q_j \\ \partial Q_i / \partial p_j & \partial Q_i / \partial q_j \end{pmatrix},\tag{1.44}$$

its inverse

$$J^{-1} = \begin{pmatrix} \partial p_i / \partial P_j & \partial p_i / \partial Q_j \\ \partial q_i / \partial P_j & \partial q_i / \partial Q_j \end{pmatrix},\tag{1.45}$$

and the symplectic unit matrix

$$E = \begin{pmatrix} 0 & \delta_{ij} \\ -\delta_{ij} & 0 \end{pmatrix},\tag{1.46}$$

we find that the Lagrange brackets (1.43) are equivalent to the Poisson brackets

$$\begin{aligned}\{P_k, Q_l\} &= \delta_{kl}, \\ \{P_k, P_l\} &= 0, \\ \{Q_k, Q_l\} &= 0.\end{aligned}\tag{1.47}$$

This follows from the fact that the $2N \times 2N$ matrix formed from the Lagrange brackets

$$\mathcal{L} \equiv \begin{pmatrix} -(Q_i, P_j) & -(Q_i, Q_j) \\ (P_i, P_j) & (P_i, Q_j) \end{pmatrix}\tag{1.48}$$

can be written as $(E^{-1}J^{-1}E)^T J^{-1}$, while an analogous matrix formed from the Poisson brackets

$$\mathcal{P} \equiv \begin{pmatrix} \{P_i, Q_j\} & -\{P_i, P_j\} \\ \{Q_i, Q_j\} & -\{Q_i, P_j\} \end{pmatrix} \quad (1.49)$$

is equal to $J(E^{-1}JE)^T$. Hence $\mathcal{L} = \mathcal{P}^{-1}$, so that (1.43) and (1.47) are equivalent to each other. Note that the Lagrange brackets (1.43) [and thus the Poisson brackets (1.47)] ensure $p_i \dot{q}_i - P_j \dot{Q}_j$ to be a total differential of some function of P_j and Q_j in the $2N$ -dimensional phase space:

$$p_i \dot{q}_i - P_j \dot{Q}_j = \frac{d}{dt} G(P_j, Q_j, t). \quad (1.50)$$

The Poisson brackets (1.47) for P_i, Q_i have the same form as those in Eqs. (1.24) for the original phase space variables p_i, q_i .

The other two equations (1.42) relate the new Hamiltonian to the old one. They can always be used to construct $H'(P_j, Q_j, t)$ from $H(p_i, q_i, t)$. The Lagrange brackets (1.43) or Poisson brackets (1.47) are therefore both necessary and sufficient for the transformation $p_i, q_i \rightarrow P_j, Q_j$ to be canonical.

A canonical transformation preserves the volume in phase space. This follows from the fact that the matrix product $J(E^{-1}JE)^T$ is equal to the $2N \times 2N$ unit matrix (1.49). Hence $\det(J) = \pm 1$ and

$$\prod_i \int [dp_i dq_i] = \prod_j \int [dP_j dQ_j]. \quad (1.51)$$

It is obvious that the process of canonical transformations is reflexive. It may be viewed just as well from the opposite side, with the roles of p_i, q_i and P_j, Q_j exchanged [we could just as well have considered the integrand in (1.40) as a complete differential in P_j, Q_j, t space].

Once a system is described in terms of new canonical coordinates P_j, Q_j , we introduce the new Poisson brackets

$$\{A, B\}' \equiv \frac{\partial A}{\partial P_j} \frac{\partial B}{\partial Q_j} - \frac{\partial B}{\partial P_j} \frac{\partial A}{\partial Q_j}, \quad (1.52)$$

and the equation of motion for an arbitrary observable quantity $O(P_j(t), Q_j(t), t)$ becomes with (20.180)

$$\frac{dO}{dt} = \{H', O\}' + \frac{\partial O}{\partial t}, \quad (1.53)$$

by complete analogy with (20.176). The new Poisson brackets automatically guarantee the canonical commutation rules

$$\begin{aligned} \{P_i, Q_j\}' &= \delta_{ij}, \\ \{P_i, P_j\}' &= 0, \\ \{Q_i, Q_j\}' &= 0. \end{aligned} \quad (1.54)$$

A standard class of canonical transformations can be constructed by introducing a *generating function* F satisfying a relation of the type (1.37), while depending explicitly on half an old and half a new set of canonical coordinates, for instance

$$F = F(q_i, Q_j, t). \quad (1.55)$$

One now considers the equation

$$\int_{t_a}^{t_b} dt [p_i \dot{q}_i - H(p_i, q_i, t)] = \int_{t_a}^{t_b} dt \left[P_j \dot{Q}_j - H'(P_j, Q_j, t) + \frac{d}{dt} F(q_i, Q_j, t) \right], \quad (1.56)$$

replaces $P_j \dot{Q}_j$ by $-\dot{P}_j Q_j + \frac{d}{dt} P_j Q_j$, defines

$$F(q_i, P_j, t) \equiv F(q_i, Q_j, t) + P_j Q_j,$$

and works out the derivatives. This yields

$$\begin{aligned} & \int_{t_a}^{t_b} dt \left\{ p_i \dot{q}_i + \dot{P}_j Q_j - [H(p_i, q_i, t) - H'(P_j, Q_j, t)] \right\} \\ &= \int_{t_a}^{t_b} dt \left\{ \frac{\partial F}{\partial q_i}(q_i, P_j, t) \dot{q}_i + \frac{\partial F}{\partial P_j}(q_i, P_j, t) \dot{P}_j + \frac{\partial F}{\partial t}(q_i, P_j, t) \right\}. \end{aligned} \quad (1.57)$$

A comparison of the two sides yields the equations for the canonical transformation

$$\begin{aligned} p_i &= \frac{\partial}{\partial q_i} F(q_i, P_j, t), \\ Q_j &= \frac{\partial}{\partial P_j} F(q_i, P_j, t). \end{aligned} \quad (1.58)$$

The second equation shows that the above relation between $F(q_i, P_j, t)$ and $F(q_i, Q_j, t)$ amounts to a Legendre transformation.

The new Hamiltonian is

$$H'(P_j, Q_j, t) = H(p_i, q_i, t) + \frac{\partial}{\partial t} F(q_i, P_j, t). \quad (1.59)$$

Instead of (1.55) we could also have chosen functions with other mixtures of arguments such as $F(q_i, P_j, t)$, $F(p_i, Q_j, t)$, $F(p_i, P_j, t)$ to generate simple canonical transformations.

A particularly important canonical transformation arises by choosing a generating function $F(q_i, P_j)$ in such a way that it leads to time-independent momenta $P_j \equiv \alpha_j$. Coordinates Q_j with this property are called *cyclic*. To find cyclic coordinates we must search for a generating function $F(q_j, P_j, t)$ which makes the transformed H' in (1.59) vanish identically. Then all derivatives with respect to the coordinates vanish and the new momenta P_j are trivially constant. Thus we seek a solution for the equation

$$\frac{\partial}{\partial t} F(q_i, P_j, t) = -H(p_i, q_i, t), \quad (1.60)$$

where the momentum variables in the Hamiltonian obey the first equation of (1.58). This leads to the following partial differential equation for $F(q_i, P_j, t)$:

$$\partial_t F(q_i, P_j, t) = -H(\partial_{q_i} F(q_i, P_j, t), q_i, t), \quad (1.61)$$

called the *Hamilton-Jacobi equation*. Here and in the sequel we shall often use the short notations for partial derivatives $\partial_t \equiv \partial/\partial t$, $\partial_{q_i} \equiv \partial/\partial q_i$.

A generating function which achieves this goal is supplied by the action functional (1.14). When following the classical solutions starting from a fixed initial point and running to all possible final points q_i at a time t , the associated actions of these solutions form a function $A(q_i, t)$. Expression (1.14) shows that, if a particle moves along a classical trajectory and the path is varied *without* keeping the endpoints fixed, the action changes as a function of the end positions (1.16) by

$$\delta \mathcal{A}[p_i, q_i] = p_i(t_b) \delta q_i(t_b) - p_i(t_a) \delta q_i(t_a). \quad (1.62)$$

From this we deduce immediately the first of the equations (1.58), now for the generating function $A(q_i, t)$:

$$p_i = \frac{\partial}{\partial q_i} A(q_i, t). \quad (1.63)$$

Moreover, the function $A(q_i, t)$ has the time derivative

$$\frac{d}{dt} A(q_i(t), t) = p_i(t) \dot{q}_i(t) - H(p_i(t), q_i(t), t). \quad (1.64)$$

Together with (1.63), this implies

$$\partial_t A(q_i, t) = -H(p_i, q_i, t). \quad (1.65)$$

If the momenta p_i on the right-hand side are replaced according to (1.63), $A(q_i, t)$ is indeed seen to be a solution of the Hamilton-Jacobi differential equation:

$$\partial_t A(q_i, t) = -H(\partial_{q_i} A(q_i, t), q_i, t). \quad (1.66)$$

1.2 Relativistic Mechanics in Curved Spacetime

The classical action of a relativistic spinless point particle in a curved four-dimensional spacetime is usually written as an integral

$$\mathcal{A} = -Mc^2 \int d\tau L(q, \dot{q}) = -Mc^2 \int d\tau \sqrt{g_{\mu\nu} \dot{q}^\mu(\tau) \dot{q}^\nu(\tau)}, \quad (1.67)$$

where τ is an arbitrary parameter of the trajectory. It can be chosen in the final trajectory to make $L(q, \dot{q}) \equiv 1$, in which case it coincides with the *proper time* of the particle. For an arbitrary time t , the Euler-Lagrange equation (1.8) reads

$$\frac{d}{dt} \left[\frac{1}{L(q, \dot{q})} g_{\mu\nu} \dot{q}^\nu \right] = \frac{1}{2L(q, \dot{q})} (\partial_\mu g_{\kappa\lambda}) \dot{q}^\kappa \dot{q}^\lambda. \quad (1.68)$$

If τ is the proper time where $L(q, \dot{q}) \equiv 1$, this simplifies to

$$\frac{d}{dt}(g_{\mu\nu}\dot{q}^\nu) = \frac{1}{2}(\partial_\mu g_{\kappa\lambda})\dot{q}^\kappa\dot{q}^\lambda, \quad (1.69)$$

or

$$g_{\mu\nu}\ddot{q}^\nu = \left(\frac{1}{2}\partial_\mu g_{\kappa\lambda} - \partial_\lambda g_{\mu\kappa}\right)\dot{q}^\kappa\dot{q}^\lambda. \quad (1.70)$$

For brevity, we have denoted partial derivatives $\partial/\partial q^\mu$ by ∂_μ . This partial derivative is supposed to apply only to the quantity right behind it. At this point one introduces the *Christoffel symbol*

$$\bar{\Gamma}_{\lambda\nu\mu} \equiv \frac{1}{2}(\partial_\lambda g_{\nu\mu} + \partial_\nu g_{\lambda\mu} - \partial_\mu g_{\lambda\nu}), \quad (1.71)$$

and the Christoffel symbol of the second kind [6]:

$$\bar{\Gamma}_{\kappa\nu}{}^\mu \equiv g^{\mu\sigma}\bar{\Gamma}_{\kappa\nu\sigma}. \quad (1.72)$$

Then (1.70) can be written as

$$\ddot{q}^\mu + \bar{\Gamma}_{\kappa\lambda}{}^\mu\dot{q}^\kappa\dot{q}^\lambda = 0. \quad (1.73)$$

Since the solutions of this equation minimize the length of a curve in spacetime, they are called *geodesics*.

1.3 Quantum Mechanics

Historically, the extension of classical mechanics to quantum mechanics became necessary in order to understand the stability of atomic orbits and the discrete nature of atomic spectra. It soon became clear that these phenomena reflect the fact that, at a sufficiently short length scale, small material particles such as electrons behave like waves, called *material waves*. The fact that waves cannot be squeezed into an arbitrarily small volume without increasing indefinitely their frequency and thus their energy, prevents the collapse of the electrons into the nucleus, which would take place in classical mechanics. The discreteness of the atomic states of an electron are a manifestation of standing material waves in the atomic potential well, by analogy with the standing waves of electromagnetism in a cavity.

1.3.1 Bragg Reflections and Interference

The most direct manifestation of the wave nature of small particles is seen in diffraction experiments on periodic structures, for example of electrons diffracted by a crystal. If an electron beam of fixed momentum $\mathbf{p}$ passes through a crystal, it emerges along sharply peaked angles. These are the well-known *Bragg reflections*. They look very similar to the interference patterns of electromagnetic waves. In fact, it

is possible to use the same mathematical framework to explain these patterns as in electromagnetism. A free particle moving with momentum

$$\mathbf{p} = (p^1, p^2, \dots, p^D) \quad (1.74)$$

through a D -dimensional euclidean space spanned by the Cartesian coordinate vectors

$$\mathbf{x} = (x^1, x^2, \dots, x^D) \quad (1.75)$$

is associated with a *plane wave*, whose field strength or *wave function* has the form

$$\Psi_{\mathbf{p}}(\mathbf{x}, t) = e^{i\mathbf{k}\mathbf{x} - i\omega t}, \quad (1.76)$$

where $\mathbf{k}$ is the *wave vector* pointing into the direction of $\mathbf{p}$ and ω is the *wave frequency*. Each scattering center, say at $\mathbf{x}'$, becomes a source of a spherical wave with the spatial behavior e^{ikR}/R (with $R \equiv |\mathbf{x} - \mathbf{x}'|$ and $k \equiv |\mathbf{k}|$) and the wavelength $\lambda = 2\pi/k$. At the detector, all field strengths have to be added to the total field strength $\Psi(\mathbf{x}, t)$. The absolute square of the total field strength, $|\Psi(\mathbf{x}, t)|^2$, is proportional to the number of electrons arriving at the detector.

The standard experiment where these rules can most simply be applied consists of an electron beam impinging vertically upon a flat screen with two parallel slits with spacing d . At a large distance R behind these, one observes the number of particles arriving per unit time (see Fig. 1.1)

$$\frac{dN}{dt} \propto |\Psi_1 + \Psi_2|^2 \approx \left| e^{ik(R + \frac{1}{2}d \sin \varphi)} + e^{ik(R - \frac{1}{2}d \sin \varphi)} \right|^2 \frac{1}{R^2}, \quad (1.77)$$

where φ is the angle of deflection from the normal.

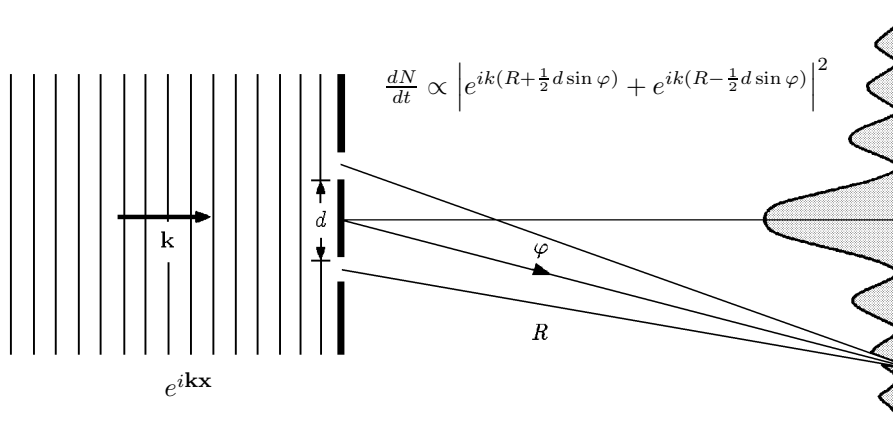


FIGURE 1.1 Probability distribution of a particle wave behind a double-slit. It is proportional to the absolute square of the sum of the two complex field strengths.

Conventionally, the wave function $\Psi(\mathbf{x}, t)$ is normalized to describe a single particle. Its absolute square gives directly the probability density of the particle at the space point $\mathbf{x}$, i.e., $d^3x |\Psi(\mathbf{x}, t)|^2$ is the probability of finding the particle in the volume element d^3x around $\mathbf{x}$.

1.3.2 Matter Waves

From the experimentally observed relation between the momentum and the size of the angular deflection φ of the diffracted beam of the particles, one deduces the relation between momentum and wave vector

$$\mathbf{p} = \hbar \mathbf{k}, \quad (1.78)$$

where $\hbar$ is the universal *Planck constant* whose dimension is equal to that of an action,

$$\hbar \equiv \frac{h}{2\pi} = 1.0545919(80) \times 10^{-27} \text{ erg sec} \quad (1.79)$$

(the number in parentheses indicating the experimental uncertainty of the last two digits before it). A similar relation holds between the energy and the frequency of the wave $\Psi(\mathbf{x}, t)$. It may be determined by an absorption process in which a light wave hits an electron and kicks it out of the surface of a metal, the well-known *photoelectric effect*. From the threshold property of this effect one learns that an electromagnetic wave oscillating in time as $e^{-i\omega t}$ can transfer to the electron the energy

$$E = \hbar \omega, \quad (1.80)$$

where the proportionality constant $\hbar$ is the same as in (1.78). The reason for this lies in the properties of electromagnetic waves. On the one hand, their frequency ω and the wave vector $\mathbf{k}$ satisfy the relation $\omega/c = |\mathbf{k}|$, where c is the light velocity defined to be $c \equiv 299\,792.458 \text{ km/s}$. The energy and momentum are related by $E/c = |\mathbf{p}|$. Thus, the quanta of electromagnetic waves, the *photons*, certainly satisfy (1.78) and the constant $\hbar$ must be the same as in Eq. (1.80).

With matter waves and photons sharing the same relations (1.78), it is suggestive to postulate also the relation (1.80) between energy and frequency to be universal for the waves of all particles, massive and massless ones. All free particles of momentum $\mathbf{p}$ are described by a *plane wave* of wavelength $\lambda = 2\pi/|\mathbf{k}| = 2\pi\hbar/|\mathbf{p}|$, with the explicit form

$$\Psi_{\mathbf{p}}(\mathbf{x}, t) = \mathcal{N} e^{i(\mathbf{p}\mathbf{x} - E_{\mathbf{p}}t)/\hbar}, \quad (1.81)$$

where $\mathcal{N}$ is some normalization constant. In a finite volume, the wave function is normalized to unity. In an infinite volume, this normalization makes the wave function vanish. To avoid this, the *current density* of the particle probability

$$\mathbf{j}(\mathbf{x}, t) \equiv -i \frac{\hbar}{2m} \psi^*(\mathbf{x}, t) \overleftrightarrow{\nabla} \psi(\mathbf{x}, t) \quad (1.82)$$

is normalized in some convenient way, where $\overleftrightarrow{\nabla}$ is a short notation for the difference between forward- and backward-derivatives

$$\begin{aligned} \psi^*(\mathbf{x}, t) \overleftrightarrow{\nabla} \psi(\mathbf{x}, t) &\equiv \psi^*(\mathbf{x}, t) \overrightarrow{\nabla} \psi(\mathbf{x}, t) - \psi^*(\mathbf{x}, t) \overleftarrow{\nabla} \psi(\mathbf{x}, t) \\ &\equiv \psi^*(\mathbf{x}, t) \nabla \psi(\mathbf{x}, t) - [\nabla \psi^*(\mathbf{x}, t)] \psi(\mathbf{x}, t). \end{aligned} \quad (1.83)$$

The energy $E_{\mathbf{p}}$ depends on the momentum of the particle along its classical way, i.e., for nonrelativistic material particles of mass M it is $E_{\mathbf{p}} = \mathbf{p}^2/2M$, for relativistic ones $E_{\mathbf{p}} = c\sqrt{\mathbf{p}^2 + M^2c^2}$, and $E_{\mathbf{p}} = c|\mathbf{p}|$ for massless particles such as photons. The common relation $E_{\mathbf{p}} = \hbar\omega$ for photons and matter waves is necessary to ensure the conservation of energy in quantum mechanics.

In general, both momentum and energy of a particle are not sharply defined as in the plane-wave function (1.81). Usually, a particle wave is some superposition of plane waves (1.81):

$$\Psi(\mathbf{x}, t) = \int \frac{d^3p}{(2\pi\hbar)^3} f(\mathbf{p}) e^{i(\mathbf{p}\mathbf{x} - E_{\mathbf{p}}t)/\hbar}. \quad (1.84)$$

By the Fourier inversion theorem, $f(\mathbf{p})$ can be calculated via the integral

$$f(\mathbf{p}) = \int d^3x e^{-i\mathbf{p}\mathbf{x}/\hbar} \Psi(\mathbf{x}, 0). \quad (1.85)$$

With an appropriate choice of $f(\mathbf{p})$ it is possible to prepare $\Psi(\mathbf{x}, t)$ in any desired form at some initial time, say at $t = 0$. For example, $\Psi(\mathbf{x}, 0)$ may be a function sharply centered around a space point $\bar{\mathbf{x}}$. Then $f(\mathbf{p})$ is approximately a pure phase $f(\mathbf{p}) \sim e^{-i\mathbf{p}\bar{\mathbf{x}}/\hbar}$, and the wave contains all momenta with equal probability. Conversely, if the particle amplitude is spread out in space, its momentum distribution is confined to a small region. The limiting $f(\mathbf{p})$ is concentrated at a specific momentum $\bar{\mathbf{p}}$. The particle is found at each point in space with equal probability, with the amplitude oscillating like $\Psi(\mathbf{x}, t) \sim e^{i(\bar{\mathbf{p}}\mathbf{x} - E_{\bar{\mathbf{p}}}t)/\hbar}$.

In general, the width of $\Psi(\mathbf{x}, 0)$ in space and of $f(\mathbf{p})$ in momentum space are inversely proportional to each other:

$$\Delta\mathbf{x} \Delta\mathbf{p} \sim \hbar. \quad (1.86)$$

This is the content of *Heisenberg's principle of uncertainty*. If the wave is localized in a finite region of space while having at the same time a fairly well-defined average momentum $\bar{\mathbf{p}}$, it is called a *wave packet*. The maximum in the associated probability density can be shown from (1.84) to move with a velocity

$$\bar{\mathbf{v}} = \partial E_{\bar{\mathbf{p}}} / \partial \bar{\mathbf{p}}. \quad (1.87)$$

This coincides with the velocity of a classical particle of momentum $\bar{\mathbf{p}}$.

1.3.3 Schrödinger Equation

Suppose now that the particle is nonrelativistic and has a mass M . The classical Hamiltonian, and thus the energy $E_{\mathbf{p}}$, are given by

$$H(\mathbf{p}) = E_{\mathbf{p}} = \frac{\mathbf{p}^2}{2M}. \quad (1.88)$$

We may therefore derive the following identity for a general wave function (1.84):

$$\int \frac{d^3p}{(2\pi\hbar)^3} f(\mathbf{p}) [H(\mathbf{p}) - E_{\bar{\mathbf{p}}}] e^{i(\mathbf{p}\mathbf{x} - E_{\bar{\mathbf{p}}}t)/\hbar} = 0. \quad (1.89)$$

The arguments *inside* the brackets can be moved in front of the integral (1.89) by observing that $\mathbf{p}$ and $E_{\mathbf{p}}$ inside the brackets are equivalent to the differential operators

$$\begin{aligned}\hat{\mathbf{p}} &= -i\hbar\partial_{\mathbf{x}}, \\ \hat{E} &= i\hbar\partial_t\end{aligned}\tag{1.90}$$

outside the integral. Then, Eq. (1.89) may be written as the differential equation

$$[H(-i\hbar\partial_{\mathbf{x}}) - i\hbar\partial_t]\Psi(\mathbf{x}, t) = 0.\tag{1.91}$$

This is the *Schrödinger equation* for the wave function of a free particle. The equation suggests that the motion of a particle with an arbitrary Hamiltonian $H(\mathbf{p}, \mathbf{x}, t)$ follows the straightforward generalization of (1.91)

$$(\hat{H} - i\hbar\partial_t)\Psi(\mathbf{x}, t) = 0,\tag{1.92}$$

where $\hat{H}$ is the differential operator

$$\hat{H} \equiv H(-i\hbar\partial_{\mathbf{x}}, \mathbf{x}, t).\tag{1.93}$$

The rule of obtaining $\hat{H}$ from the classical Hamiltonian $H(\mathbf{p}, \mathbf{x}, t)$ by the substitutions $\mathbf{x} \rightarrow \hat{\mathbf{x}}$ and $\mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar\partial_{\mathbf{x}}$ will be referred to as the *correspondence principle*.² The substitution rule for $\mathbf{p}$ runs also under the name *Jordan rule*.

This simple correspondence principle holds only in Cartesian coordinates. A slight generalization is possible to coordinates $q_i(t)$ which are of the *quasi-Cartesian* type. For these, the so-called *dynamical metric*, or *Hessian*, defined in the Lagrangian formalism by

$$g_{ij}(q) \equiv \frac{\partial^2}{\partial \dot{q}_i \partial \dot{q}_j} L(q, \dot{q}),\tag{1.94}$$

and in the Hamiltonian formalism by

$$g^{ij}(q) \equiv \frac{\partial^2}{\partial p_i \partial p_j} H(p, q).\tag{1.95}$$

Then the momentum operators are, as in (1.90),

$$\hat{p}_i \equiv -i\hbar \frac{\partial}{\partial q_i}.\tag{1.96}$$

For such quasi-Cartesian generalized coordinates, the system may be quantized alternatively à la Heisenberg by assuming $p_i(t)$ and $q_i(t)$ to be Heisenberg operators $\hat{p}_{iH}(t)$ and $\hat{q}_{iH}(t)$ satisfying the canonical commutation rules (1.25):

$$\begin{aligned}[\hat{p}_{iH}(t), \hat{q}_{jH}(t)] &= -i\hbar\delta_{ij}, \\ [\hat{p}_{iH}(t), \hat{p}_{jH}(t)] &= 0, \\ [\hat{q}_{iH}(t), \hat{q}_{jH}(t)] &= 0.\end{aligned}\tag{1.97}$$

²Our formulation of this principle is slightly stronger than the historical one used at the initial stage of quantum mechanics, which gave certain correspondence rules between classical and quantum-mechanical relations.

This peculiarity of the canonical quantization rules will be discussed further in Sections 1.13–1.15.

The Schrödinger operators (1.90) of momentum and energy satisfy with $\mathbf{x}$ and t the so-called canonical commutation relations

$$[\hat{p}_i, x_j] = -i\hbar, \quad [\hat{E}, t] = 0 = i\hbar. \quad (1.98)$$

The linear combinations of the solutions of the Schrödinger equation (1.92) form a *Hilbert space* at each time t . If the Hamiltonian does not depend explicitly on time, the Hilbert space can be spanned by the energy eigenstates $\Psi_{E_n}(\mathbf{x}, t) = e^{-iE_n t/\hbar} \Psi_{E_n}(\mathbf{x})$, where $\Psi_{E_n}(\mathbf{x})$ are time-independent *stationary states* that solve the time-independent Schrödinger equation

$$\hat{H}(\hat{\mathbf{p}}, \mathbf{x}) \Psi_{E_n}(\mathbf{x}) = E_n \Psi_{E_n}(\mathbf{x}). \quad (1.99)$$

The validity of the Schrödinger theory (1.92) is confirmed by experiment, most notably for the Coulomb Hamiltonian

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2M} - \frac{e^2}{r}. \quad (1.100)$$

It governs the quantum mechanics of the hydrogen atom in the center-of-mass coordinate system of the electron and the proton, where M is the reduced mass of the two particles.

Since the square of the wave function $|\Psi(\mathbf{x}, t)|^2$ specifies the probability density of a single particle in a finite volume, the integral over the entire volume must be normalized to unity:

$$\int d^3x |\Psi(\mathbf{x}, t)|^2 = 1. \quad (1.101)$$

For a stable particle, this normalization must remain the same at all times. If $\Psi(\mathbf{x}, t)$ follows the Schrödinger equation (1.92), this is assured if, and only if, the Hamiltonian operator is Hermitian,³ i.e., if any two wave functions Ψ_1, Ψ_2 satisfy the equality

$$\int d^3x [\hat{H}\Psi_2(\mathbf{x}, t)]^* \Psi_1(\mathbf{x}, t) = \int d^3x \Psi_2^*(\mathbf{x}, t) \hat{H}\Psi_1(\mathbf{x}, t). \quad (1.102)$$

The left-hand side contains the *Hermitian-adjoint* of the operator $\hat{H}$, denoted by $\hat{H}^\dagger$, and defined by the identity

$$\int d^3x \Psi_2^*(\mathbf{x}, t) \hat{H}^\dagger \Psi_1(\mathbf{x}, t) \equiv \int d^3x [\hat{H}\Psi_2(\mathbf{x}, t)]^* \Psi_1(\mathbf{x}, t) \quad (1.103)$$

³Problems arising from a possible unboundedness or from discontinuities of the Hamiltonian and other quantum-mechanical operators, also restrictions of the domains of definition, are ignored here since they are well understood. Correspondingly we do not distinguish between Hermitian and self-adjoint operators (see J. von Neumann, *Mathematische Grundlagen der Quantenmechanik*, Springer, Berlin, 1932).

for all square-integrable wave functions $\Psi_1(\mathbf{x}, t), \Psi_2(\mathbf{x}, t)$. An operator $\hat{H}$ is *Hermitian* if it coincides with its Hermitian-adjoint $\hat{H}^\dagger$:

$$\hat{H} = \hat{H}^\dagger. \quad (1.104)$$

Let us calculate the time change of the integral over two arbitrary wave functions, $\int d^3x \Psi_2^*(\mathbf{x}, t) \Psi_1(\mathbf{x}, t)$. With the Schrödinger equation (1.92), this time change vanishes indeed as long as $\hat{H}$ is Hermitian:

$$i\hbar \frac{d}{dt} \int d^3x \Psi_2^*(\mathbf{x}, t) \Psi_1(\mathbf{x}, t) = \int d^3x \Psi_2^*(\mathbf{x}, t) \hat{H} \Psi_1(\mathbf{x}, t) - \int d^3x [\hat{H} \Psi_2(\mathbf{x}, t)]^* \Psi_1(\mathbf{x}, t) = 0. \quad (1.105)$$

This also implies the time independence of the normalization integral $\int d^3x |\Psi(\mathbf{x}, t)|^2 = 1$.

Conversely, if $\hat{H}$ is not Hermitian, one can always find an eigenstate of $\hat{H}$ whose norm changes with time: any eigenstate of $(H - H^\dagger)/i$ has this property.

Since $\hat{\mathbf{p}} = -i\hbar\partial_{\mathbf{x}}$ and $\mathbf{x}$ are themselves Hermitian operators, $\hat{H}$ will automatically be a Hermitian operator if it is a sum of a kinetic and a potential energy:

$$H(\mathbf{p}, \mathbf{x}, t) = T(\mathbf{p}, t) + V(\mathbf{x}, t). \quad (1.106)$$

This is always the case for nonrelativistic particles in Cartesian coordinates $\mathbf{x}$. If $\mathbf{p}$ and $\mathbf{x}$ appear in one and the same term of H , for instance as $\mathbf{p}^2 \mathbf{x}^2$, the correspondence principle does not lead to a unique quantum-mechanical operator $\hat{H}$. Then there seem to be, in principle, several Hermitian operators which, in the above example, can be constructed from the product of two $\hat{\mathbf{p}}$ and two $\hat{\mathbf{x}}$ operators [for instance $\alpha \hat{\mathbf{p}}^2 \hat{\mathbf{x}}^2 + \beta \hat{\mathbf{x}}^2 \hat{\mathbf{p}}^2 + \gamma \hat{\mathbf{p}} \hat{\mathbf{x}}^2 \hat{\mathbf{p}}$ with $\alpha + \beta + \gamma = 1$]. They all correspond to the same classical $\mathbf{p}^2 \mathbf{x}^2$. At first sight it appears as though only a comparison with experiment could select the correct operator ordering. This is referred to as the operator-ordering problem of *quantum mechanics* which has plagued many researchers in the past. If the ordering problem is caused by the geometry of the space in which the particle moves, there exists a surprisingly simple geometric principle which specifies the ordering in the physically correct way. These are explained in Chapter 10 of the textbook [1]. Here we avoid such ambiguities by assuming $H(\mathbf{p}, \mathbf{x}, t)$ to have the standard form (1.106), unless otherwise stated.

1.3.4 Particle Current Conservation

The conservation of the total probability (1.101) is a consequence of a more general *local conservation law* linking the *current density* of the particle probability

$$\mathbf{j}(\mathbf{x}, t) \equiv -i\frac{\hbar}{2m} \psi(\mathbf{x}, t) \overleftrightarrow{\nabla} \psi(\mathbf{x}, t) \quad (1.107)$$

with the *probability density*

$$\rho(\mathbf{x}, t) = \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) \quad (1.108)$$

via the relation

$$\partial_t \rho(\mathbf{x}, t) = -\nabla \cdot \mathbf{j}(\mathbf{x}, t). \quad (1.109)$$

By integrating this *current conservation law* over a volume V enclosed by a surface S , and using Green's theorem, one finds

$$\int_V d^3x \partial_t \rho(\mathbf{x}, t) = - \int_V d^3x \nabla \cdot \mathbf{j}(\mathbf{x}, t) = - \int_S d\mathbf{S} \cdot \mathbf{j}(\mathbf{x}, t), \quad (1.110)$$

where $d\mathbf{S}$ are the directed infinitesimal surface elements. This equation states that the probability in a volume decreases by the same amount by which probability leaves the surface via the current $\mathbf{j}(\mathbf{x}, t)$.

By extending the integral (1.110) over the entire space and assuming the currents to vanish at spatial infinity, we recover the conservation of the total probability (1.101).

More general dynamical systems with N particles in euclidean space are parametrized in terms of $3N$ Cartesian coordinates $\mathbf{x}_\nu$ ($\nu = 1, \dots, N$). The Hamiltonian has the form

$$H(\mathbf{p}_\nu, \mathbf{x}_\nu, t) = \sum_{\nu=1}^N \frac{\mathbf{p}_\nu^2}{2M_\nu} + V(\mathbf{x}_\nu, t), \quad (1.111)$$

where the arguments $\mathbf{p}_\nu, \mathbf{x}_\nu$ in H and V stand for all $\mathbf{p}_\nu$'s, $\mathbf{x}_\nu$ with $\nu = 1, 2, 3, \dots, N$. The wave function $\Psi(\mathbf{x}_\nu, t)$ satisfies the N -particle Schrödinger equation

$$\left\{ - \sum_{\nu=1}^N \left[\frac{\hbar^2}{2M_\nu} \partial_{\mathbf{x}_\nu}^2 + V(\mathbf{x}_\nu, t) \right] \right\} \Psi(\mathbf{x}_\nu, t) = i\hbar \partial_t \Psi(\mathbf{x}_\nu, t). \quad (1.112)$$

1.4 Dirac's Bra-Ket Formalism

Mathematically speaking, the wave function $\Psi(\mathbf{x}, t)$ may be considered as a vector in an infinite-dimensional complex vector space called *Hilbert space*. The configuration space variable $\mathbf{x}$ plays the role of a continuous “index” of these vectors. An obvious contact with the usual vector notation may be established. In vector analysis, a D -dimensional vector $\mathbf{v}$ is specified by D components v_i with a subscript $i = 1, \dots, D$. In field theory we may consider the wave functions $\Psi(\mathbf{x}, t)$ as functional vectors and consider their argument $\mathbf{x}$ as analogs of a subscript:

$$\Psi(\mathbf{x}, t) \equiv \Psi_{\mathbf{x}}(t). \quad (1.113)$$

The usual norm of a complex vector is defined by

$$|\mathbf{v}|^2 = \sum_i v_i^* v_i. \quad (1.114)$$

The continuous version of this is

$$|\Psi|^2 = \int d^3x \Psi_{\mathbf{x}}^*(t) \Psi_{\mathbf{x}}(t) = \int d^3x \Psi^*(\mathbf{x}, t) \Psi(\mathbf{x}, t). \quad (1.115)$$

The normalization condition (1.101) requires that the wave functions have the norm $|\Psi| = 1$, i.e., that they are unit vectors in Hilbert space.

1.4.1 Basis Transformations

In a vector space, there are many possible choices of orthonormal basis vectors b_i^a labeled by $a = 1, \dots, D$, in terms of which⁴

$$v_i = \sum_a b_i^a v_a, \quad (1.116)$$

with the components v_a given by the scalar products

$$v_a \equiv \sum_i b_i^{a*} v_i. \quad (1.117)$$

The latter equation is a consequence of the *orthogonality relation*⁵

$$\sum_i b_i^{a*} b_i^{a'} = \delta^{aa'}, \quad (1.118)$$

which in a finite-dimensional vector space implies the *completeness relation*

$$\sum_a b_i^{a*} b_j^a = \delta^{ij}. \quad (1.119)$$

In the space of wave functions (1.113) there exists a special set of basis functions called *local basis functions* of particular importance. It may be constructed in the following fashion: Imagine the continuum of space points to be coarse-grained into a cubic lattice of mesh size ϵ , at positions

$$\mathbf{x}_{\mathbf{n}} = (n_1, n_2, n_3)\epsilon, \quad n_{1,2,3} = 0, \pm 1, \pm 2, \dots \quad (1.120)$$

Let $h^{\mathbf{n}}(\mathbf{x})$ be a function that vanishes everywhere in space, except in a cube of size ϵ^3 centered around $\mathbf{x}_{\mathbf{n}}$, i.e., for each component x_i of $\mathbf{x}$,

$$h^{\mathbf{n}}(\mathbf{x}) = \begin{cases} 1/\sqrt{\epsilon^3} & |x_i - x_{\mathbf{n}i}| \leq \epsilon/2, \quad i = 1, 2, 3. \\ 0 & \text{otherwise.} \end{cases} \quad (1.121)$$

These functions are certainly orthonormal:

$$\int d^3x h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta^{\mathbf{n}\mathbf{n}'}. \quad (1.122)$$

Consider now the expansion

$$\Psi(\mathbf{x}, t) = \sum_{\mathbf{n}} h^{\mathbf{n}}(\mathbf{x}) \Psi_{\mathbf{n}}(t) \quad (1.123)$$

⁴Mathematicians would expand more precisely $v_i = \sum_a b_i^a v_a^{(b)}$, but physicists prefer to shorten the notation by distinguishing the different components via different types of subscripts, using for the initial components $i, j, k, \dots$ and for the b -transformed components $a, b, c, \dots$.

⁵An orthogonality relation implies usually a unit norm and is thus really an *orthonormality relation*, but this name is rarely used.

with the coefficients

$$\Psi_{\mathbf{n}}(t) = \int d^3x h^{\mathbf{n}}(\mathbf{x})^* \Psi(\mathbf{x}, t) \approx \sqrt{\epsilon^3} \Psi(\mathbf{x}_{\mathbf{n}}, t). \quad (1.124)$$

It provides an excellent approximation to the true wave function $\Psi(\mathbf{x}, t)$, as long as the mesh size ϵ is much smaller than the scale over which $\Psi(\mathbf{x}, t)$ varies. In fact, if $\Psi(\mathbf{x}, t)$ is integrable, the integral over the sum (1.123) will always converge to $\Psi(\mathbf{x}, t)$. The same convergence of discrete approximations is found in any scalar product, and thus in any observable probability amplitude. They can all be calculated with arbitrary accuracy knowing the discrete components of the type (1.124) in the limit $\epsilon \rightarrow 0$. The functions $h^{\mathbf{n}}(\mathbf{x})$ may therefore be used as an approximate basis in the same way as the previous basis functions $f^a(\mathbf{x}), g^b(\mathbf{x})$, with any desired accuracy depending on the choice of ϵ .

In general, there are many possible orthonormal basis functions $f^a(\mathbf{x})$ in Hilbert space which satisfy the orthonormality relation

$$\int d^3x f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \quad (1.125)$$

in terms of which we can expand

$$\Psi(\mathbf{x}, t) = \sum_a f^a(\mathbf{x}) \Psi_a(t), \quad (1.126)$$

with the coefficients

$$\Psi_a(t) = \int d^3x f^a(\mathbf{x})^* \Psi(\mathbf{x}, t). \quad (1.127)$$

Suppose we use another orthonormal basis $\tilde{f}^b(\mathbf{x})$ with the orthonormality relation

$$\int d^3x \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}, \quad \sum_b \tilde{f}^b(\mathbf{x}) \tilde{f}^b(\mathbf{x}')^* = \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (1.128)$$

to re-expand

$$\Psi(\mathbf{x}, t) = \sum_b \tilde{f}^b(\mathbf{x}) \tilde{\Psi}_b(t), \quad (1.129)$$

with the components

$$\tilde{\Psi}_b(t) = \int d^3x \tilde{f}^b(\mathbf{x})^* \Psi(\mathbf{x}, t). \quad (1.130)$$

Inserting (1.126) shows that the components are related to each other by

$$\tilde{\Psi}_b(t) = \sum_a \left[\int d^3x \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}) \right] \Psi_a(t). \quad (1.131)$$

1.4.2 Bracket Notation

It is useful to write the scalar products between two wave functions occurring in the above basis transformations in the so-called *Dirac bracket notation* as

$$\langle \tilde{b} | a \rangle \equiv \int d^3x \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}). \quad (1.132)$$

In this notation, the components (1.127) and (1.130) of a state vector $\Psi(\mathbf{x}, t)$ are

$$\begin{aligned}\Psi_a(t) &= \langle a | \Psi(t) \rangle, \\ \tilde{\Psi}_b(t) &= \langle \tilde{b} | \Psi(t) \rangle.\end{aligned}\tag{1.133}$$

The transformation formula (1.131) takes the form

$$\langle \tilde{b} | \Psi(t) \rangle = \sum_a \langle \tilde{b} | a \rangle \langle a | \Psi(t) \rangle.\tag{1.134}$$

The right-hand side of this equation may be formally viewed as a result of inserting the abstract relation

$$\sum_a |a\rangle \langle a| = 1\tag{1.135}$$

between $\langle \tilde{b} |$ and $|\Psi(t)\rangle$ on the left-hand side:

$$\langle \tilde{b} | \Psi(t) \rangle = \langle \tilde{b} | 1 | \Psi(t) \rangle = \sum_a \langle \tilde{b} | a \rangle \langle a | \Psi(t) \rangle.\tag{1.136}$$

Since this expansion is possible only if the functions $f^b(\mathbf{x})$ form a complete basis, the relation (1.135) is an alternative abstract way of stating the completeness of the basis functions. It may be referred to as a *completeness relation à la Dirac*.

Since the scalar products are written in the form of brackets $\langle a | a' \rangle$, Dirac called the formal objects $\langle a |$ and $|a'\rangle$, from which the brackets are composed, *bra* and *ket*, respectively. In the Dirac bracket notation, the orthonormality of the basis $f^a(\mathbf{x})$ and $g^b(\mathbf{x})$ may be expressed as follows:

$$\begin{aligned}\langle a | a' \rangle &= \int d^3x f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \\ \langle \tilde{b} | \tilde{b}' \rangle &= \int d^3x \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}.\end{aligned}\tag{1.137}$$

In the same spirit we introduce abstract bra and ket vectors associated with the basis functions $h^{\mathbf{n}}(\mathbf{x})$ of Eq. (1.121), denoting them by $\langle \mathbf{x}_{\mathbf{n}} |$ and $|\mathbf{x}_{\mathbf{n}}\rangle$, respectively, and writing the orthogonality relation (1.122) in bracket notation as

$$\langle \mathbf{x}_{\mathbf{n}} | \mathbf{x}_{\mathbf{n}'} \rangle \equiv \int d^3x h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta_{\mathbf{n}\mathbf{n}'}.\tag{1.138}$$

The components $\Psi_{\mathbf{n}}(t)$ may be considered as the scalar products

$$\Psi_{\mathbf{n}}(t) \equiv \langle \mathbf{x}_{\mathbf{n}} | \Psi(t) \rangle \approx \sqrt{\epsilon^3} \Psi(\mathbf{x}_{\mathbf{n}}, t).\tag{1.139}$$

Changes of basis vectors, for instance from $|\mathbf{x}_{\mathbf{n}}\rangle$ to the states $|a\rangle$, can be performed according to the rules developed above by inserting a completeness relation à la Dirac of the type (1.135). Thus we may expand

$$\Psi_{\mathbf{n}}(t) = \langle \mathbf{x}_{\mathbf{n}} | \Psi(t) \rangle = \sum_a \langle \mathbf{x}_{\mathbf{n}} | a \rangle \langle a | \Psi(t) \rangle.\tag{1.140}$$

Also the inverse relation is true:

$$\langle a|\Psi(t)\rangle = \sum_{\mathbf{n}} \langle a|\mathbf{x}_{\mathbf{n}}\rangle \langle \mathbf{x}_{\mathbf{n}}|\Psi(t)\rangle. \quad (1.141)$$

This is, of course, just an approximation to the integral

$$\int d^3x h^{\mathbf{n}}(\mathbf{x})^* \langle \mathbf{x}|\Psi(t)\rangle. \quad (1.142)$$

The completeness of the basis $h^{\mathbf{n}}(\mathbf{x})$ may therefore be expressed via the abstract relation

$$\sum_{\mathbf{n}} |\mathbf{x}_{\mathbf{n}}\rangle \langle \mathbf{x}_{\mathbf{n}}| \approx 1. \quad (1.143)$$

The approximate sign turns into an equality sign in the limit of zero mesh size, $\epsilon \rightarrow 0$.

1.4.3 Continuum Limit

In ordinary calculus, finer and finer sums are eventually replaced by integrals. The same thing is done here. We define new continuous scalar products

$$\langle \mathbf{x}|\Psi(t)\rangle \approx \frac{1}{\sqrt{\epsilon^3}} \langle \mathbf{x}_{\mathbf{n}}|\Psi(t)\rangle, \quad (1.144)$$

where $\mathbf{x}_{\mathbf{n}}$ are the lattice points closest to $\mathbf{x}$. With (1.139), the right-hand side is equal to $\Psi(\mathbf{x}_{\mathbf{n}}, t)$. In the limit $\epsilon \rightarrow 0$, $\mathbf{x}$ and $\mathbf{x}_{\mathbf{n}}$ coincide and we have

$$\langle \mathbf{x}|\Psi(t)\rangle \equiv \Psi(\mathbf{x}, t). \quad (1.145)$$

The completeness relation can be used to write

$$\begin{aligned} \langle a|\Psi(t)\rangle &\approx \sum_{\mathbf{n}} \langle a|\mathbf{x}_{\mathbf{n}}\rangle \langle \mathbf{x}_{\mathbf{n}}|\Psi(t)\rangle \\ &\approx \sum_{\mathbf{n}} \epsilon^3 \langle a|\mathbf{x}\rangle \langle \mathbf{x}|\Psi(t)\rangle \Big|_{\mathbf{x}=\mathbf{x}_{\mathbf{n}}}, \end{aligned} \quad (1.146)$$

which becomes in the limit $\epsilon \rightarrow 0$:

$$\langle a|\Psi(t)\rangle = \int d^3x \langle a|\mathbf{x}\rangle \langle \mathbf{x}|\Psi(t)\rangle. \quad (1.147)$$

This may be viewed as the result of inserting the formal completeness relation of the limiting local bra and ket basis vectors $\langle \mathbf{x}|$ and $|\mathbf{x}\rangle$,

$$\int d^3x |\mathbf{x}\rangle \langle \mathbf{x}| = 1, \quad (1.148)$$

evaluated between the vectors $\langle a|$ and $|\Psi(t)\rangle$.

With the limiting local basis, the wave functions can be treated as components of the state vectors $|\Psi(t)\rangle$ with respect to the local basis $|\mathbf{x}\rangle$ in the same way as any other set of components in an arbitrary basis $|a\rangle$. In fact, the expansion

$$\langle a|\Psi(t)\rangle = \int d^3x \langle a|\mathbf{x}\rangle \langle \mathbf{x}|\Psi(t)\rangle \quad (1.149)$$

may be viewed as a re-expansion of a component of $|\Psi(t)\rangle$ in one basis, namely $|a\rangle$, into those of another basis, $|\mathbf{x}\rangle$, just as in (1.134).

In order to express all these transformation properties in a most compact notation, it has become customary to deal with an arbitrary physical state vector in a *basis-independent* way and denote it by a ket vector $|\Psi(t)\rangle$. This vector may be specified in any convenient basis by multiplying it with the corresponding completeness relation

$$\sum_a |a\rangle \langle a| = 1, \quad (1.150)$$

resulting in the expansion

$$|\Psi(t)\rangle = \sum_a |a\rangle \langle a|\Psi(t)\rangle. \quad (1.151)$$

This can be multiplied with any bra vector, say $\langle b|$, from the left to obtain the expansion formula (1.136):

$$\langle b|\Psi(t)\rangle = \sum_a \langle b|a\rangle \langle a|\Psi(t)\rangle. \quad (1.152)$$

The continuum version of the completeness relation (1.143) reads

$$\int d^3x |\mathbf{x}\rangle \langle \mathbf{x}| = 1. \quad (1.153)$$

It leads to the expansion

$$|\Psi(t)\rangle = \int d^3x |\mathbf{x}\rangle \langle \mathbf{x}|\Psi(t)\rangle, \quad (1.154)$$

in which the wave function $\Psi(\mathbf{x}, t) = \langle \mathbf{x}|\Psi(t)\rangle$ plays the role of an $\mathbf{x}$ th component of the state vector $|\Psi(t)\rangle$ in the local basis $|\mathbf{x}\rangle$. This, in turn, is the limit of the discrete basis vectors $|\mathbf{x}_n\rangle$,

$$|\mathbf{x}\rangle \approx \frac{1}{\sqrt{\epsilon^3}} |\mathbf{x}_n\rangle, \quad (1.155)$$

with $\mathbf{x}_n$ being the lattice points closest to $\mathbf{x}$.

A vector can be described equally well in bra or in ket form. To apply the above formalism consistently, we observe that the scalar products

$$\begin{aligned} \langle a|\tilde{b}\rangle &= \int d^3x f^a(\mathbf{x})^* \tilde{f}^b(\mathbf{x}), \\ \tilde{\langle b|a\rangle} &= \int d^3x \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}) \end{aligned} \quad (1.156)$$

satisfy the identity

$$\langle \tilde{b}|a\rangle \equiv \langle a|\tilde{b}\rangle^*. \quad (1.157)$$

Therefore, when expanding a ket vector as

$$|\Psi(t)\rangle = \sum_a |a\rangle \langle a|\Psi(t)\rangle, \quad (1.158)$$

or a bra vector as

$$\langle \Psi(t)| = \sum_a \langle \Psi(t)|a\rangle \langle a|, \quad (1.159)$$

a multiplication of the first equation with the bra $\langle \mathbf{x}|$ and of the second with the ket $|\mathbf{x}\rangle$ produces equations which are complex-conjugate to each other.

1.4.4 Generalized Functions

Dirac's bra-ket formalism is elegant and easy to handle. As far as the vectors $|\mathbf{x}\rangle$ are concerned there is, however, one inconsistency with some fundamental postulates of quantum mechanics: When introducing state vectors, a unit norm was required to permit a consistent probability interpretation of single-particle states. The limiting states $|\mathbf{x}\rangle$ introduced above do not satisfy this requirement. In fact, the scalar product between two different states $\langle \mathbf{x}|$ and $|\mathbf{x}'\rangle$ is

$$\langle \mathbf{x}|\mathbf{x}'\rangle \approx \frac{1}{\epsilon^3} \langle \mathbf{x}_{\mathbf{n}}|\mathbf{x}_{\mathbf{n}'}\rangle = \frac{1}{\epsilon^3} \delta_{\mathbf{n}\mathbf{n}'}, \quad (1.160)$$

where $\mathbf{x}_{\mathbf{n}}$ and $\mathbf{x}_{\mathbf{n}'}$ are the lattice points closest to $\mathbf{x}$ and $\mathbf{x}'$. For $\mathbf{x} \neq \mathbf{x}'$, the states are orthogonal. For $\mathbf{x} = \mathbf{x}'$, on the other hand, the limit $\epsilon \rightarrow 0$ is infinite, approached in such a way that

$$\epsilon^3 \sum_{\mathbf{n}'} \frac{1}{\epsilon^3} \delta_{\mathbf{n}\mathbf{n}'} = 1. \quad (1.161)$$

Therefore, the limiting state $|\mathbf{x}\rangle$ is not a properly normalizable vector in Hilbert space. For the sake of elegance, it is useful to weaken the requirement of normalizability (1.101) by admitting the limiting states $|\mathbf{x}\rangle$ to the physical Hilbert space. In fact, one admits all states which can be obtained by a limiting sequence from properly normalized state vectors.

The scalar product between states $\langle \mathbf{x}|\mathbf{x}'\rangle$ is not a proper function. It is denoted by the symbol $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ and called *Dirac δ -function*:

$$\langle \mathbf{x}|\mathbf{x}'\rangle \equiv \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (1.162)$$

The right-hand side vanishes everywhere, except in the infinitely small box of width ϵ around $\mathbf{x} \approx \mathbf{x}'$. Thus the δ -function satisfies

$$\delta^{(3)}(\mathbf{x} - \mathbf{x}') = 0 \quad \text{for} \quad \mathbf{x} \neq \mathbf{x}'. \quad (1.163)$$

At $\mathbf{x} = \mathbf{x}'$, it is so large that its volume integral is unity:

$$\int d^3x' \delta^{(3)}(\mathbf{x} - \mathbf{x}') = 1. \quad (1.164)$$

Obviously, there exists no proper function that can satisfy both requirements, (1.163) and (1.164). Only the finite- ϵ approximations in (1.160) to the δ -function are proper functions. In this respect, the scalar product $\langle \mathbf{x} | \mathbf{x}' \rangle$ behaves just like the states $|\mathbf{x}\rangle$ themselves: Both are $\epsilon \rightarrow 0$ -limits of properly defined mathematical objects.

Note that the integral Eq. (1.164) implies the following property of the δ -function:

$$\delta^{(3)}(a(\mathbf{x} - \mathbf{x}')) = \frac{1}{|a|} \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (1.165)$$

In one dimension, this leads to the more general relation

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i), \quad (1.166)$$

where x_i are the simple zeros of $f(x)$.

In mathematics, one calls the δ -function a *generalized function* or a *distribution*. It is a linear functional defined for arbitrary smooth complex-valued *test functions* $f(\mathbf{x})$ for which it produces a complex number. This number is the numerical value of the function at some desired point $\mathbf{x}$:

$$\delta_{\mathbf{x}}[f] \equiv \int d^3x \delta^{(3)}(\mathbf{x} - \mathbf{x}') f(\mathbf{x}') = f(\mathbf{x}). \quad (1.167)$$

Test functions are arbitrarily often differentiable functions with a sufficiently fast falloff at spatial infinity.

There exists a rich body of mathematical literature on distributions [4]. These form a linear space. By comparison with ordinary functions, the linear space of distributions is restricted in an essential way by the fact that products of δ -functions or any other distributions remain undefined. However, in Chapter 10 of the textbook [1] it was found that the consistency of different formulations of quantum mechanics forces us to go beyond these restricted rules. An important property of quantum mechanics is *coordinate invariance*. If we require this property also for the equivalent path-integral formulation of quantum mechanics, we can *derive* an extension of the existing theory of distributions. This procedure uniquely specifies integrals over products of distributions.

In quantum mechanics, the role of test functions is played by the wave packets $\Psi(\mathbf{x}, t)$. By admitting the generalized states $|\mathbf{x}\rangle$ to the Hilbert space, we also admit the scalar products $\langle \mathbf{x} | \mathbf{x}' \rangle$ to the space of wave functions, and thus all distributions, although they are not normalizable.

1.4.5 Schrödinger Equation in Dirac Notation

In terms of the Dirac bra-ket notation, the Schrödinger equation can be expressed in a basis-independent way as an operator equation

$$\hat{H}|\Psi(t)\rangle \equiv H(\hat{\mathbf{p}}, \hat{\mathbf{x}}, t)|\Psi(t)\rangle = i\hbar \partial_t |\Psi(t)\rangle, \quad (1.168)$$

to be supplemented by the following specifications of the canonical operators:

$$\langle \mathbf{x} | \hat{\mathbf{p}} \equiv -i\hbar \partial_{\mathbf{x}} \langle \mathbf{x} |, \quad (1.169)$$

$$\langle \mathbf{x} | \hat{\mathbf{x}} \equiv \mathbf{x} \langle \mathbf{x} |. \quad (1.170)$$

Any matrix element can be obtained from these equations by multiplication from the right with an arbitrary ket vector; for instance with the local basis vector $|\mathbf{x}'\rangle$:

$$\langle \mathbf{x} | \hat{\mathbf{p}} | \mathbf{x}' \rangle = -i\hbar \partial_{\mathbf{x}} \langle \mathbf{x} | \mathbf{x}' \rangle = -i\hbar \partial_{\mathbf{x}} \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (1.171)$$

$$\langle \mathbf{x} | \hat{\mathbf{x}} | \mathbf{x}' \rangle = \mathbf{x} \langle \mathbf{x} | \mathbf{x}' \rangle = \mathbf{x} \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (1.172)$$

The original differential form of the Schrödinger equation (1.92) follows by multiplying the basis-independent Schrödinger equation (1.168) with the bra vector $\langle \mathbf{x} |$ from the left:

$$\begin{aligned} \langle \mathbf{x} | H(\hat{\mathbf{p}}, \hat{\mathbf{x}}, t) | \Psi(t) \rangle &= H(-i\hbar \partial_{\mathbf{x}}, \mathbf{x}, t) \langle \mathbf{x} | \Psi(t) \rangle \\ &= i\hbar \partial_t \langle \mathbf{x} | \Psi(t) \rangle. \end{aligned} \quad (1.173)$$

Obviously, $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$ are Hermitian matrices in any basis,

$$\langle a | \hat{\mathbf{p}} | a' \rangle = \langle a' | \hat{\mathbf{p}} | a \rangle^*, \quad (1.174)$$

$$\langle a | \hat{\mathbf{x}} | a' \rangle = \langle a' | \hat{\mathbf{x}} | a \rangle^*, \quad (1.175)$$

and so is the Hamiltonian

$$\langle a | \hat{H} | a' \rangle = \langle a' | \hat{H} | a \rangle^*, \quad (1.176)$$

as long as it has the form (1.106).

The most general basis-independent operator that can be constructed in the generalized Hilbert space spanned by the states $|\mathbf{x}\rangle$ is some function of $\hat{\mathbf{p}}, \hat{\mathbf{x}}, t$,

$$\hat{O}(t) \equiv O(\hat{\mathbf{p}}, \hat{\mathbf{x}}, t). \quad (1.177)$$

In general, such an operator is called Hermitian if all its matrix elements have this property. In the basis-independent Dirac notation, the definition (1.102) of a Hermitian-adjoint operator $\hat{O}^\dagger(t)$ implies the equality of the matrix elements

$$\langle a | \hat{O}^\dagger(t) | a' \rangle \equiv \langle a' | \hat{O}(t) | a \rangle^*. \quad (1.178)$$

Thus we can rephrase Eqs. (1.174)–(1.176) in the basis-independent form

$$\begin{aligned} \hat{\mathbf{p}} &= \hat{\mathbf{p}}^\dagger, \\ \hat{\mathbf{x}} &= \hat{\mathbf{x}}^\dagger, \\ \hat{H} &= \hat{H}^\dagger. \end{aligned} \quad (1.179)$$

The stationary states in Eq. (1.99) have a Dirac ket representation $|E_n\rangle$, and satisfy the time-independent operator equation

$$\hat{H} |E_n\rangle = E_n |E_n\rangle. \quad (1.180)$$

1.4.6 Momentum States

Let us now look at the momentum $\hat{\mathbf{p}}$. Its eigenstates are given by the eigenvalue equation

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle. \quad (1.181)$$

By multiplying this with $\langle \mathbf{x}|$ from the left and using (1.169), we find the differential equation

$$\langle \mathbf{x}|\hat{\mathbf{p}}|\mathbf{p}\rangle = -i\hbar\partial_{\mathbf{x}}\langle \mathbf{x}|\mathbf{p}\rangle = \mathbf{p}\langle \mathbf{x}|\mathbf{p}\rangle. \quad (1.182)$$

The solution is

$$\langle \mathbf{x}|\mathbf{p}\rangle \propto e^{i\mathbf{p}\mathbf{x}/\hbar}. \quad (1.183)$$

Up to a normalization factor, this is just a plane wave introduced before in Eq. (1.76) to describe free particles of momentum $\mathbf{p}$.

In order for the states $|\mathbf{p}\rangle$ to have a finite norm, the system must be confined to a finite volume, say a cubic box of length L and volume L^3 . Assuming periodic boundary conditions, the momenta are discrete with values

$$\mathbf{p}^{\mathbf{m}} = \frac{2\pi\hbar}{L}(m_1, m_2, m_3), \quad m_i = 0, \pm 1, \pm 2, \dots \quad (1.184)$$

Then we adjust the factor in front of $\exp(i\mathbf{p}^{\mathbf{m}}\mathbf{x}/\hbar)$ to achieve unit normalization

$$\langle \mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle = \frac{1}{\sqrt{L^3}} \exp(i\mathbf{p}^{\mathbf{m}}\mathbf{x}/\hbar), \quad (1.185)$$

and the discrete states $|\mathbf{p}^{\mathbf{m}}\rangle$ satisfy

$$\int d^3x |\langle \mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle|^2 = 1. \quad (1.186)$$

The states $|\mathbf{p}^{\mathbf{m}}\rangle$ are complete:

$$\sum_{\mathbf{m}} |\mathbf{p}^{\mathbf{m}}\rangle \langle \mathbf{p}^{\mathbf{m}}| = 1. \quad (1.187)$$

We may use this relation and the matrix elements $\langle \mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle$ to expand any wave function within the box as

$$\Psi(\mathbf{x}, t) = \langle \mathbf{x}|\Psi(t)\rangle = \sum_{\mathbf{m}} \langle \mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle \langle \mathbf{p}^{\mathbf{m}}|\Psi(t)\rangle. \quad (1.188)$$

If the box is very large, the sum over the discrete momenta $\mathbf{p}^{\mathbf{m}}$ can be approximated by an integral over momentum space [7]:

$$\sum_{\mathbf{m}} \approx \int \frac{d^3p L^3}{(2\pi\hbar)^3}. \quad (1.189)$$

In this limit, the states $|\mathbf{p}^{\mathbf{m}}\rangle$ may be used to define a continuum of basis vectors with an improper normalization

$$|\mathbf{p}\rangle \approx \sqrt{L^3} |\mathbf{p}^{\mathbf{m}}\rangle, \quad (1.190)$$

in the same way as $|\mathbf{x}_n\rangle$ was used in (1.155) to define $|\mathbf{x}\rangle \sim (1/\sqrt{\epsilon^3})|\mathbf{x}^n\rangle$. The momentum states $|\mathbf{p}\rangle$ satisfy the orthogonality relation

$$\langle \mathbf{p}|\mathbf{p}'\rangle = (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}'), \quad (1.191)$$

with $\delta^{(3)}(\mathbf{p} - \mathbf{p}')$ being again the Dirac δ -function. Their completeness relation reads

$$\int \frac{d^3p}{(2\pi\hbar)^3} |\mathbf{p}\rangle \langle \mathbf{p}| = 1, \quad (1.192)$$

such that the expansion (1.188) becomes

$$\Psi(\mathbf{x}, t) = \int \frac{d^3p}{(2\pi\hbar)^3} \langle \mathbf{x}|\mathbf{p}\rangle \langle \mathbf{p}|\Psi(t)\rangle, \quad (1.193)$$

with the momentum eigenfunctions

$$\langle \mathbf{x}|\mathbf{p}\rangle = e^{i\mathbf{p}\mathbf{x}/\hbar}. \quad (1.194)$$

This coincides precisely with the Fourier decomposition introduced above in the description of a general particle wave $\Psi(\mathbf{x}, t)$ in (1.84) and (1.85), if we identify

$$\langle \mathbf{p}|\Psi(t)\rangle = f(\mathbf{p})e^{-iE_{\mathbf{p}}t/\hbar}. \quad (1.195)$$

The frequent appearance of factors $2\pi\hbar$ with δ -functions and integration measures in momentum space makes it convenient to define the modified δ -functions and integration measures

$$\delta^{(D)}(\mathbf{p}) \equiv (2\pi\hbar)^D \delta^{(D)}(\mathbf{p}), \quad d^D p \equiv \frac{d^D p}{(2\pi\hbar)^D}, \quad (1.196)$$

the latter in analogy with $\hbar \equiv h/2\pi$. Then we may write orthogonality and completeness relations as

$$\langle \mathbf{p}|\mathbf{p}'\rangle = \delta^{(3)}(\mathbf{p} - \mathbf{p}'), \quad (1.197)$$

and

$$\int d^3p |\mathbf{p}\rangle \langle \mathbf{p}| = 1. \quad (1.198)$$

The bra-ket formalism accommodates naturally the technique of Fourier transforms. The Fourier inversion formula is found by simply inserting into $\langle \mathbf{p}|\Psi(t)\rangle$ a completeness relation $\int d^3x |\mathbf{x}\rangle \langle \mathbf{x}| = 1$ which yields

$$\begin{aligned} \langle \mathbf{p}|\Psi(t)\rangle &= \int d^3x \langle \mathbf{p}|\mathbf{x}\rangle \langle \mathbf{x}|\Psi(t)\rangle \\ &= \int d^3x e^{-i\mathbf{p}\mathbf{x}/\hbar} \Psi(\mathbf{x}, t). \end{aligned} \quad (1.199)$$

The amplitudes $\langle \mathbf{p}|\Psi(t)\rangle$ are referred to as *momentum space wave functions*.

By inserting the completeness relation

$$\int d^3x |\mathbf{x}\rangle\langle\mathbf{x}| = 1 \quad (1.200)$$

between the momentum states on the left-hand side of the orthogonality relation (1.191), we obtain the Fourier representation of the δ -function (1.191):

$$\begin{aligned} \langle\mathbf{p}|\mathbf{p}'\rangle &= \int d^3x \langle\mathbf{p}|\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{p}'\rangle \\ &= \int d^3x e^{-i(\mathbf{p}-\mathbf{p}')\mathbf{x}/\hbar} = (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}'). \end{aligned} \quad (1.201)$$

1.4.7 Incompleteness and Poisson's Summation Formula

For many physical applications it is important to find out what happens to the completeness relation (1.153) if one restricts the integral to a subset of positions. Most relevant will be the one-dimensional integral,

$$\int dx |x\rangle\langle x| = 1, \quad (1.202)$$

restricted to a sum over equally spaced points at $x_n = n \cdot a$:

$$\sum_{n=-N}^N |x_n\rangle\langle x_n| = 1. \quad (1.203)$$

Taking this sum between momentum eigenstates $|p\rangle$, we obtain

$$\sum_{n=-N}^N \langle p|x_n\rangle\langle x_n|p'\rangle = \sum_{n=-N}^N e^{i(p-p')na/\hbar}. \quad (1.204)$$

For $N \rightarrow \infty$ we can perform the sum with the help of *Poisson's summation formula*:⁶

$$\sum_{n=-\infty}^{\infty} e^{2\pi i \mu n} = \sum_{m=-\infty}^{\infty} \delta(\mu - m). \quad (1.205)$$

Identifying μ with $(p - p')a/2\pi\hbar$, we find using Eq. (1.165):

$$\sum_{n=-\infty}^{\infty} \langle p|x_n\rangle\langle x_n|p'\rangle = \sum_{m=-\infty}^{\infty} \delta\left(\frac{a(p-p')}{2\pi\hbar} - m\right) = \sum_{m=-\infty}^{\infty} \frac{2\pi\hbar}{a} \delta\left(p-p' - \frac{2\pi\hbar m}{a}\right). \quad (1.206)$$

In order to prove the Poisson formula (1.205), we observe that the sum $s(\mu) \equiv \sum_m \delta(\mu - m)$ on the right-hand side is periodic in μ with a unit period and has the Fourier series $s(\mu) = \sum_{n=-\infty}^{\infty} s_n e^{2\pi i \mu n}$. The Fourier coefficients are given by

⁶For a proof of this formula see p. 28 of the textbook [1].

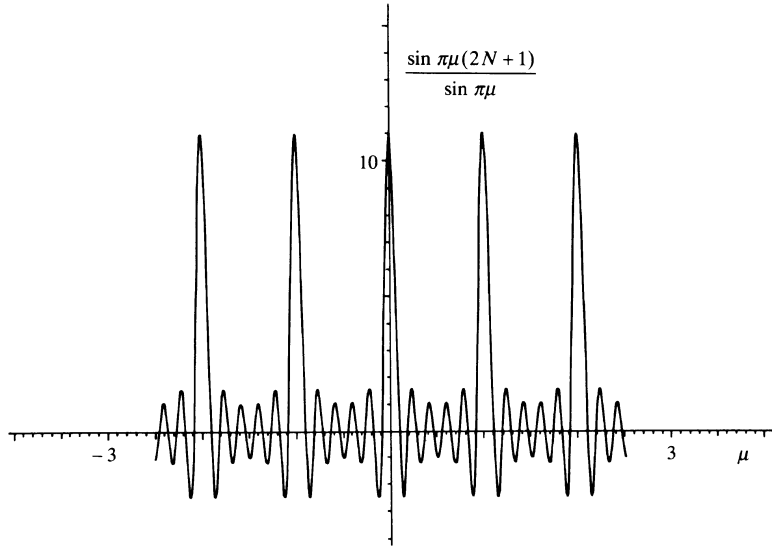


FIGURE 1.2 Relevant function $\sum_{n=-N}^N e^{2\pi i \mu n}$ in Poisson's summation formula. In the limit $N \rightarrow \infty$, μ is squeezed to integer values.

$s_n = \int_{-1/2}^{1/2} d\mu s(\mu) e^{-2\pi i \mu n} \equiv 1$. These are precisely the Fourier coefficients on the left-hand side.

For a finite N , the sum over n on the left-hand side of (1.205) yields

$$\begin{aligned} \sum_{n=-N}^N e^{2\pi i \mu n} &= 1 + (e^{2\pi i \mu} + e^{2 \cdot 2\pi i \mu} + \dots + e^{N \cdot 2\pi i \mu} + \text{c.c.}) \\ &= -1 + \left(\frac{1 - e^{2\pi i \mu(N+1)}}{1 - e^{2\pi i \mu}} + \text{c.c.} \right) \\ &= 1 + \frac{e^{2\pi i \mu} - e^{2\pi i \mu(N+1)}}{1 - e^{2\pi i \mu}} + \text{c.c.} = \frac{\sin \pi \mu(2N+1)}{\sin \pi \mu}. \end{aligned} \quad (1.207)$$

This function is well known in wave optics (see Fig. 1.2). It determines the diffraction pattern of light behind a grating with $2N+1$ slits. It has large peaks at $\mu = 0, \pm 1, \pm 2, \pm 3, \dots$ and $N-1$ small maxima between each pair of neighboring peaks, at $\nu = (1+4k)/2(2N+1)$ for $k = 1, \dots, N-1$. There are zeros at $\nu = (1+2k)/(2N+1)$ for $k = 1, \dots, N-1$.

Inserting $\mu = (p-p')a/2\pi\hbar$ into (1.207), we obtain

$$\sum_{n=-N}^N \langle p|x_n\rangle \langle x_n|p'\rangle = \frac{\sin(p-p')a(2N+1)/2\hbar}{\sin(p-p')a/2\hbar}. \quad (1.208)$$

Let us see how the right-hand side of (1.207) turns into the right-hand side of (1.205) in the limit $N \rightarrow \infty$. In this limit, the area under each large peak can be calculated by an integral over the central large peak plus a number n of small maxima next to it:

$$\int_{-n/2N}^{n/2N} d\mu \frac{\sin \pi \mu(2N+1)}{\sin \pi \mu} = \int_{-n/2N}^{n/2N} d\mu \frac{\sin 2\pi \mu N \cos \pi \mu + \cos 2\pi \mu N \sin \pi \mu}{\sin \pi \mu}. \quad (1.209)$$

Keeping a fixed ratio $n/N \ll 1$, we may replace in the integrand $\sin \pi\mu$ by $\pi\mu$ and $\cos \pi\mu$ by 1. Then the integral becomes, for $N \rightarrow \infty$ at fixed n/N ,

$$\begin{aligned} \int_{-n/2N}^{n/2N} d\mu \frac{\sin \pi\mu(2N+1)}{\sin \pi\mu} &\xrightarrow{N \rightarrow \infty} \int_{-n/2N}^{n/2N} d\mu \frac{\sin 2\pi\mu N}{\pi\mu} + \int_{-n/2N}^{n/2N} d\mu \cos 2\pi\mu N \\ &\xrightarrow{N \rightarrow \infty} \frac{1}{\pi} \int_{-\pi n}^{\pi n} dx \frac{\sin x}{x} + \frac{1}{2\pi N} \int_{-\pi n}^{\pi n} dx \cos x \xrightarrow{N \rightarrow \infty} 1, \end{aligned} \quad (1.210)$$

where we have used the integral formula

$$\int_{-\infty}^{\infty} dx \frac{\sin x}{x} = \pi. \quad (1.211)$$

In the limit $N \rightarrow \infty$, we find indeed (1.205) and thus (1.213).

There exists another useful way of expressing Poisson's formula. Consider an arbitrary smooth function $f(\mu)$ which possesses a convergent sum

$$\sum_{m=-\infty}^{\infty} f(m). \quad (1.212)$$

Then Poisson's formula (1.205) implies that the sum can be rewritten as an integral and an auxiliary sum:

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i \mu n} f(\mu). \quad (1.213)$$

The auxiliary sum over n squeezes μ to the integer numbers.

1.5 Observables

Changes of basis vectors are an important tool in analyzing the physically observable content of a wave vector. Let $A = A(\mathbf{p}, \mathbf{x})$ be an arbitrary time-independent real function of the phase space variables $\mathbf{p}$ and $\mathbf{x}$. Important examples for such an A are $\mathbf{p}$ and $\mathbf{x}$ themselves, the Hamiltonian $H(\mathbf{p}, \mathbf{x})$, and the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$. Quantum-mechanically, there will be an observable operator associated with each such quantity. It is obtained by simply replacing the variables $\mathbf{p}$ and $\mathbf{x}$ in A by the corresponding operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$:

$$\hat{A} \equiv A(\hat{\mathbf{p}}, \hat{\mathbf{x}}). \quad (1.214)$$

This replacement rule is the extension of the correspondence principle for the Hamiltonian operator (1.93) to more general functions in phase space, converting them into observable operators. It must be assumed that the replacement leads to a unique Hermitian operator, i.e., that there is no ordering problem of the type discussed in context with the Hamiltonian (1.106).⁷ If there are ambiguities, the naive

⁷Note that this is true for the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$.

correspondence principle is insufficient to determine the observable operator. Then the correct ordering must be decided by comparison with experiment, unless it can be specified by means of simple geometric principles. The problem is solved in the textbook [1].

Once an observable operator $\hat{A}$ is Hermitian, it has the useful property that the set of all eigenvectors $|a\rangle$, obtained by solving the equation

$$\hat{A}|a\rangle = a|a\rangle, \quad (1.215)$$

can be used as a basis to span the Hilbert space. Among the eigenvectors, there is always a choice of orthonormal vectors $|a\rangle$ fulfilling the completeness relation

$$\sum_a |a\rangle\langle a| = 1. \quad (1.216)$$

The vectors $|a\rangle$ can be used to extract physical information on the observable A from an arbitrary state vector $|\Psi(t)\rangle$. For this we expand this vector in the basis $|a\rangle$:

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle. \quad (1.217)$$

The components

$$\langle a|\Psi(t)\rangle \quad (1.218)$$

yield the probability amplitude for measuring the eigenvalue a for the observable quantity A .

The wave function $\Psi(\mathbf{x}, t)$ itself is an example of this interpretation. If we write it as

$$\Psi(\mathbf{x}, t) = \langle \mathbf{x}|\Psi(t)\rangle, \quad (1.219)$$

it gives the probability amplitude for measuring the eigenvalues $\mathbf{x}$ of the position operator $\hat{\mathbf{x}}$, i.e., $|\Psi(\mathbf{x}, t)|^2$ is the probability density in $\mathbf{x}$ -space.

The expectation value of the observable operator (1.214) in the state $|\Psi(t)\rangle$ is defined as the matrix element

$$\langle \Psi(t)|\hat{A}|\Psi(t)\rangle \equiv \int d^3x \langle \Psi(t)|\mathbf{x}\rangle A(-i\hbar\nabla, \mathbf{x}) \langle \mathbf{x}|\Psi(t)\rangle. \quad (1.220)$$

1.5.1 Uncertainty Relation

We have observed before [see the discussion after (1.84) and (1.85)] that the amplitudes in real space and those in momentum space have widths inversely proportional to each other, due to the properties of Fourier analysis. If a wave packet is localized in real space with a width $\Delta\mathbf{x}$, its momentum space wave function has a width $\Delta\mathbf{p}$ given by

$$\Delta\mathbf{x} \Delta\mathbf{p} \sim \hbar. \quad (1.221)$$

From the Hilbert space point of view this uncertainty relation can be shown to be a consequence of the fact that the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ do not commute with each other, but its components satisfy the canonical commutation rules

$$\begin{aligned} [\hat{p}_i, \hat{x}_j] &= -i\hbar\delta_{ij}, \\ [\hat{x}_i, \hat{x}_j] &= 0, \\ [\hat{p}_i, \hat{p}_j] &= 0. \end{aligned} \tag{1.222}$$

In general, if an observable operator $\hat{A}$ is measured to have a sharp value a in one state, this state must be an eigenstate of $\hat{A}$ with an eigenvalue a :

$$\hat{A}|a\rangle = a|a\rangle. \tag{1.223}$$

This follows from the expansion

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle, \tag{1.224}$$

in which $|\langle a|\Psi(t)\rangle|^2$ is the probability to measure an arbitrary eigenvalue a . If this probability is sharply focused at a specific value of a , the state necessarily coincides with $|a\rangle$.

Given the set of all eigenstates $|a\rangle$ of $\hat{A}$, we may ask under what circumstances another observable, say $\hat{B}$, can be measured sharply in each of these states. The requirement implies that the states $|a\rangle$ are also eigenstates of $\hat{B}$,

$$\hat{B}|a\rangle = b_a|a\rangle, \tag{1.225}$$

with some a -dependent eigenvalue b_a . If this is true for all $|a\rangle$,

$$\hat{B}\hat{A}|a\rangle = b_a a|a\rangle = a b_a|a\rangle = \hat{A}\hat{B}|a\rangle, \tag{1.226}$$

the operators $\hat{A}$ and $\hat{B}$ necessarily commute:

$$[\hat{A}, \hat{B}] = 0. \tag{1.227}$$

Conversely, it can be shown that a vanishing commutator is also sufficient for two observable operators to be simultaneously diagonalizable, and thus to allow for simultaneous sharp measurements.

1.5.2 Density Matrix and Wigner Function

An important object for calculating observable properties of a quantum-mechanical system is the quantum mechanical density operator associated with a pure state

$$\hat{\rho}(t) \equiv |\Psi(t)\rangle\langle\Psi(t)|, \tag{1.228}$$

and the associated density matrix associated with a pure state

$$\rho(\mathbf{x}_1, \mathbf{x}_2; t) = \langle \mathbf{x}_1 | \Psi(t) \rangle \langle \Psi(t) | \mathbf{x}_2 \rangle. \quad (1.229)$$

The expectation value of any function $f(\mathbf{x}, \hat{\mathbf{p}})$ can be calculated from the trace

$$\langle \Psi(t) | f(\mathbf{x}, \hat{\mathbf{p}}) | \Psi(t) \rangle = \text{tr}[f(\mathbf{x}, \hat{\mathbf{p}}) \hat{\rho}(t)] = \int d^3x \langle \Psi(t) | \mathbf{x} \rangle f(\mathbf{x}, -i\hbar \nabla) \langle \mathbf{x} | \Psi(t) \rangle. \quad (1.230)$$

If we decompose the states $|\Psi(t)\rangle$ into stationary eigenstates $|E_n\rangle$ of the Hamiltonian operator $\hat{H}$ [recall (1.180)], $|\Psi(t)\rangle = \sum_n |E_n\rangle \langle E_n | \Psi(t) \rangle$, then the density matrix has the expansion

$$\hat{\rho}(t) \equiv \sum_{n,m} |E_n\rangle \rho_{nm}(t) \langle E_m| = \sum_{n,m} |E_n\rangle \langle E_n | \Psi(t) \rangle \langle \Psi(t) | E_m \rangle \langle E_m|. \quad (1.231)$$

Wigner showed that the Fourier transform of the density matrix, the *Wigner function*

$$W(\mathbf{X}, \mathbf{p}; t) \equiv \int \frac{d^3\Delta\mathbf{x}}{(2\pi\hbar)^3} e^{i\mathbf{p}\Delta\mathbf{x}/\hbar} \rho(\mathbf{X} + \Delta\mathbf{x}/2, \mathbf{X} - \Delta\mathbf{x}/2; t) \quad (1.232)$$

satisfies, for a single particle of mass M in a potential $V(\mathbf{x})$, the Wigner-Liouville equation

$$\left(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} \right) W(\mathbf{X}, \mathbf{p}; t) = W_t(\mathbf{X}, \mathbf{p}; t), \quad \mathbf{v} \equiv \frac{\mathbf{p}}{M}, \quad (1.233)$$

where

$$W_t(\mathbf{X}, \mathbf{p}; t) \equiv \frac{2}{\hbar} \int \frac{d^3q}{(2\pi\hbar)^3} W(\mathbf{X}, \mathbf{p} - \mathbf{q}; t) \int d^3\Delta\mathbf{x} V(\mathbf{X} - \Delta\mathbf{x}/2) e^{i\mathbf{q}\Delta\mathbf{x}/\hbar}. \quad (1.234)$$

In the limit $\hbar \rightarrow 0$, we may expand $W(\mathbf{X}, \mathbf{p} - \mathbf{q}; t)$ in powers of $\mathbf{q}$, and $V(\mathbf{X} - \Delta\mathbf{x}/2)$ in powers of $\Delta\mathbf{x}$, which we rewrite in front of the exponential $e^{i\mathbf{q}\Delta\mathbf{x}/\hbar}$ as powers of $-i\hbar \nabla_{\mathbf{q}}$. Then we perform the integral over $\Delta\mathbf{x}$ to obtain $(2\pi\hbar)^3 \delta^{(3)}(\mathbf{q})$, and perform the integral over $\mathbf{q}$ to obtain the classical *Liouville equation* for the probability density of the particle in phase space

$$\left(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} \right) W(\mathbf{X}, \mathbf{p}; t) = -F(\mathbf{X}) \nabla_{\mathbf{p}} W(\mathbf{X}, \mathbf{p}; t), \quad \mathbf{v} \equiv \frac{\mathbf{p}}{M}. \quad (1.235)$$

Here $F(\mathbf{X}) \equiv -\nabla_{\mathbf{x}} V(\mathbf{X})$ is the force associated with the potential $V(\mathbf{X})$.

1.5.3 Generalization to Many Particles

All this development can be extended to systems of N distinguishable mass points with Cartesian coordinates $\mathbf{x}_1, \dots, \mathbf{x}_N$. If $H(\mathbf{p}_\nu, \mathbf{x}_\nu, t)$ is the Hamiltonian, the Schrödinger equation becomes

$$H(\hat{\mathbf{p}}_\nu, \hat{\mathbf{x}}_\nu, t) |\Psi(t)\rangle = i\hbar \partial_t |\Psi(t)\rangle. \quad (1.236)$$

We may introduce a complete local basis $|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle$ with the properties

$$\begin{aligned} \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \mathbf{x}'_1, \dots, \mathbf{x}'_N \rangle &= \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_N - \mathbf{x}'_N), \\ \int d^3x_1 \cdots d^3x_N |\mathbf{x}_1, \dots, \mathbf{x}_N\rangle \langle \mathbf{x}_1, \dots, \mathbf{x}_N| &= 1, \end{aligned} \quad (1.237)$$

and define

$$\begin{aligned} \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \hat{\mathbf{p}}_\nu &= -i\hbar \partial_{\mathbf{x}_\nu} \langle \mathbf{x}_1, \dots, \mathbf{x}_N |, \\ \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \hat{\mathbf{x}}_\nu &= \mathbf{x}_\nu \langle \mathbf{x}_1, \dots, \mathbf{x}_N |. \end{aligned} \quad (1.238)$$

The Schrödinger equation for N particles (1.112) follows from (1.236) by multiplying it from the left with the bra vectors $\langle \mathbf{x}_1, \dots, \mathbf{x}_N |$. In the same way, all other formulas given above can be generalized to N -body state vectors.

1.6 Time Evolution Operator. Definition

If the Hamiltonian operator possesses no explicit time dependence, the basis-independent Schrödinger equation (1.168) can be integrated to find the wave function $|\Psi(t)\rangle$ at any time t_b from the state at any other time t_a :

$$|\Psi(t_b)\rangle = e^{-i(t_b-t_a)\hat{H}/\hbar} |\Psi(t_a)\rangle. \quad (1.239)$$

The operator

$$\hat{U}(t_b, t_a) = e^{-i(t_b-t_a)\hat{H}/\hbar} \quad (1.240)$$

is called the *time evolution operator*. It satisfies the differential equation

$$i\hbar \partial_{t_b} \hat{U}(t_b, t_a) = \hat{H} \hat{U}(t_b, t_a). \quad (1.241)$$

Its inverse is obtained by interchanging the order of t_b and t_a :

$$\hat{U}^{-1}(t_b, t_a) \equiv e^{i(t_b-t_a)\hat{H}/\hbar} = \hat{U}(t_a, t_b). \quad (1.242)$$

As an exponential of i times a Hermitian operator, $\hat{U}$ is a *unitary operator* satisfying

$$\hat{U}^\dagger = \hat{U}^{-1}. \quad (1.243)$$

Indeed:

$$\hat{U}^\dagger(t_b, t_a) = e^{i(t_b-t_a)\hat{H}^\dagger/\hbar} = e^{i(t_b-t_a)\hat{H}/\hbar} = \hat{U}^{-1}(t_b, t_a). \quad (1.244)$$

If $H(\hat{\mathbf{p}}, \hat{\mathbf{x}}, t)$ depends explicitly on time, the integration of the Schrödinger equation (1.168) is somewhat more involved. The solution may be found iteratively: For $t_b > t_a$, the time interval is sliced into a large number $N + 1$ of small pieces of thickness ϵ with $\epsilon \equiv (t_b - t_a)/(N + 1)$, slicing once at each time $t_n = t_a + n\epsilon$ for

$n = 0, \dots, N + 1$. We then use the Schrödinger equation (1.168) to relate the wave function in each slice approximately to the previous one:

$$\begin{aligned} |\Psi(t_a + \epsilon)\rangle &\approx \left(1 - \frac{i}{\hbar} \int_{t_a}^{t_a + \epsilon} dt \hat{H}(t)\right) |\Psi(t_a)\rangle, \\ |\Psi(t_a + 2\epsilon)\rangle &\approx \left(1 - \frac{i}{\hbar} \int_{t_a + \epsilon}^{t_a + 2\epsilon} dt \hat{H}(t)\right) |\Psi(t_a + \epsilon)\rangle, \\ &\vdots \\ |\Psi(t_a + (N + 1)\epsilon)\rangle &\approx \left(1 - \frac{i}{\hbar} \int_{t_a + N\epsilon}^{t_a + (N + 1)\epsilon} dt \hat{H}(t)\right) |\Psi(t_a + N\epsilon)\rangle. \end{aligned} \quad (1.245)$$

From the combination of these equations we extract the evolution operator as a product

$$\hat{U}(t_b, t_a) \approx \left(1 - \frac{i}{\hbar} \int_{t_N}^{t_b} dt'_{N+1} \hat{H}(t'_{N+1})\right) \times \dots \times \left(1 - \frac{i}{\hbar} \int_{t_a}^{t_1} dt'_1 \hat{H}(t'_1)\right). \quad (1.246)$$

By multiplying out the product and going to the limit $N \rightarrow \infty$ we find the series

$$\begin{aligned} \hat{U}(t_b, t_a) = & 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} dt'_1 \hat{H}(t'_1) + \left(\frac{-i}{\hbar}\right)^2 \int_{t_a}^{t_b} dt'_2 \int_{t_a}^{t'_2} dt'_1 \hat{H}(t'_2) \hat{H}(t'_1) \\ & + \left(\frac{-i}{\hbar}\right)^3 \int_{t_a}^{t_b} dt'_3 \int_{t_a}^{t'_3} dt'_2 \int_{t_a}^{t'_2} dt'_1 \hat{H}(t'_3) \hat{H}(t'_2) \hat{H}(t'_1) + \dots, \end{aligned} \quad (1.247)$$

known as the *Neumann-Liouville expansion* or *Dyson series*.

Note that each integral has the time arguments in the Hamilton operators ordered *causally*: Operators with later times stand to the left of those with earlier times. It is useful to introduce a *time-ordering operator* which, when applied to an arbitrary product of operators,

$$\hat{O}_n(t_n) \dots \hat{O}_1(t_1), \quad (1.248)$$

reorders the times chronologically. More explicitly, we define

$$\hat{T}(\hat{O}_n(t_n) \dots \hat{O}_1(t_1)) \equiv \hat{O}_{i_n}(t_{i_n}) \dots \hat{O}_{i_1}(t_{i_1}), \quad (1.249)$$

where $t_{i_n}, \dots, t_{i_1}$ are the times $t_n, \dots, t_1$ relabeled in the causal order, so that

$$t_{i_n} > t_{i_{n-1}} > \dots > t_{i_1}. \quad (1.250)$$

Any *c*-number factors in (1.249) can be pulled out in front of the $\hat{T}$ -operator. With this formal operator, the Neumann-Liouville expansion can be rewritten in a more compact way. Take, for instance, the third term in (1.247)

$$\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 \hat{H}(t_2) \hat{H}(t_1). \quad (1.251)$$

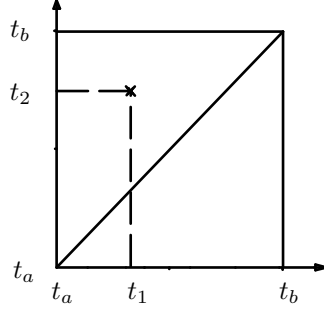


FIGURE 1.3 Illustration of time-ordering procedure in Eq. (1.251).

The integration covers the triangle above the diagonal in the square $t_1, t_2 \in [t_a, t_b]$ in the (t_1, t_2) plane (see Fig. 29.5). By comparing this with the missing integral over the lower triangle

$$\int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1 \hat{H}(t_2) \hat{H}(t_1), \quad (1.252)$$

we see that the two expressions coincide except for the order of the operators. This can be corrected with the use of a time-ordering operator $\hat{T}$. The expression

$$\hat{T} \int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1 \hat{H}(t_2) \hat{H}(t_1) \quad (1.253)$$

is equal to (1.251), since it may be rewritten as

$$\int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1 \hat{H}(t_1) \hat{H}(t_2), \quad (1.254)$$

or, after interchanging the order of integration, as

$$\int_{t_a}^{t_b} dt_1 \int_{t_a}^{t_1} dt_2 \hat{H}(t_1) \hat{H}(t_2). \quad (1.255)$$

Apart from the dummy integration variables $t_2 \leftrightarrow t_1$, this double integral coincides with (1.251). Since the time arguments are properly ordered, (1.251) can trivially be multiplied with the time-ordering operator. The conclusion of this discussion is that (1.251) can alternatively be written as

$$\frac{1}{2} \hat{T} \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 \hat{H}(t_2) \hat{H}(t_1). \quad (1.256)$$

On the right-hand side, the integrations now run over the full square in the t_1, t_2 -plane so that the two integrals can be factorized into

$$\frac{1}{2} \hat{T} \left(\int_{t_a}^{t_b} dt \hat{H}(t) \right)^2. \quad (1.257)$$

Similarly, we may rewrite the n th-order term of (1.247) as

$$\frac{1}{n!} \hat{T} \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_b} dt_{n-1} \cdots \int_{t_a}^{t_b} dt_1 \hat{H}(t_n) \hat{H}(t_{n-1}) \cdots \hat{H}(t_1) = \frac{1}{n!} \hat{T} \left[\int_{t_a}^{t_b} dt \hat{H}(t) \right]^n. \quad (1.258)$$

The time evolution operator $\hat{U}(t_b, t_a)$ has therefore the series expansion

$$\begin{aligned} \hat{U}(t_b, t_a) &= 1 - \frac{i}{\hbar} \hat{T} \int_{t_a}^{t_b} dt \hat{H}(t) + \frac{1}{2!} \left(\frac{-i}{\hbar} \right)^2 \hat{T} \left(\int_{t_a}^{t_b} dt \hat{H}(t) \right)^2 + \dots \\ &+ \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n \hat{T} \left(\int_{t_a}^{t_b} dt \hat{H}(t) \right)^n + \dots \end{aligned} \quad (1.259)$$

The right-hand side of $\hat{T}$ contains simply the power series expansion of the exponential so that we can write

$$\hat{U}(t_b, t_a) = \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{H}(t) \right\}. \quad (1.260)$$

If $\hat{H}$ does not depend on time, the time-ordering operation is superfluous, the integral can be done trivially, and we recover the previous result (1.240).

Note that a small variation $\delta \hat{H}(t)$ of $\hat{H}(t)$ changes $\hat{U}(t_b, t_a)$ by

$$\begin{aligned} \delta \hat{U}(t_b, t_a) &= -\frac{i}{\hbar} \int_{t_a}^{t_b} dt' \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t'}^{t_b} dt \hat{H}(t) \right\} \delta \hat{H}(t') \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t'} dt \hat{H}(t) \right\} \\ &= -\frac{i}{\hbar} \int_{t_a}^{t_b} dt' \hat{U}(t_b, t') \delta \hat{H}(t') \hat{U}(t', t_a). \end{aligned} \quad (1.261)$$

A simple application for this relation is given in Appendix 1A.

1.7 Time Evolution Operator. Properties

By construction, $\hat{U}(t_b, t_a)$ has some important properties:

a) Fundamental composition law

If two time translations are performed successively, the corresponding operators $\hat{U}$ are related by

$$\hat{U}(t_b, t_a) = \hat{U}(t_b, t') \hat{U}(t', t_a), \quad t' \in (t_a, t_b). \quad (1.262)$$

This composition law makes the operators $\hat{U}$ a representation of the abelian group of time translations. For time-independent Hamiltonians with $\hat{U}(t_b, t_a)$ given by (1.240), the proof of (1.262) is trivial. In the general case (1.260), it follows from the simple manipulation valid for $t_b > t_a$:

$$\hat{T} \exp \left(-\frac{i}{\hbar} \int_{t'}^{t_b} \hat{H}(t) dt \right) \hat{T} \exp \left(-\frac{i}{\hbar} \int_{t_a}^{t'} \hat{H}(t) dt \right)$$

$$\begin{aligned}
&= \hat{T} \left[\exp \left(-\frac{i}{\hbar} \int_{t'}^{t_b} \hat{H}(t) dt \right) \exp \left(-\frac{i}{\hbar} \int_{t_a}^{t'} \hat{H}(t) dt \right) \right] \\
&= \hat{T} \exp \left(-\frac{i}{\hbar} \int_{t_a}^{t_b} \hat{H}(t) dt \right).
\end{aligned} \tag{1.263}$$

b) *Unitarity*

The expression (1.260) for the time evolution operator $\hat{U}(t_b, t_a)$ was derived only for the *causal* (or *retarded*) time arguments, i.e., for t_b later than t_a . We may, however, define $\hat{U}(t_b, t_a)$ also for the *anticausal* (or *advanced*) case where t_b lies before t_a . To be consistent with the above composition law (1.262), we must have

$$\hat{U}(t_b, t_a) \equiv \hat{U}(t_a, t_b)^{-1}. \tag{1.264}$$

Indeed, when considering two states at successive times

$$|\Psi(t_a)\rangle = \hat{U}(t_a, t_b) |\Psi(t_b)\rangle, \tag{1.265}$$

the order of succession is inverted by multiplying both sides by $\hat{U}^{-1}(t_a, t_b)$:

$$|\Psi(t_b)\rangle = \hat{U}(t_a, t_b)^{-1} |\Psi(t_a)\rangle, \quad t_b < t_a. \tag{1.266}$$

The operator on the right-hand side is defined to be the time evolution operator $\hat{U}(t_b, t_a)$ from the later time t_a to the earlier time t_b .

If the Hamiltonian is independent of time, with the time evolution operator being

$$\hat{U}(t_a, t_b) = e^{-i(t_a - t_b)\hat{H}/\hbar}, \quad t_a > t_b, \tag{1.267}$$

the unitarity of the operator $\hat{U}(t_b, t_a)$ is obvious:

$$\hat{U}^\dagger(t_b, t_a) = \hat{U}(t_b, t_a)^{-1}, \quad t_b < t_a. \tag{1.268}$$

Let us verify this property for a general time-dependent Hamiltonian. There, a direct solution of the Schrödinger equation (1.168) for the state vector shows that the operator $\hat{U}(t_b, t_a)$ for $t_b < t_a$ has a representation just like (1.260), except for a reversed time order of its arguments. One writes this in the form [compare (1.260)]

$$\hat{U}(t_b, t_a) = \hat{\bar{T}} \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} \hat{H}(t) dt \right\}, \tag{1.269}$$

where $\hat{\bar{T}}$ denotes the time-antiordeing operator, with an obvious definition analog to (1.249), apart from the opposite order (1.250). This operator satisfies the relation

$$\left[\hat{T} \left(\hat{O}_1(t_1) \hat{O}_2(t_2) \right) \right]^\dagger = \hat{\bar{T}} \left(\hat{O}_2^\dagger(t_2) \hat{O}_1^\dagger(t_1) \right), \tag{1.270}$$

with an obvious generalization to the product of n operators. We can therefore conclude right away that

$$\hat{U}^\dagger(t_b, t_a) = \hat{U}(t_a, t_b), \quad t_b > t_a. \tag{1.271}$$

With $\hat{U}(t_a, t_b) \equiv \hat{U}(t_b, t_a)^{-1}$, this proves the unitarity relation (1.268), in general.

c) *Schrödinger equation for $\hat{U}(t_b, t_a)$*

Since the operator $\hat{U}(t_b, t_a)$ rules the relation between arbitrary wave functions at different times,

$$|\Psi(t_b)\rangle = \hat{U}(t_b, t_a)|\Psi(t_a)\rangle, \quad (1.272)$$

the Schrödinger equation (1.236) implies that the operator $\hat{U}(t_b, t_a)$ satisfies the corresponding equations

$$i\hbar\partial_t\hat{U}(t, t_a) = \hat{H}\hat{U}(t, t_a), \quad (1.273)$$

$$i\hbar\partial_t\hat{U}(t, t_a)^{-1} = -\hat{U}(t, t_a)^{-1}\hat{H}, \quad (1.274)$$

with the initial condition

$$\hat{U}(t_a, t_a) = 1. \quad (1.275)$$

1.8 Heisenberg Picture of Quantum Mechanics

The unitary time evolution operator $\hat{U}(t, t_a)$ may be used to give a different formulation of quantum mechanics bearing the closest resemblance to classical mechanics. This formulation, called the *Heisenberg picture* of quantum mechanics, is in a way more closely related to classical mechanics than the Schrödinger formulation. Many classical equations remain valid by simply replacing the canonical variables $p_i(t)$ and $q_i(t)$ in phase space by Heisenberg *operators*, to be denoted by $p_{Hi}(t)$, $q_{Hi}(t)$. Originally, Heisenberg postulated that they are matrices, but later it became clear that these matrices are functional matrix elements of operators, whose indices can be partly continuous. The classical equations of motion hold for the Heisenberg operators, as a consequence of the canonical commutation rules (1.97). It is important that $q_i(t)$ are Cartesian coordinates. In this case we shall always use the notation x_i for the position variable, as in Section 1.4, rather than q_i . And the corresponding Heisenberg operators are really $\hat{x}_{Hi}(t)$. Suppressing the subscripts i , the canonical equal-time commutation rules are

$$\begin{aligned} [\hat{p}_H(t), \hat{x}_H(t)] &= -i\hbar, \\ [\hat{p}_H(t), \hat{p}_H(t)] &= 0, \\ [\hat{x}_H(t), \hat{x}_H(t)] &= 0. \end{aligned} \quad (1.276)$$

According to Heisenberg, classical equations involving Poisson brackets remain valid if the Poisson brackets are replaced by $i/\hbar$ times the matrix commutators at equal times. The canonical commutation relations (1.276) are a special case of this rule, recalling the fundamental Poisson brackets (1.24). The Hamilton equations of motion (1.23) turn into the Heisenberg equations

$$\begin{aligned} \frac{d}{dt}\hat{p}_H(t) &= \frac{i}{\hbar} [\hat{H}_H, \hat{p}_H(t)], \\ \frac{d}{dt}\hat{x}_H(t) &= \frac{i}{\hbar} [\hat{H}_H, \hat{x}_H(t)], \end{aligned} \quad (1.277)$$

where

$$\hat{H}_H \equiv H(\hat{p}_H(t), \hat{x}_H(t), t) \quad (1.278)$$

is the Hamiltonian in the Heisenberg picture. Similarly, the equation of motion for an arbitrary observable function $O(p_i(t), x_i(t), t)$ derived in (1.19) goes over into the matrix commutator equation for the Heisenberg operator

$$\hat{O}_H(t) \equiv O(\hat{p}_H(t), \hat{x}_H(t), t), \quad (1.279)$$

namely,

$$\frac{d}{dt}\hat{O}_H = \frac{i}{\hbar}[\hat{H}_H, \hat{O}_H] + \frac{\partial}{\partial t}\hat{O}_H. \quad (1.280)$$

These rules are referred to as *Heisenberg's correspondence principle*.

The relation between Schrödinger's and Heisenberg's picture is supplied by the time evolution operator. Let $\hat{O}$ be an arbitrary observable in the Schrödinger description

$$\hat{O}(t) \equiv O(\hat{p}, \hat{x}, t). \quad (1.281)$$

If the states $|\Psi_a(t)\rangle$ are an arbitrary complete set of solutions of the Schrödinger equation, where a runs through discrete and continuous indices, the operator $\hat{O}(t)$ can be specified in terms of its functional matrix elements

$$O_{ab}(t) \equiv \langle \Psi_a(t) | \hat{O}(t) | \Psi_b(t) \rangle. \quad (1.282)$$

We can now use the unitary operator $\hat{U}(t, 0)$ to go to a new time-independent basis $|\Psi_{Ha}\rangle$, defined by

$$|\Psi_a(t)\rangle \equiv \hat{U}(t, 0) |\Psi_{Ha}\rangle. \quad (1.283)$$

Simultaneously, we transform the Schrödinger operators of the canonical coordinates $\hat{p}$ and $\hat{x}$ into the time-dependent canonical *Heisenberg operators* $\hat{p}_H(t)$ and $\hat{x}_H(t)$ via

$$\hat{p}_H(t) \equiv \hat{U}(t, 0)^{-1} \hat{p} \hat{U}(t, 0), \quad (1.284)$$

$$\hat{x}_H(t) \equiv \hat{U}(t, 0)^{-1} \hat{x} \hat{U}(t, 0). \quad (1.285)$$

At the time $t = 0$, the Heisenberg operators $\hat{p}_H(t)$ and $\hat{x}_H(t)$ coincide with the time-independent Schrödinger operators $\hat{p}$ and $\hat{x}$, respectively. An arbitrary observable $\hat{O}(t)$ is transformed into the associated Heisenberg operator as

$$\begin{aligned} \hat{O}_H(t) &\equiv \hat{U}(t, t_a)^{-1} O(\hat{p}, \hat{x}, t) \hat{U}(t, t_a) \\ &\equiv O(\hat{p}_H(t), \hat{x}_H(t), t). \end{aligned} \quad (1.286)$$

The Heisenberg matrices $O_H(t)_{ab}$ are then obtained from the Heisenberg operators $\hat{O}_H(t)$ by sandwiching $\hat{O}_H(t)$ between the time-independent basis vectors $|\Psi_{Ha}\rangle$:

$$O_H(t)_{ab} \equiv \langle \Psi_{Ha} | \hat{O}_H(t) | \Psi_{Hb} \rangle. \quad (1.287)$$

Note that the time dependence of these matrix elements is now completely due to the time dependence of the operators,

$$\frac{d}{dt}O_H(t)_{ab} \equiv \langle \Psi_{Ha} | \frac{d}{dt}\hat{O}_H(t) | \Psi_{Hb} \rangle. \quad (1.288)$$

This is in contrast to the Schrödinger representation (1.282), where the right-hand side would have contained two more terms from the time dependence of the wave functions. Due to the absence of such terms in (1.288) it is possible to study the equation of motion of the Heisenberg matrices independently of the basis by considering directly the Heisenberg operators. It is straightforward to verify that they do indeed satisfy the rules of Heisenberg's correspondence principle. Consider the time derivative of an arbitrary observable $\hat{O}_H(t)$,

$$\begin{aligned} \frac{d}{dt}\hat{O}_H(t) &= \left(\frac{d}{dt}\hat{U}^{-1}(t, t_a) \right) \hat{O}(t) \hat{U}(t, t_a) \\ &+ \hat{U}^{-1}(t, t_a) \left(\frac{\partial}{\partial t} \hat{O}(t) \right) \hat{U}(t, t_a) + \hat{U}^{-1}(t, t_a) \hat{O}(t) \left(\frac{d}{dt} \hat{U}(t, t_a) \right), \end{aligned} \quad (1.289)$$

which can be rearranged to

$$\begin{aligned} &\left[\left(\frac{d}{dt} \hat{U}^{-1}(t, t_a) \right) \hat{U}(t, t_a) \right] \hat{U}^{-1}(t, t_a) \hat{O}(t) \hat{U}(t, t_a) \\ &+ \left[\hat{U}^{-1}(t, t_a) \hat{O}(t) \hat{U}(t, t_a) \right] \hat{U}^{-1}(t, t_a) \frac{d}{dt} \hat{U}(t, t_a) + \hat{U}^{-1}(t, t_a) \left(\frac{\partial}{\partial t} \hat{O}(t) \right) \hat{U}(t, t_a). \end{aligned}$$

Using (1.273), we obtain

$$\frac{d}{dt}\hat{O}_H(t) = \frac{i}{\hbar} \left[\hat{U}^{-1} \hat{H} \hat{U}, \hat{O}_H \right] + \hat{U}^{-1} \left(\frac{\partial}{\partial t} \hat{O}(t) \right) \hat{U}. \quad (1.290)$$

After inserting (1.286), we find the equation of motion for the Heisenberg operator:

$$\frac{d}{dt}\hat{O}_H(t) = \frac{i}{\hbar} \left[\hat{H}_H, \hat{O}_H(t) \right] + \left(\frac{\partial}{\partial t} \hat{O} \right)_H(t). \quad (1.291)$$

By sandwiching this equation between the complete time-independent basis states $|\Psi_a\rangle$ in Hilbert space, it holds for the matrices and turns into the Heisenberg equation of motion. For the phase space variables $p_H(t)$, $x_H(t)$ themselves, these equations reduce, of course, to the Hamilton equations of motion (1.277).

Thus we have shown that Heisenberg's matrix quantum mechanics is completely equivalent to Schrödinger's quantum mechanics, and that the Heisenberg matrices obey the same Hamilton equations as the classical observables.

1.9 Interaction Picture and Perturbation Expansion

For some physical systems, the Hamiltonian operator can be split into two contributions

$$\hat{H} = \hat{H}_0 + \hat{V}, \quad (1.292)$$

where $\hat{H}_0$ is a so-called *free Hamiltonian* operator for which the Schrödinger equation $\hat{H}_0|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle$ can be solved, while $\hat{V}$ is an interaction potential which slightly perturbs these solutions. In this case it is useful to describe the system in Dirac's *interaction picture*. We remove the temporal evolution of the unperturbed Schrödinger solutions and define the states

$$|\psi_I(t)\rangle \equiv e^{i\hat{H}_0 t/\hbar}|\psi(t)\rangle. \quad (1.293)$$

Their time evolution comes entirely from the interaction potential $\hat{V}$. It is governed by the time evolution operator

$$\hat{U}_I(t_b, t_a) \equiv e^{i\hat{H}_0 t_b/\hbar} e^{-i\hat{H} t_b/\hbar} e^{i\hat{H} t_a/\hbar} e^{-i\hat{H}_0 t_a/\hbar}, \quad (1.294)$$

and reads

$$|\psi_I(t_b)\rangle = \hat{U}_I(t_b, t_a)|\psi_I(t_a)\rangle. \quad (1.295)$$

If $\hat{V} = 0$, the states $|\psi_I(t_b)\rangle$ are time-independent and coincide with the Heisenberg states (1.283) of the operator $\hat{H}_0$.

The operator $\hat{U}_I(t_b, t_a)$ satisfies the equation of motion

$$i\hbar\partial_{t_b}\hat{U}_I(t_b, t_a) = \hat{V}_I(t_b)\hat{U}_I(t_b, t_a), \quad (1.296)$$

where

$$\hat{V}_I(t) \equiv e^{i\hat{H}_0 t/\hbar}\hat{V}e^{-i\hat{H}_0 t/\hbar} \quad (1.297)$$

is the potential in the interaction picture. This equation of motion can be turned into an integral equation

$$\hat{U}_I(t_b, t_a) = 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{V}_I(t) \hat{U}_I(t, t_a). \quad (1.298)$$

Inserting Eq. (1.297), this reads

$$\hat{U}_I(t_b, t_a) = 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0 t/\hbar} \hat{U}_I(t, t_a). \quad (1.299)$$

This equation can be iterated to find a perturbation expansion for the operator $\hat{U}_I(t_b, t_a)$ in powers of the interaction potential:

$$\begin{aligned} \hat{U}_I(t_b, t_a) &= 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0 t/\hbar} \\ &\quad + \left(-\frac{i}{\hbar}\right)^2 \int_{t_a}^{t_b} dt \int_{t_a}^t dt' e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0(t-t')/\hbar} \hat{V} e^{-i\hat{H}_0 t'/\hbar} + \dots \end{aligned} \quad (1.300)$$

Inserting on the left-hand side the operator (1.294), this can also be rewritten as

$$e^{-iH(t_b-t_a)/\hbar} = e^{-iH_0(t_b-t_a)/\hbar} - \frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{-i\hat{H}_0(t_b-t)/\hbar} V e^{-i\hat{H}_0(t-t_a)/\hbar} \\ + \left(-\frac{i}{\hbar}\right)^2 \int_{t_a}^{t_b} dt \int_{t_a}^t dt' e^{-i\hat{H}_0(t_b-t)/\hbar} V e^{-i\hat{H}_0(t-t')/\hbar} V e^{-i\hat{H}_0(t'-t_a)/\hbar} + \dots \quad (1.301)$$

This expansion is seen to be the recursive solution of the integral equation

$$e^{-iH(t_b-t_a)/\hbar} = e^{-iH_0(t_b-t_a)/\hbar} - \frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{-i\hat{H}_0(t_b-t)/\hbar} V e^{-i\hat{H}(t-t_a)/\hbar}. \quad (1.302)$$

Note that the lowest-order correction agrees with the previous formula (1.261).

A compact way of writing the expansion (1.301) is

$$e^{-iH(t_b-t_a)/\hbar} = e^{-iH_0(t_b-t_a)/\hbar} \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{-i\hat{H}_0(t_b-t)/\hbar} V e^{-i\hat{H}_0(t-t_a)/\hbar} \right\}. \quad (1.303)$$

The right-hand exponential can be expanded with the help of *Lie's expansion formula*

$$e^{-iA} B e^{iA} = 1 - i[A, B] + \frac{i^2}{2!} [A, [A, B]] + \dots \quad (1.304)$$

It forms the basis of the Campbell-Baker-Hausdorff expansion to be derived later in Appendix 4A.

Equation (1.303) can be used as a basis for deriving a perturbative formula that yields the energy of an interacting system. Let $|\psi_{E_0}\rangle$ be an eigenstate of the free Schrödinger equation $\hat{H}_0|\psi_{E_0}\rangle = E_0|\psi_{E_0}\rangle$. If this state is subjected for an infinite amount of time to the time-independent interaction V , it will turn into an eigenstate $|\psi_E\rangle$ of the full Hamiltonian $\hat{H}$ of Eq. (1.292). This has an energy $E = E_0 + \Delta E$, where ΔE is determined by the exponential⁸

$$e^{-i\Delta E(t_b-t_a)/\hbar} = \langle \psi_{E_0} | \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} dt e^{-i\hat{H}_0(t_b-t)/\hbar} V e^{-i\hat{H}_0(t-t_a)/\hbar} \right\} | \psi_{E_0} \rangle. \quad (1.305)$$

1.10 Time Evolution Amplitude

In the subsequent development, an important role will be played by the matrix elements of the time evolution operator in the localized basis states,

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) \equiv \langle \mathbf{x}_b | \hat{U}(t_b, t_a) | \mathbf{x}_a \rangle. \quad (1.306)$$

They are referred to as *time evolution* amplitudes. The functional matrix $(\mathbf{x}_b t_b | \mathbf{x}_a t_a)$ is also called the *propagator* of the system. For a system with a time-independent Hamiltonian operator where $\hat{U}(t_b, t_a)$ is given by (1.267), the propagator is simply

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \langle \mathbf{x}_b | \exp[-i\hat{H}(t_b - t_a)/\hbar] | \mathbf{x}_a \rangle. \quad (1.307)$$

⁸See Eqs. (3.506) and (3.515) of the textbook [2].

Due to the operator equations (1.273), the propagator satisfies the Schrödinger equation

$$[H(-i\hbar\partial_{\mathbf{x}_b}, \mathbf{x}_b, t_b) - i\hbar\partial_{t_b}](\mathbf{x}_b t_b | \mathbf{x}_a t_a) = 0. \quad (1.308)$$

In the quantum theory of nonrelativistic particles, only the propagators from earlier to later times are relevant. It is therefore customary to introduce the so-called *causal* or *retarded* time evolution operator:

$$\hat{U}^R(t_b, t_a) \equiv \begin{cases} \hat{U}(t_b, t_a), & t_b \geq t_a, \\ 0, & t_b < t_a, \end{cases} \quad (1.309)$$

and, associated with it, the *causal* or *retarded* time evolution amplitude:

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a)^R \equiv \langle \mathbf{x}_b | \hat{U}^R(t_b, t_a) | \mathbf{x}_a \rangle. \quad (1.310)$$

This differs from (1.306) only for t_b earlier than t_a . Since all formulas in the subsequent text will be used only for t_b later than t_a , we shall often omit the superscript R . To abbreviate the case distinction in (1.309), it is convenient to use the *Heaviside function* defined by

$$\Theta(t) \equiv \begin{cases} 1 & \text{for } t > 0, \\ 0 & \text{for } t \leq 0, \end{cases} \quad (1.311)$$

and write

$$U^R(t_b, t_a) \equiv \Theta(t_b - t_a) \hat{U}(t_b, t_a), \quad (\mathbf{x}_b t_b | \mathbf{x}_a t_a)^R \equiv \Theta(t_b - t_a) (\mathbf{x}_b t_b | \mathbf{x}_a t_a). \quad (1.312)$$

There exists also another Heaviside function which differs from (1.311) only by the value at $t_b = t_a$:

$$\Theta^R(t) \equiv \begin{cases} 1 & \text{for } t \geq 0, \\ 0 & \text{for } t < 0. \end{cases} \quad (1.313)$$

Both Heaviside functions have the property that their derivative yields Dirac's δ -function

$$\partial_t \Theta(t) = \delta(t). \quad (1.314)$$

In those cases where it is not important which Θ -function is used, we shall ignore the superscript R .

The retarded propagator satisfies the Schrödinger equation

$$[H(-i\hbar\partial_{\mathbf{x}_b}, \mathbf{x}_b, t_b)^R - i\hbar\partial_{t_b}](\mathbf{x}_b t_b | \mathbf{x}_a t_a)^R = -i\hbar\delta(t_b - t_a)\delta^{(3)}(\mathbf{x}_b - \mathbf{x}_a). \quad (1.315)$$

The nonzero right-hand side arises from the time derivative of the Heaviside function in (1.312):

$$-i\hbar [\partial_{t_b} \Theta(t_b - t_a)] (\mathbf{x}_b t_b | \mathbf{x}_a t_a) = -i\hbar \delta(t_b - t_a) (\mathbf{x}_b t_b | \mathbf{x}_a t_a) = -i\hbar \delta(t_b - t_a) (\mathbf{x}_b t_a | \mathbf{x}_a t_a), \quad (1.316)$$

together with the initial condition $\langle \mathbf{x}_b t_a | \mathbf{x}_a t_a \rangle = \langle \mathbf{x}_b | \mathbf{x}_a \rangle = \delta^{(3)}(\mathbf{x}_b - \mathbf{x}_a)$, that follows from (1.275).

If the Hamiltonian does not depend on time, the propagator depends only on the time difference $t = t_b - t_a$. The retarded propagator vanishes for $t < 0$. Functions $f(t)$ with this property have a characteristic Fourier transform. The integral

$$\tilde{f}(E) \equiv \int_0^\infty dt f(t) e^{iEt/\hbar} \quad (1.317)$$

is an analytic function in the upper half of the complex energy plane. This analyticity property is necessary and sufficient to produce a factor $\Theta(t)$ when inverting the Fourier transform via the energy integral

$$f(t) \equiv \int_{-\infty}^\infty \frac{dE}{2\pi\hbar} \tilde{f}(E) e^{-iEt/\hbar}. \quad (1.318)$$

For $t < 0$, the contour of integration may be closed by an infinite semicircle in the upper half-plane at no extra cost. Since the contour encloses no singularities, it can be contracted to a point, yielding $f(t) = 0$.

The Heaviside function $\Theta(t)$ itself is the simplest retarded function, with a Fourier representation containing only a single pole just below the origin of the complex energy plane:

$$\Theta(t) = \int_{-\infty}^\infty \frac{dE}{2\pi} \frac{i}{E + i\eta} e^{-iEt}, \quad (1.319)$$

where η is an infinitesimally small positive number. The integral representation is undefined for $t = 0$ and there are, in fact, infinitely many possible definitions for the Heaviside function depending on the value assigned to the function at the origin. A special role is played by the average of the Heaviside functions (1.313) and (1.311), which is equal to $1/2$ at the origin:

$$\bar{\Theta}(t) \equiv \begin{cases} 1 & \text{for } t > 0, \\ \frac{1}{2} & \text{for } t = 0, \\ 0 & \text{for } t < 0. \end{cases} \quad (1.320)$$

Usually, the difference in the value at the origin does not matter since the Heaviside function appears only in integrals accompanied by some smooth function $f(t)$. This makes the Heaviside function a distribution with respect to smooth test functions $f(t)$ as defined in Eq. (1.167). All three distributions $\Theta_r(t)$, $\Theta^l(t)$, and $\bar{\Theta}(t)$ define the same linear functional of the test functions by the integral

$$\Theta[f] = \int dt \Theta(t - t') f(t'). \quad (1.321)$$

They are one and the same element in the linear space of all distributions.

As indicated after Eq. (1.167), a consistent theory of path integrals specifies, in addition, integrals over products of distribution and thus gives rise to an important extension of the theory of distributions. In this, the Heaviside function $\bar{\Theta}(t - t')$ plays the main role.

While discussing the concept of distributions let us introduce, for later use, the closely related distribution

$$\epsilon(t - t') \equiv \Theta(t - t') - \Theta(t' - t) = \bar{\Theta}(t - t') - \bar{\Theta}(t' - t), \quad (1.322)$$

which is a step function jumping at the origin from -1 to 1 as follows:

$$\epsilon(t - t') = \begin{cases} 1 & \text{for } t > t', \\ 0 & \text{for } t = t', \\ -1 & \text{for } t < t'. \end{cases} \quad (1.323)$$

1.11 Fixed-Energy Amplitude

The Fourier-transform of the retarded time evolution amplitude (1.310)

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \int_{-\infty}^{\infty} dt_b e^{iE(t_b - t_a)/\hbar} (\mathbf{x}_b t_b | \mathbf{x}_a t_a)^R = \int_{t_a}^{\infty} dt_b e^{iE(t_b - t_a)/\hbar} (\mathbf{x}_b t_b | \mathbf{x}_a t_a) \quad (1.324)$$

is called the *fixed-energy amplitude*.

If the Hamiltonian does not depend on time, we insert here Eq. (1.307) and find that the fixed-energy amplitudes are matrix elements

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \langle \mathbf{x}_b | \hat{R}(E) | \mathbf{x}_a \rangle \quad (1.325)$$

of the so-called *resolvent operator*

$$\hat{R}(E) = \frac{i\hbar}{E - \hat{H} + i\eta}, \quad (1.326)$$

which is the Fourier transform of the retarded time evolution operator (1.309):

$$\hat{R}(E) = \int_{-\infty}^{\infty} dt_b e^{iE(t_b - t_a)/\hbar} \hat{U}^R(t_b, t_a) = \int_{t_a}^{\infty} dt_b e^{iE(t_b - t_a)/\hbar} \hat{U}(t_b, t_a). \quad (1.327)$$

Let us suppose that the time-independent Schrödinger equation is completely solved, i.e., that one knows all solutions $|\psi_n\rangle$ of the equation

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle. \quad (1.328)$$

These satisfy the completeness relation

$$\sum_n |\psi_n\rangle \langle \psi_n| = 1, \quad (1.329)$$

which can be inserted on the right-hand side of (1.307) between the Dirac brackets leading to the *spectral representation*

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \sum_n \psi_n(\mathbf{x}_b) \psi_n^*(\mathbf{x}_a) \exp[-iE_n(t_b - t_a)/\hbar], \quad (1.330)$$

with

$$\psi_n(\mathbf{x}) = \langle \mathbf{x} | \psi_n \rangle \quad (1.331)$$

being the wave functions associated with the eigenstates $|\psi_n\rangle$. Applying the Fourier transform (1.324), we obtain

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \sum_n \psi_n(\mathbf{x}_b) \psi_n^*(\mathbf{x}_a) R_n(E) = \sum_n \psi_n(\mathbf{x}_b) \psi_n^*(\mathbf{x}_a) \frac{i\hbar}{E - E_n + i\eta}. \quad (1.332)$$

The matrix elements of the resolvent operator

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \langle \mathbf{x}_b | \frac{1}{E - \hat{H} + i\eta} | \mathbf{x}_a \rangle \quad (1.333)$$

are the Green functions of the Schrödinger equation, since they satisfy

$$(\hat{H} - E)(\mathbf{x} | \mathbf{x}')_E = -i\hbar \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (1.334)$$

For this reason we may also denote the resolvent operator $i\hbar/(E - \hat{H})$ as $\hat{G}(E)$.

The fixed-energy amplitude (1.324) contains as much information on the system as the time evolution amplitude, which is recovered from it by the inverse Fourier transformation

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} e^{-iE(t_b - t_a)/\hbar} (\mathbf{x}_b | \mathbf{x}_a)_E. \quad (1.335)$$

The small $i\eta$ -shift in the energy E in (1.332) may be thought of as being attached to each of the energies E_n , which are thus placed by an infinitesimal piece *below* the real energy axis. Then the exponential behavior of the wave functions is slightly damped, going to zero at infinite time:

$$e^{-i(E_n - i\eta)t/\hbar} \rightarrow 0. \quad (1.336)$$

This so-called $i\eta$ -prescription ensures the causality of the Fourier representation (11.6). When doing the Fourier integral (11.6), the exponential $e^{iE(t_b - t_a)/\hbar}$ makes it always possible to close the integration contour along the energy axis by an infinite semicircle in the complex energy plane. The semicircle lies in the upper half-plane for $t_b < t_a$ and in the lower half-plane for $t_b > t_a$. The $i\eta$ -prescription guarantees that for $t_b < t_a$ there is no pole inside the closed contour so that the propagator vanishes. For $t_b > t_a$, on the other hand, the poles in the lower half-plane give, via Cauchy's residue theorem, the spectral representation (1.330) of the propagator. An $i\eta$ -prescription will appear in another context in Section 7.1.3.

If the eigenstates are nondegenerate, the residues at the poles of (1.332) render directly the products of eigenfunctions (barring degeneracies which must be discussed separately). For a system with a continuum of energy eigenvalues, there is a cut in the complex energy plane which may be thought of as a closely spaced sequence of poles. In general, the wave functions are recovered from the discontinuity of the amplitudes $(\mathbf{x}_b | \mathbf{x}_a)_E$ across the cut, using the formula

$$\text{disc} \left(\frac{i\hbar}{E - E_n} \right) \equiv \frac{i\hbar}{E - E_n + i\eta} - \frac{i\hbar}{E - E_n - i\eta} = 2\pi\hbar \delta(E - E_n). \quad (1.337)$$

Here we have employed the relation valid inside integrals over E :⁹

$$\frac{1}{E - E_n \pm i\eta} = \frac{\mathcal{P}}{E - E_n} \mp i\pi\delta(E - E_n), \quad (1.338)$$

where the symbol $\mathcal{P}$ indicates that the principal value of the integral over E must be taken.

The energy integral over the discontinuity of the fixed-energy amplitude (1.332) $(\mathbf{x}_b|\mathbf{x}_a)_E$ reproduces the completeness relation (1.329) evaluated between the local states $\langle\mathbf{x}_b|$ and $|\mathbf{x}_a\rangle$:

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \text{disc}(\mathbf{x}_b|\mathbf{x}_a)_E = \sum_n \psi_n(\mathbf{x}_b)\psi_n^*(\mathbf{x}_a) = \langle\mathbf{x}_b|\mathbf{x}_a\rangle = \delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a). \quad (1.339)$$

The completeness relation may be viewed as a consequence of the following property of the resolvent operator:

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \text{disc} \hat{R}(E) = \hat{1}. \quad (1.340)$$

In general, a system possesses also a continuous spectrum, in which case the completeness relation contains a spectral integral and (1.329) has the form

$$\sum_n |\psi_n\rangle\langle\psi_n| + \int d\nu |\psi_\nu\rangle\langle\psi_\nu| = 1. \quad (1.341)$$

The continuum causes a branch cut along the E -axis in the complex energy plane, and (1.339) includes an integral over the discontinuity along the cut. The cut will often be omitted in the formulas, for brevity.

1.12 Free-Particle Amplitudes

For a free particle with a Hamiltonian operator $\hat{H} = \hat{\mathbf{p}}^2/2M$, the spectrum is continuous. The eigenfunctions are (1.194) with energies $E(\mathbf{p}) = \mathbf{p}^2/2M$. Inserting the completeness relation (1.192) into Eq. (1.307), we obtain the Fourier representation of the time evolution amplitude of a free particle

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \frac{d^D p}{(2\pi\hbar)^D} \exp \left\{ \frac{i}{\hbar} \left[\mathbf{p}(\mathbf{x}_b - \mathbf{x}_a) - \frac{\mathbf{p}^2}{2M}(t_b - t_a) \right] \right\}. \quad (1.342)$$

The momentum integrals can easily be done. First we perform a quadratic completion in the exponent and rewrite it as

$$\mathbf{p}(\mathbf{x}_b - \mathbf{x}_a) - \frac{1}{2M}\mathbf{p}^2(t_b - t_a) = \frac{1}{2M} \left(\mathbf{p} - \frac{1}{M} \frac{\mathbf{x}_b - \mathbf{x}_a}{t_b - t_a} \right)^2 (t_b - t_a) - \frac{M}{2} \frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a}. \quad (1.343)$$

⁹This is often referred to as *Sochocki's formula*. It is the beginning of an expansion in powers of $\eta > 0$: $1/(x \pm i\eta) = \mathcal{P}/x \mp i\pi\delta(x) + \eta[\pi\delta'(x) \pm id_x\mathcal{P}/x] + \mathcal{O}(\eta^2)$.

Then we replace the integration variables $\mathbf{p}$ by the shifted momenta $\mathbf{p}' = \mathbf{p} - (\mathbf{x}_b - \mathbf{x}_a)/(t_b - t_a)M$, which can be integrated out to arrive at the amplitude

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = F(t_b - t_a) \exp \left[\frac{i}{\hbar} \frac{M}{2} \frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a} \right], \quad (1.344)$$

where $F(t_b - t_a)$ is the integral over the shifted momenta

$$F(t_b - t_a) \equiv \int \frac{d^D p'}{(2\pi\hbar)^D} \exp \left\{ -\frac{i}{\hbar} \frac{\mathbf{p}'^2}{2M} (t_b - t_a) \right\}. \quad (1.345)$$

This can be performed using the *Fresnel integral formula*

$$\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \exp \left(i \frac{a}{2} p^2 \right) = \frac{1}{\sqrt{|a|}} \begin{cases} \sqrt{i}, & a > 0, \\ 1/\sqrt{i}, & a < 0. \end{cases} \quad (1.346)$$

Here the square-root $\sqrt{i}$ denotes the phase factor $e^{i\pi/4}$: This follows from the Gauss formula

$$\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \exp \left(-\frac{\alpha}{2} p^2 \right) = \frac{1}{\sqrt{\alpha}}, \quad \text{Re } \alpha > 0, \quad (1.347)$$

by continuing α analytically from positive values into the right complex half-plane. As long as $\text{Re } \alpha > 0$, this is straightforward. On the boundaries, i.e., on the positive and negative imaginary axes, one has to be careful. At $\alpha = \pm ia + \eta$ with $a \gtrless 0$ and infinitesimal $\eta > 0$, the integral is certainly convergent yielding (1.346). But the integral also converges for $\eta = 0$, as can easily be seen by substituting $x^2 = z$ (see Appendix 1B).

Note that differentiation of Eq. (1.347) with respect to α yields the more general Gaussian integral formula

$$\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} p^{2n} \exp \left(-\frac{\alpha}{2} p^2 \right) = \frac{1}{\sqrt{\alpha}} \frac{(2n-1)!!}{\alpha^n} \quad \text{Re } \alpha > 0, \quad (1.348)$$

where $(2n-1)!!$ is defined as the product $(2n-1) \cdot (2n-3) \cdots 1$. For odd powers p^{2n+1} , the integral vanishes. In the Fresnel formula (1.346), an extra integrand p^{2n} produces a factor $(i/a)^n$.

Since the Fresnel formula is a special analytically continued case of the Gauss formula, we shall in the sequel always speak of Gaussian integrations and use Fresnel's name only if the imaginary nature of the quadratic exponent is emphasized.

Applying this formula to (1.345), we obtain

$$F(t_b - t_a) = \frac{1}{\sqrt{2\pi i \hbar (t_b - t_a)/M}}^D, \quad (1.349)$$

so that the full time evolution amplitude of a free massive point particle is

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \frac{1}{\sqrt{2\pi i \hbar (t_b - t_a)/M}}^D \exp \left[\frac{i}{\hbar} \frac{M}{2} \frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a} \right]. \quad (1.350)$$

In the limit $t_b \rightarrow t_a$, the left-hand side becomes the scalar product $\langle \mathbf{x}_b | \mathbf{x}_a \rangle = \delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a)$, implying the following limiting formula for the δ -function:

$$\delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a) = \lim_{t_b - t_a \rightarrow 0} \frac{1}{\sqrt{2\pi i \hbar (t_b - t_a)/M}^D} \exp \left[\frac{i}{\hbar} \frac{M}{2} \frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a} \right]. \quad (1.351)$$

Inserting Eq. (1.344) into (1.324), we have for the fixed-energy amplitude the integral representation

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \int_0^\infty d(t_b - t_a) \int \frac{d^D p}{(2\pi \hbar)^D} \exp \left\{ \frac{i}{\hbar} \left[\mathbf{p}(\mathbf{x}_b - \mathbf{x}_a) + (t_b - t_a) \left(E - \frac{\mathbf{p}^2}{2M} \right) \right] \right\}. \quad (1.352)$$

Performing the time integration yields

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \int \frac{d^D p}{(2\pi \hbar)^D} \exp [i \mathbf{p}(\mathbf{x}_b - \mathbf{x}_a)] \frac{i \hbar}{E - \mathbf{p}^2/2M + i\eta}, \quad (1.353)$$

where we have inserted a damping factor $e^{-\eta(t_b - t_a)}$ into the integral to ensure convergence at large $t_b - t_a$. For a more explicit result it is more convenient to calculate the Fourier transform (1.350):

$$(\mathbf{x}_b | \mathbf{x}_a)_E = \int_0^\infty d(t_b - t_a) \frac{1}{\sqrt{2\pi i \hbar (t_b - t_a)/M}^D} \exp \left\{ \frac{i}{\hbar} \left[E(t_b - t_a) + \frac{M}{2} \frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a} \right] \right\}. \quad (1.354)$$

For $E < 0$, we set

$$\kappa \equiv \sqrt{-2ME/\hbar^2}, \quad (1.355)$$

and perform the integral with the help of the formula¹⁰

$$\int_0^\infty dt t^{\nu-1} e^{-i\gamma t + i\beta/t} = 2 \left(\frac{\beta}{\gamma} \right)^{\nu/2} e^{-i\nu\pi/2} K_{-\nu}(2\sqrt{\beta\gamma}), \quad (1.356)$$

where $K_\nu(z)$ is the *modified Bessel function* which satisfies $K_\nu(z) = K_{-\nu}(z)$.¹¹ The result is

$$(\mathbf{x}_b | \mathbf{x}_a)_E = -i \frac{2M}{\hbar} \frac{\kappa^{D-2}}{(2\pi)^{D/2}} \frac{K_{D/2-1}(\kappa R)}{(\kappa R)^{D/2-1}}, \quad (1.357)$$

where $R \equiv |\mathbf{x}_b - \mathbf{x}_a|$. The simplest modified Bessel function is¹²

$$K_{1/2}(z) = K_{-1/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z}, \quad (1.358)$$

¹⁰I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980. Use any of Formulas 3.471.10, 3.471.11, or 8.432.6.

¹¹*Ibid.*, Formula 8.486.16.

¹²M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Formula 10.2.17.

so that we find the amplitudes for $D = 1, 2, 3$:

$$-i\frac{M}{\hbar}\frac{1}{\kappa}e^{-\kappa R}, \quad -i\frac{M}{\hbar}\frac{1}{\pi}K_0(\kappa R), \quad -i\frac{M}{\hbar}\frac{1}{2\pi R}e^{-\kappa R}. \quad (1.359)$$

At $R = 0$, the amplitude (1.357) is finite for all $D \leq 2$, and we can use the small-argument behavior of the associated Bessel function¹³

$$K_\nu(z) = K_{-\nu}(z) \approx \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} \quad \text{for } \text{Re } \nu > 0, \quad (1.360)$$

to obtain

$$(\mathbf{x}|\mathbf{x})_E = -i\frac{2M}{\hbar}\frac{\kappa^{D-2}}{(4\pi)^{D/2}}\Gamma(1-D/2). \quad (1.361)$$

This result can be continued analytically to $D > 2$, which is often of interest.

For $E > 0$ we set

$$k \equiv \sqrt{2ME/\hbar^2}, \quad (1.362)$$

and use the formula¹⁴

$$\int_0^\infty dt t^{\nu-1} e^{i\gamma t + i\beta/t} = i\pi \left(\frac{\beta}{\gamma}\right)^{\nu/2} e^{-i\nu\pi/2} H_{-\nu}^{(1)}(2\sqrt{\beta\gamma}), \quad (1.363)$$

where $H_\nu^{(1)}(z)$ is the Hankel function, to find

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \frac{M\pi}{\hbar} \frac{k^{D-2}}{(2\pi)^{D/2}} \frac{H_{D/2-1}(kR)}{(kR)^{D/2-1}}. \quad (1.364)$$

The relation¹⁵

$$K_\nu(-iz) = \frac{\pi}{2} i e^{i\nu\pi/2} H_\nu^{(1)}(z) \quad (1.365)$$

connects the two results (1.357) and (1.364) with each other when continuing the energy from negative to positive values, which replaces κ by $e^{-i\pi/2}k = -ik$.

For large distances, the asymptotic behavior¹⁶

$$K_\nu(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z}, \quad H_\nu^{(1)}(z) \approx \sqrt{\frac{2}{\pi z}} e^{i(z-\nu\pi/2-\pi/4)} \quad (1.366)$$

shows that the fixed-energy amplitude behaves for $E < 0$ like

$$(\mathbf{x}_b|\mathbf{x}_a)_E \approx -i\frac{M}{\hbar}\kappa^{D-2} \frac{1}{(2\pi)^{(D-1)/2}} \frac{1}{(\kappa R)^{(D-1)/2}} e^{-\kappa R/\hbar}, \quad (1.367)$$

and for $E > 0$ like

$$(\mathbf{x}_b|\mathbf{x}_a)_E \approx \frac{M}{\hbar} k^{D-2} \frac{1}{(2\pi i)^{(D-1)/2}} \frac{1}{(kR)^{(D-1)/2}} e^{ikR/\hbar}. \quad (1.368)$$

For $D = 1$ and 3 , these asymptotic expressions hold for all R .

¹³*Ibid.*, Formula 9.6.9.

¹⁴*Ibid.*, Formulas 3.471.11 or 8.421.7.

¹⁵*Ibid.*, Formula 8.407.1.

¹⁶*Ibid.*, Formulas 8.451.6 or 8.451.3.

1.13 Quantum Mechanics of General Lagrangian Systems

An extension of the quantum-mechanical formalism to systems described by a set of completely general Lagrange coordinates $q_1, \dots, q_N$ is not straightforward. Only in the special case that q_i ($i = 1, \dots, N$) represent merely a curvilinear reparametrization of a D -dimensional euclidean space parametrized by x^i , the above correspondence rules are sufficient to quantize the system. Then the number N of coordinates is equal to the dimension D , and a variable change from x^i to q_j in the Schrödinger equation leads to the correct quantum mechanics. It will be useful to label the curvilinear coordinates by Greek superscripts, and write q^μ instead of latin subscripts in q_j . This will help us to write all ensuing equations in a form that is manifestly covariant under coordinate transformations. In the original definition of generalized coordinates in Eq. (1.1), this was unnecessary since transformation properties were ignored. For the Cartesian coordinates we shall use Latin indices alternatively as sub- or superscripts. The coordinate transformation $x^i = x^i(q^\mu)$ implies the relation between the derivatives $\partial_\mu \equiv \partial/\partial q^\mu$ and $\partial_i \equiv \partial/\partial x^i$:

$$\partial_\mu = e^i{}_\mu(q) \partial_i, \quad (1.369)$$

with the transformation matrix

$$e^i{}_\mu(q) \equiv \partial_\mu x^i(q) \quad (1.370)$$

called *basis D-ad* (in 3 dimensions basis triad, in 4 dimensions basis tetrad, etc.). Let $e_i{}^\mu(q) = \partial q^\mu / \partial x^i$ be the inverse matrix (assuming it exists) called the *reciprocal D-ad*, satisfying with $e^i{}_\mu$ the orthogonality and completeness relations

$$e^i{}_\mu e_i{}^\nu = \delta_\mu{}^\nu, \quad e^i{}_\mu e_j{}^\mu = \delta^i_j. \quad (1.371)$$

Then (1.369) is inverted to

$$\partial_i = e_i{}^\mu(q) \partial_\mu \quad (1.372)$$

and yields the curvilinear transform of the Cartesian quantum-mechanical momentum operators

$$\hat{p}_i = -i\hbar \partial_i = -i\hbar e_i{}^\mu(q) \partial_\mu. \quad (1.373)$$

The free-particle Hamiltonian operator

$$\hat{H}_0 = \hat{T} = \frac{1}{2M} \hat{\mathbf{p}}^2 = -\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \quad (1.374)$$

goes over into

$$\hat{H}_0 = -\frac{\hbar^2}{2M} \Delta, \quad (1.375)$$

where Δ is the Laplacian expressed in curvilinear coordinates:

$$\begin{aligned} \Delta &= \partial_i^2 = e^{i\mu} \partial_\mu e_i{}^\nu \partial_\nu \\ &= e^{i\mu} e_i{}^\nu \partial_\mu \partial_\nu + (e^{i\mu} \partial_\mu e_i{}^\nu) \partial_\nu. \end{aligned} \quad (1.376)$$

At this point one introduces the *metric tensor*

$$g_{\mu\nu}(q) \equiv e_{i\mu}(q)e^i{}_\nu(q), \quad (1.377)$$

its inverse

$$g^{\mu\nu}(q) = e^{i\mu}(q)e_i{}^\nu(q) \quad (1.378)$$

defined by $g^{\mu\nu}g_{\nu\lambda} = \delta^\mu{}_\lambda$, and the so-called *affine connection*

$$\Gamma_{\mu\nu}{}^\lambda(q) = -e^i{}_\nu(q)\partial_\mu e_i{}^\lambda(q) = e_i{}^\lambda(q)\partial_\mu e^i{}_\nu(q). \quad (1.379)$$

Then the Laplacian takes the form

$$\Delta = g^{\mu\nu}(q)\partial_\mu\partial_\nu - \Gamma_\mu{}^{\mu\nu}(q)\partial_\nu, \quad (1.380)$$

with $\Gamma_\mu{}^{\lambda\nu}$ being defined as the *contraction*

$$\Gamma_\mu{}^{\lambda\nu} \equiv g^{\lambda\kappa}\Gamma_{\mu\kappa}{}^\nu. \quad (1.381)$$

The reason why (1.377) is called a metric tensor is obvious: An infinitesimal square distance between two points in the original Cartesian coordinates

$$ds^2 \equiv d\mathbf{x}^2 \quad (1.382)$$

becomes, in curvilinear coordinates,

$$ds^2 = \frac{\partial \mathbf{x}}{\partial q^\mu} \frac{\partial \mathbf{x}}{\partial q^\nu} dq^\mu dq^\nu = g_{\mu\nu}(q) dq^\mu dq^\nu. \quad (1.383)$$

The infinitesimal volume element $d^D x$ is given by

$$d^D x = \sqrt{g} d^D q, \quad (1.384)$$

where

$$g(q) \equiv \det(g_{\mu\nu}(q)) \quad (1.385)$$

is the determinant of the metric tensor. Using this determinant, we form the quantity

$$\Gamma_\mu \equiv g^{-1/2}(\partial_\mu g^{1/2}) = \frac{1}{2}g^{\lambda\kappa}(\partial_\mu g_{\lambda\kappa}) \quad (1.386)$$

and see that it is equal to the once-contracted connection

$$\Gamma_\mu = \Gamma_{\mu\lambda}{}^\lambda. \quad (1.387)$$

With the inverse metric (1.378) we have furthermore

$$\Gamma_\mu{}^{\mu\nu} = -\partial_\mu g^{\mu\nu} - \Gamma_\mu{}^{\nu\mu}. \quad (1.388)$$

We now take advantage of the fact that the derivatives $\partial_\mu, \partial_\nu$ applied to the coordinate transformation $x^i(q)$ commute, causing $\Gamma_{\mu\nu}^\lambda$ to be symmetric in $\mu\nu$, i.e., $\Gamma_{\mu\nu}^\lambda = \Gamma_{\nu\mu}^\lambda$ and hence $\Gamma_\mu^{\nu\mu} = \Gamma^\nu$. Together with (1.386) we find the rotation

$$\Gamma_\mu^{\mu\nu} = -\frac{1}{\sqrt{g}}(\partial_\mu g^{\mu\nu} \sqrt{g}), \quad (1.389)$$

which allows the Laplace operator Δ to be rewritten in the more compact form

$$\Delta = \frac{1}{\sqrt{g}} \partial_\mu g^{\mu\nu} \sqrt{g} \partial_\nu. \quad (1.390)$$

This expression is called the *Laplace-Beltrami operator*.

Thus we have shown that, for a Hamiltonian in a euclidean space,

$$H(\hat{\mathbf{p}}, \mathbf{x}) = \frac{1}{2M} \hat{\mathbf{p}}^2 + V(\mathbf{x}), \quad (1.391)$$

the Schrödinger equation in curvilinear coordinates becomes

$$\hat{H}\psi(q, t) \equiv \left[-\frac{\hbar^2}{2M} \Delta + V(q) \right] \psi(q, t) = i\hbar \partial_t \psi(q, t), \quad (1.392)$$

where $V(q)$ is short for $V(\mathbf{x}(q))$. The scalar product of two wave functions $\int d^D x \psi_2^*(\mathbf{x}, t) \psi_1(\mathbf{x}, t)$, which determines the transition amplitudes of the system, transforms into

$$\int d^D q \sqrt{g} \psi_2^*(q, t) \psi_1(q, t). \quad (1.393)$$

It is important to realize that this Schrödinger equation would *not* be obtained by a straightforward application of the canonical formalism to the coordinate-transformed version of the Cartesian Lagrangian

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{M}{2} \dot{\mathbf{x}}^2 - V(\mathbf{x}). \quad (1.394)$$

With the velocities transforming like

$$\dot{x}^i = e^i_\mu(q) \dot{q}^\mu, \quad (1.395)$$

the Lagrangian becomes

$$L(q, \dot{q}) = \frac{M}{2} g_{\mu\nu}(q) \dot{q}^\mu \dot{q}^\nu - V(q). \quad (1.396)$$

Up to a factor M , the metric is equal to the Hessian metric of the system, which depends here only on q^μ [recall (1.12)]:

$$H_{\mu\nu}(q) = M g_{\mu\nu}(q). \quad (1.397)$$

The canonical momenta are

$$p_\mu \equiv \frac{\partial L}{\partial \dot{q}^\mu} = M g_{\mu\nu} \dot{q}^\nu. \quad (1.398)$$

The associated quantum-mechanical momentum operators $\hat{p}_\mu$ have to be Hermitian in the scalar product (1.393). They must satisfy the canonical commutation rules (1.276):

$$\begin{aligned} [\hat{p}_\mu, \hat{q}^\nu] &= -i\hbar \delta_\mu^\nu, \\ [\hat{q}^\mu, \hat{q}^\nu] &= 0, \\ [\hat{p}_\mu, \hat{p}_\nu] &= 0. \end{aligned} \quad (1.399)$$

An obvious solution is

$$\hat{p}_\mu = -i\hbar g^{-1/4} \partial_\mu g^{1/4}, \quad \hat{q}^\mu = q^\mu. \quad (1.400)$$

The commutation rules are true for $-i\hbar g^{-z} \partial_\mu g^z$ with any power z , but only $z = 1/4$ produces a Hermitian momentum operator:

$$\begin{aligned} \int d^3q \sqrt{g} \Psi_2^*(q, t) [-i\hbar g^{-1/4} \partial_\mu g^{1/4} \Psi_1(q, t)] &= \int d^3q g^{1/4} \Psi_2^*(q, t) [-i\hbar \partial_\mu g^{1/4} \Psi_1(q, t)] \\ &= \int d^3q \sqrt{g} [-i\hbar g^{-1/4} \partial_\mu g^{1/4} \Psi_2(q, t)]^* \Psi_1(q, t), \end{aligned} \quad (1.401)$$

as is easily verified by partial integration.

In terms of the quantity (1.386), this can also be rewritten as

$$\hat{p}_\mu = -i\hbar (\partial_\mu + \tfrac{1}{2} \Gamma_\mu). \quad (1.402)$$

Consider now the classical Hamiltonian associated with the Lagrangian (1.396), which by (1.398) is simply

$$H = p_\mu \dot{q}^\mu - L = \frac{1}{2M} g_{\mu\nu}(q) p^\mu p^\nu + V(q). \quad (1.403)$$

When trying to turn this expression into a Hamiltonian operator, we encounter the operator-ordering problem discussed in connection with Eq. (1.106). The correspondence principle requires replacing the momenta p_μ by the momentum operators $\hat{p}_\mu$, but it does not specify the position of these operators with respect to the coordinates q^μ contained in the inverse metric $g^{\mu\nu}(q)$. An important constraint is provided by the required hermiticity of the Hamiltonian operator, but this is not sufficient for a unique specification. We may, for instance, define the canonical Hamiltonian operator as

$$\hat{H}_{\text{can}} \equiv \frac{1}{2M} \hat{p}^\mu g_{\mu\nu}(q) \hat{p}^\nu + V(q), \quad (1.404)$$

in which the momentum operators have been arranged symmetrically around the inverse metric to achieve hermiticity. This operator, however, is not equal to the

correct Schrödinger operator in (1.392). The kinetic term contains what we may call the *canonical Laplacian*

$$\Delta_{\text{can}} = (\partial_\mu + \tfrac{1}{2}\Gamma_\mu) g^{\mu\nu}(q) (\partial_\nu + \tfrac{1}{2}\Gamma_\nu). \quad (1.405)$$

It differs from the Laplace-Beltrami operator (1.390) in (1.392) by

$$\Delta - \Delta_{\text{can}} = -\tfrac{1}{2}\partial_\mu(g^{\mu\nu}\Gamma_\nu) - \tfrac{1}{4}g^{\mu\nu}\Gamma_\nu\Gamma_\mu. \quad (1.406)$$

The correct Hamiltonian operator could be obtained by suitably distributing pairs of dummy factors of $g^{1/4}$ and $g^{-1/4}$ symmetrically between the canonical operators, for example by taking [8]:

$$\hat{H} = \frac{1}{2M} g^{-1/4} \hat{p}_\mu g^{1/4} g^{\mu\nu}(q) g^{1/4} \hat{p}_\nu g^{-1/4} + V(q). \quad (1.407)$$

This operator has the same classical limit (1.403) as (1.404). The correspondence principle does not specify how the classical factors have to be ordered before being replaced by operators.

The simplest system exhibiting the breakdown of the canonical quantization rules is a free particle in a plane described by radial coordinates $q^1 = r, q^2 = \varphi$:

$$x^1 = r \cos \varphi, \quad x^2 = r \sin \varphi. \quad (1.408)$$

Since the infinitesimal square distance is $ds^2 = dr^2 + r^2 d\varphi^2$, the metric reads

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}_{\mu\nu}. \quad (1.409)$$

It has a determinant

$$g = r^2 \quad (1.410)$$

and an inverse

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & r^{-2} \end{pmatrix}^{\mu\nu}. \quad (1.411)$$

The Laplace-Beltrami operator becomes

$$\Delta = \frac{1}{r} \partial_r r \partial_r + \frac{1}{r^2} \partial_\varphi^2. \quad (1.412)$$

The canonical Laplacian, on the other hand, reads

$$\begin{aligned} \Delta_{\text{can}} &= (\partial_r + 1/2r)^2 + \frac{1}{r^2} \partial_\varphi^2 \\ &= \partial_r^2 + \frac{1}{r} \partial_r - \frac{1}{4r^2} + \frac{1}{r^2} \partial_\varphi^2. \end{aligned} \quad (1.413)$$

The discrepancy (1.406) is therefore

$$\Delta_{\text{can}} - \Delta = -\frac{1}{4r^2}. \quad (1.414)$$

Note that this discrepancy arises even though there is no apparent ordering problem in the naively quantized canonical expression $\hat{p}^\mu g_{\mu\nu}(q) \hat{p}^\nu$ in (1.413). Only the need to introduce dummy $g^{1/4}$ - and $g^{-1/4}$ -factors creates such problems, and a specification of the order is required to obtain the correct result.

If the Lagrangian coordinates q_i do not merely reparametrize a euclidean space but specify the points of a general geometry, we cannot proceed as above and derive the Laplace-Beltrami operator by a coordinate transformation of a Cartesian Laplacian. With the canonical quantization rules being unreliable in curvilinear coordinates there are, at first sight, severe difficulties in quantizing such a system. This is why the literature contains many proposals for handling this problem [9]. Fortunately, a large class of non-Cartesian systems allows for a unique quantum-mechanical description on completely different grounds. These systems have the common property that their Hamiltonian can be expressed in terms of the generators of a group of motion in the general coordinate frame. For symmetry reasons, the correspondence principle must then be imposed on the commutators of the group generators rather than upon the Poisson brackets of the canonical variables p and q . The brackets containing two group generators specify the structure of the group, while those containing a generator and a coordinate specify the defining representation of the group in configuration space. The replacement of these brackets by commutation rules constitutes the proper generalization of the canonical quantization from Cartesian to non-Cartesian coordinates. It is called *group quantization*. The replacement rule will be referred to as the *group correspondence principle*. The canonical commutation rules in euclidean space may be viewed as a special case of the commutation rules between group generators, i.e., of the *Lie algebra* of the group. In a Cartesian coordinate frame, the group of motion is the euclidean group containing translations and rotations. The generators of translations and rotations are the momenta and the angular momenta, respectively. According to the group correspondence principle, the Poisson brackets between the generators and the coordinates have to be replaced by commutation rules. Thus, in a euclidean space, the commutation rules between group generators and coordinates lead to the canonical quantization rules, and this appears to be the deeper reason why the canonical rules are correct. This is true in particular for systems whose energy depends on generators of the group of motion other than those of translations, for instance on the angular momenta. Then the commutators between the group generators must be used for quantization, rather than the canonical commutators between positions and momenta.

The prime examples for such systems are provided by a particle on the surface of a sphere or by a spinning top. The quantization of both will now be discussed.

1.14 Particle on the Surface of a Sphere

For a particle moving on the surface of a sphere of radius r with coordinates

$$x^1 = r \sin \theta \cos \varphi, \quad x^2 = r \sin \theta \sin \varphi, \quad x^3 = r \cos \theta, \quad (1.415)$$

the Lagrangian reads

$$L = \frac{Mr^2}{2}(\dot{\theta}^2 + \sin^2 \theta \dot{\varphi}^2). \quad (1.416)$$

The canonical momenta are

$$p_\theta = Mr^2 \dot{\theta}, \quad p_\varphi = Mr^2 \sin^2 \theta \dot{\varphi}, \quad (1.417)$$

and the classical Hamiltonian is given by

$$H = \frac{1}{2Mr^2} \left(p_\theta^2 + \frac{1}{\sin^2 \theta} p_\varphi^2 \right). \quad (1.418)$$

According to the canonical quantization rules, the momenta should become operators

$$\hat{p}_\theta = -i\hbar \frac{1}{\sin^{1/2} \theta} \partial_\theta \sin^{1/2} \theta, \quad \hat{p}_\varphi = -i\hbar \partial_\varphi. \quad (1.419)$$

But as explained in the previous section, these momentum operators are not expected to give the correct Hamiltonian operator when inserted into the Hamiltonian (1.418). Moreover, there exists no proper coordinate transformation from the surface of the sphere to Cartesian coordinates¹⁷ such that a particle on a sphere cannot be treated via the safe Cartesian quantization rules (1.276):

$$\begin{aligned} [\hat{p}_i, \hat{x}^j] &= -i\hbar \delta_i^j, \\ [\hat{x}^i, \hat{x}^j] &= 0, \\ [\hat{p}_i, \hat{p}_j] &= 0. \end{aligned} \quad (1.420)$$

The only help comes from the group properties of the motion on the surface of the sphere. The angular momentum

$$\mathbf{L} = \mathbf{x} \times \mathbf{p} \quad (1.421)$$

can be quantized uniquely in Cartesian coordinates. It becomes an operator

$$\hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}, \quad (1.422)$$

whose components satisfy the commutation rules of the Lie algebra of the rotation group

$$[\hat{L}_i, \hat{L}_j] = i\hbar \hat{L}_k \quad (i, j, k \text{ cyclic}). \quad (1.423)$$

Note that there is no factor-ordering problem since the $\hat{x}^i$'s and the $\hat{p}_i$'s appear with different indices in each $\hat{L}_k$. An important property of the angular momentum

¹⁷There exist, however, certain infinitesimal nonholonomic coordinate transformations which are multivalued and can be used to transform infinitesimal distances in a flat space into those in a curved one. They are introduced and applied in the textbook entitled *Multivalued Fields* cited in Ref. [5] leading once more to the same quantum mechanics as the one described here.

operator is its homogeneity in $\mathbf{x}$. It has the consequence that, when going from Cartesian to spherical coordinates

$$x^1 = r \sin \theta \cos \varphi, \quad x^2 = r \sin \theta \sin \varphi, \quad x^3 = r \cos \theta, \quad (1.424)$$

the radial coordinate cancels, making the angular momentum a differential operator involving only the angles θ, φ :

$$\begin{aligned} \hat{L}_1 &= i\hbar (\sin \varphi \partial_\theta + \cot \theta \cos \varphi \partial_\varphi), \\ \hat{L}_2 &= -i\hbar (\cos \varphi \partial_\theta - \cot \theta \sin \varphi \partial_\varphi), \\ \hat{L}_3 &= -i\hbar \partial_\varphi. \end{aligned} \quad (1.425)$$

There is then a natural way of quantizing the system which makes use of these operators $\hat{L}_i$. We re-express the classical Hamiltonian (1.418) in terms of the classical angular momenta

$$\begin{aligned} L_1 &= Mr^2 \left(-\sin \varphi \dot{\theta} - \sin \theta \cos \theta \cos \varphi \dot{\varphi} \right), \\ L_2 &= Mr^2 \left(\cos \varphi \dot{\theta} - \sin \theta \cos \theta \sin \varphi \dot{\varphi} \right), \\ L_3 &= Mr^2 \sin^2 \theta \dot{\varphi} \end{aligned} \quad (1.426)$$

as

$$H = \frac{1}{2Mr^2} \mathbf{L}^2, \quad (1.427)$$

and replace the angular momenta by the operators (1.425). The result is the Hamiltonian operator:

$$\hat{H} = \frac{1}{2Mr^2} \hat{\mathbf{L}}^2 = -\frac{\hbar^2}{2Mr^2} \left[\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\varphi^2 \right]. \quad (1.428)$$

The eigenfunctions diagonalizing the rotation-invariant operator $\hat{\mathbf{L}}^2$ are well known. They can be chosen to diagonalize simultaneously one component of $\hat{L}_i$, for instance the third one, $\hat{L}_3$, in which case they are equal to the spherical harmonics

$$Y_{lm}(\theta, \varphi) = (-1)^m \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\varphi}, \quad (1.429)$$

with $P_l^m(z)$ being the associated Legendre polynomials

$$P_l^m(z) = \frac{1}{2^l l!} (1-z^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (z^2-1)^l. \quad (1.430)$$

The spherical harmonics are orthonormal with respect to the rotation-invariant scalar product

$$\int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi Y_{lm}^*(\theta, \varphi) Y_{l'm'}(\theta, \varphi) = \delta_{ll'} \delta_{mm'}. \quad (1.431)$$

Two important lessons can be learned from this group quantization. First, the correct Hamiltonian operator (1.428) does not agree with the canonically quantized one which would be obtained by inserting Eqs. (1.419) into (1.418). The correct result would, however, arise by distributing dummy factors

$$g^{-1/4} = r^{-1} \sin^{-1/2} \theta, \quad g^{1/4} = r \sin^{1/2} \theta \quad (1.432)$$

between the canonical momentum operators as observed earlier in Eq. (1.407). Second, just as in the case of polar coordinates, the correct Hamiltonian operator is equal to

$$\hat{H} = -\frac{\hbar^2}{2M} \Delta, \quad (1.433)$$

where Δ is the Laplace-Beltrami operator associated with the metric

$$g_{\mu\nu} = r^2 \begin{pmatrix} 1 & 0 \\ 0 & \sin^2 \theta \end{pmatrix}, \quad (1.434)$$

i.e.,

$$\Delta = \frac{1}{r^2} \left[\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\varphi^2 \right]. \quad (1.435)$$

1.15 Spinning Top

For a spinning top, the optimal starting point is again not the classical Lagrangian but the Hamiltonian expressed in terms of the classical angular momenta. In the symmetric case in which two moments of inertia coincide, it is written as

$$H = \frac{1}{2I_\xi} (L_\xi^2 + L_\eta^2) + \frac{1}{2I_\zeta} L_\zeta^2, \quad (1.436)$$

where L_ξ, L_η, L_ζ are the components of the orbital angular momentum in the directions of the principal body axes, and $I_\xi, I_\eta \equiv I_\xi, I_\zeta$ denotes the corresponding moments of inertia. The classical angular momentum of an aggregate of mass points is given by

$$\mathbf{L} = \sum_\nu \mathbf{x}_\nu \times \mathbf{p}_\nu, \quad (1.437)$$

where the sum over ν runs over all mass points. The angular momentum possesses a unique operator

$$\hat{\mathbf{L}} = \sum_\nu \hat{\mathbf{x}}_\nu \times \hat{\mathbf{p}}_\nu, \quad (1.438)$$

with the commutation rules (1.423) between the components $\hat{L}_i$. Since rotations do not change the distances between the mass points, they commute with the constraints of the rigid body. If the center of mass of the rigid body is placed at the origin, the only dynamical degrees of freedom are the orientations in space. They can uniquely be specified by the rotation matrix which brings the body from some standard orientation to the actual one. We may choose the standard orientation

to have the principal body axes aligned with the x, y, z -directions, respectively. An arbitrary orientation is obtained by applying all finite rotations to each point of the body. They are specified by the 3×3 orthonormal matrices R_{ij} . The space of these matrices has three degrees of freedom. It can be decomposed, omitting the matrix indices as

$$R(\alpha, \beta, \gamma) = R_3(\alpha)R_2(\beta)R_3(\gamma), \quad (1.439)$$

where $R_3(\alpha)$, $R_3(\gamma)$ are rotations around the z -axis by angles α , γ , respectively, and $R_2(\beta)$ is a rotation around the y -axis by β . These rotation matrices can be expressed as exponentials

$$R_i(\delta) \equiv e^{-i\delta L_i/\hbar}, \quad (1.440)$$

where δ is the rotation angle and L_i are the 3×3 matrix generators of the rotations with the elements

$$(L_i)_{jk} = -i\hbar\epsilon_{ijk}. \quad (1.441)$$

It is easy to check that these generators satisfy the commutation rules (1.423) of angular momentum operators. The angles α, β, γ are referred to as *Euler angles*.

The 3×3 rotation matrices make it possible to express the infinitesimal rotations around the three coordinate axes as differential operators of the three Euler angles. Let $\psi(R)$ be the wave function of the spinning top describing the probability amplitude of the different orientations which arise from a standard orientation by the rotation matrix $R = R(\alpha, \beta, \gamma)$. Then a further rotation by $R(\alpha', \beta', \gamma')$ transforms the wave function into $\psi'(R) = \psi(R^{-1}(\alpha', \beta', \gamma')R)$. The transformation may be described by a unitary differential operator

$$\hat{U}(\alpha', \beta', \gamma') \equiv e^{-i\alpha' \hat{L}_3/\hbar} e^{-i\beta' \hat{L}_2/\hbar} e^{-i\gamma' \hat{L}_3/\hbar}, \quad (1.442)$$

where $\hat{L}_i$ is the representation of the generators in terms of differential operators. To calculate these we note that the 3×3 -matrix $R^{-1}(\alpha, \beta, \gamma)$ has the following derivatives

$$\begin{aligned} -i\hbar\partial_\alpha R^{-1} &= R^{-1}L_3, \\ -i\hbar\partial_\beta R^{-1} &= R^{-1}(\cos\alpha L_2 - \sin\alpha L_1), \\ -i\hbar\partial_\gamma R^{-1} &= R^{-1}[\cos\beta L_3 + \sin\beta(\cos\alpha L_1 + \sin\alpha L_2)]. \end{aligned} \quad (1.443)$$

The first relation is trivial, the second follows from the rotation of the generator

$$e^{-i\alpha L_3/\hbar} L_2 e^{i\alpha L_3/\hbar} = \cos\alpha L_2 - \sin\alpha L_1, \quad (1.444)$$

which is a consequence of Lie's expansion formula (4.105), together with the commutation rules (1.441) of the 3×3 matrices L_i . The third requires, in addition, the rotation

$$e^{-i\beta L_2/\hbar} L_3 e^{i\beta L_2/\hbar} = \cos\beta L_3 + \sin\beta L_1. \quad (1.445)$$

Inverting the relations (1.443), we find the differential operators generating the rotations [10]:

$$\begin{aligned}\hat{L}_1 &= i\hbar \left(\cos \alpha \cot \beta \partial_\alpha + \sin \alpha \partial_\beta - \frac{\cos \alpha}{\sin \beta} \partial_\gamma \right), \\ \hat{L}_2 &= i\hbar \left(\sin \alpha \cot \beta \partial_\alpha - \cos \alpha \partial_\beta - \frac{\sin \alpha}{\sin \beta} \partial_\gamma \right), \\ \hat{L}_3 &= -i\hbar \partial_\alpha.\end{aligned}\tag{1.446}$$

After exponentiating these differential operators we derive

$$\hat{U}(\alpha', \beta', \gamma') R(\alpha, \beta, \gamma) \hat{U}^{-1}(\alpha', \beta', \gamma') = R^{-1}(\alpha', \beta', \gamma') R(\alpha, \beta, \gamma),\tag{1.447}$$

implying that $\psi'(R) = \hat{U}(\alpha', \beta', \gamma') \psi(R)$, as desired.

In the Hamiltonian (1.436), we need the components of $\hat{\mathbf{L}}$ along the body axes. They are obtained by rotating the 3×3 matrices L_i by $R(\alpha, \beta, \gamma)$ into

$$\begin{aligned}L_\xi &= RL_1R^{-1} = \cos \gamma \cos \beta (\cos \alpha L_1 + \sin \alpha L_2) \\ &\quad + \sin \gamma (\cos \alpha L_2 - \sin \alpha L_1) - \cos \gamma \sin \beta L_3, \\ L_\eta &= RL_2R^{-1} = -\sin \gamma \cos \beta (\cos \alpha L_1 + \sin \alpha L_2) \\ &\quad + \cos \gamma (\cos \alpha L_2 - \sin \alpha L_1) + \sin \gamma \sin \beta L_3, \\ L_\zeta &= RL_3R^{-1} = \cos \beta L_3 + \sin \beta (\cos \alpha L_1 + \sin \alpha L_2),\end{aligned}\tag{1.448}$$

and by replacing $L_i \rightarrow \hat{L}_i$ in the final expressions. Inserting (1.446), we find the operators

$$\begin{aligned}\hat{L}_\xi &= i\hbar \left(-\cos \gamma \cot \beta \partial_\gamma - \sin \gamma \partial_\beta + \frac{\cos \gamma}{\sin \beta} \partial_\alpha \right), \\ \hat{L}_\eta &= i\hbar \left(\sin \gamma \cot \beta \partial_\gamma - \cos \gamma \partial_\beta - \frac{\sin \gamma}{\sin \beta} \partial_\alpha \right), \\ \hat{L}_\zeta &= -i\hbar \partial_\gamma.\end{aligned}\tag{1.449}$$

Note that these commutation rules have an opposite sign with respect to those in Eqs. (1.423) of the operators $\hat{L}_i$.¹⁸

$$[\hat{L}_\xi, \hat{L}_\eta] = -i\hbar \hat{L}_\zeta, \quad \xi, \eta, \zeta = \text{cyclic}.\tag{1.450}$$

The sign is most simply understood by writing

$$\hat{L}_\xi = a_\xi^i \hat{L}_i, \quad \hat{L}_\eta = a_\eta^i \hat{L}_i, \quad \hat{L}_\zeta = a_\zeta^i \hat{L}_i,\tag{1.451}$$

¹⁸When applied to functions which do not depend on α , then, after replacing $\beta \rightarrow \theta$ and $\gamma \rightarrow \varphi$, the operators agree with those in (1.425), up to the sign of $\hat{L}_1$.

where $a_\xi^i, a_\eta^i, a_\zeta^i$, are the components of the body axes. Under rotations these behave like $[\hat{L}_i, a_\xi^j] = i\hbar\epsilon_{ijk}a_\xi^k$, i.e., they are vector operators. It is easy to check that this property produces the sign reversal in (1.450) with respect to (1.423).

The correspondence principle is now applied to the Hamiltonian in Eq. (1.436) by placing operator hats on the L_a 's. The energy spectrum and the wave functions can then be obtained by using only the group commutators between $\hat{L}_\xi, \hat{L}_\eta, \hat{L}_\zeta$. The spectrum is

$$E_{L\Lambda} = \hbar^2 \left[\frac{1}{2I_\xi} L(L+1) + \left(\frac{1}{2I_\zeta} - \frac{1}{2I_\xi} \right) \Lambda^2 \right], \quad (1.452)$$

where $L(L+1)$ with $L = 0, 1, 2, \dots$ are the eigenvalues of $\hat{\mathbf{L}}^2$, and $\Lambda = -L, \dots, L$ are the eigenvalues of $\hat{L}_\zeta$. The wave functions are the representation functions of the rotation group. If the Euler angles α, β, γ are used to specify the orientation of the body axes, the wave functions are

$$\psi_{L\Lambda m}(\alpha, \beta, \gamma) = D_{m\Lambda}^L(-\alpha, -\beta, -\gamma). \quad (1.453)$$

Here m are the eigenvalues of $\hat{L}_3$, i.e., the magnetic quantum numbers, and $D_{m\Lambda}^L(\alpha, \beta, \gamma)$ are the representation matrices of angular momentum L . In accordance with (1.442), we may decompose

$$D_{mm'}^L(\alpha, \beta, \gamma) = e^{-i(m\alpha+m'\gamma)} d_{mm'}^L(\beta), \quad (1.454)$$

with the matrices

$$\begin{aligned} d_{mm'}^L(\beta) &= \left[\frac{(L+m')!(L-m)!}{(L+m)!(L-m')!} \right]^{1/2} \\ &\times \left(\cos \frac{\beta}{2} \right)^{m+m'} \left(-\sin \frac{\beta}{2} \right)^{m-m'} P_{L-m'}^{(m'-m, m'+m)}(\cos \beta). \end{aligned} \quad (1.455)$$

For $j = 1/2$, these form the spinor representation of the rotations around the y -axis

$$d_{m'm}^{1/2}(\beta) = \begin{pmatrix} \cos \beta/2 & -\sin \beta/2 \\ \sin \beta/2 & \cos \beta/2 \end{pmatrix}. \quad (1.456)$$

The indices have the order $+1/2, -1/2$. The full spinor representation function $D^{1/2}(\alpha, \beta, \gamma)$ in (1.454) is most easily obtained by inserting, into the general expression (1.442), the representation matrices of spin $1/2$ for the generators $\hat{L}_i$ with the commutation rules (1.423), which are, of course, the famous *Pauli spin matrices*:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.457)$$

Thus we can write

$$D^{1/2}(\alpha, \beta, \gamma) = e^{-i\alpha\sigma_3/2} e^{-i\beta\sigma_2/2} e^{-i\gamma\sigma_3/2}. \quad (1.458)$$

The first and the third factor yield the pure phase factors in (1.454). The function $d_{m'm}^{1/2}(\beta)$ is obtained by a simple power series expansion of $e^{-i\beta\sigma^2/2}$, using the fact that $(\sigma^2)^{2n} = 1$ and $(\sigma^2)^{2n+1} = \sigma^2$:

$$e^{-i\beta\sigma^2/2} = \cos \beta/2 - i \sin \beta/2 \sigma^2, \quad (1.459)$$

which is equal to (1.456).

For $j = 1$, the representation functions (1.455) form the vector representation

$$d_{m'm}^1(\beta) = \begin{pmatrix} \frac{1}{2}(1 + \cos \beta) & -\frac{1}{\sqrt{2}} \sin \beta & \frac{1}{2}(1 - \cos \beta) \\ \frac{1}{\sqrt{2}} \sin \beta & \cos \beta & -\frac{1}{\sqrt{2}} \sin \beta \\ \frac{1}{2}(1 - \cos \beta) & \frac{1}{\sqrt{2}} \sin \beta & \frac{1}{2}(1 + \cos \beta) \end{pmatrix}, \quad (1.460)$$

where the indices have the order $+1/2, -1/2$. The vector representation goes over into the ordinary rotation matrices $R_{ij}(\beta)$ by mapping the states $|1m\rangle$ onto the spherical unit vectors $\epsilon(0) = \hat{\mathbf{z}}$, $\epsilon(\pm 1) = \mp(\hat{\mathbf{x}} \pm i\hat{\mathbf{y}})/2$ using the matrix elements $\langle i|1m\rangle = \epsilon^i(m)$. Hence $R(\beta)\epsilon(m) = \sum_{m'=-1}^1 \epsilon(m') d_{m'm}^1(\beta)$.

The representation functions $D^1(\alpha, \beta, \gamma)$ can also be obtained by inserting into the general exponential (1.442) the representation matrices of spin 1 for the generators $\hat{L}_i$ with the commutation rules (1.423). In Cartesian coordinates, these are simply $(\hat{L}_i)_{jk} = -i\epsilon_{ijk}$, where ϵ_{ijk} is the completely antisymmetric tensor with $\epsilon_{123} = 1$. In the spherical basis, these become $(\hat{L}_i)_{mm'} = \langle m|i\rangle(\hat{L}_i)_{ij}\langle j|m'\rangle = \epsilon_i^*(m)(\hat{L}_i)_{ij}\epsilon_j(m')$. The exponential $(e^{-i\beta\hat{L}_2})_{mm'}$ is equal to (1.460).

The functions $P_l^{(\alpha, \beta)}(z)$ are the Jacobi polynomials [11], which can be expressed in terms of hypergeometric functions as

$$P_l^{(\alpha, \beta)} \equiv \frac{(-1)^l}{l!} \frac{\Gamma(l + \beta + 1)}{\Gamma(\beta + 1)} F(-l, l + 1 + \alpha + \beta; 1 + \beta; (1 + z)/2), \quad (1.461)$$

where

$$F(a, b; c; z) \equiv 1 + \frac{ab}{c}z + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \dots \quad (1.462)$$

The rotation functions $d_{mm'}^L(\beta)$ satisfy the differential equation

$$\left(-\frac{d^2}{d\beta^2} - \cot \beta \frac{d}{d\beta} + \frac{m^2 + m'^2 - 2mm' \cos \beta}{\sin^2 \beta} \right) d_{mm'}^L(\beta) = L(L+1) d_{mm'}^L(\beta). \quad (1.463)$$

The scalar products of two wave functions have to be calculated with a measure of integration that is invariant under rotations:

$$\langle \psi_2 | \psi_1 \rangle \equiv \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} d\alpha d\beta \sin \beta d\gamma \psi_2^*(\alpha, \beta, \gamma) \psi_1(\alpha, \beta, \gamma). \quad (1.464)$$

The above eigenstates (1.454) satisfy the orthogonality relation

$$\begin{aligned} \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} d\alpha d\beta \sin \beta d\gamma D_{m'_1 m_1}^{L_1*}(\alpha, \beta, \gamma) D_{m'_2 m_2}^{L_2}(\alpha, \beta, \gamma) \\ = \delta_{m'_1 m'_2} \delta_{m_1 m_2} \delta_{L_1 L_2} \frac{8\pi^2}{2L_1 + 1}. \end{aligned} \quad (1.465)$$

Let us also contrast in this example the correct quantization via the commutation rules between group generators with the canonical approach. That would start out with the classical Lagrangian (1.416), or its non-symmetric version corresponding to the Hamiltonian (1.436). The non-symmetric Lagrangian would be the following function of the angular velocities $\omega_\xi, \omega_\eta, \omega_\zeta$, measured along the principal axes of the spinning top,

$$L = \frac{1}{2}[I_\xi(\omega_\xi^2 + \omega_\eta^2) + I_\zeta\omega_\zeta^2]. \quad (1.466)$$

To express $\omega_\xi, \omega_\eta, \omega_\zeta$ in terms of Euler angles of the top α, β, γ , we note that the components of angular momentum in the rest frame $\omega_1, \omega_2, \omega_3$ are obtained from the relation

$$\omega_k L_k = i\dot{R}R^{-1} \quad (1.467)$$

as

$$\begin{aligned} \omega_1 &= -\dot{\beta} \sin \alpha + \dot{\gamma} \sin \beta \cos \alpha, \\ \omega_2 &= \dot{\beta} \cos \alpha + \dot{\gamma} \sin \beta \sin \alpha, \\ \omega_3 &= \dot{\gamma} \cos \beta + \dot{\alpha}. \end{aligned} \quad (1.468)$$

After the rotation (1.448) into the body-fixed system, these become

$$\begin{aligned} \omega_\xi &= \dot{\beta} \sin \gamma - \dot{\alpha} \sin \beta \cos \gamma, \\ \omega_\eta &= \dot{\beta} \cos \gamma + \dot{\alpha} \sin \beta \sin \gamma, \\ \omega_\zeta &= \dot{\alpha} \cos \beta + \dot{\gamma}. \end{aligned} \quad (1.469)$$

Explicitly, the Lagrangian is

$$L = \frac{1}{2}[I_\xi(\dot{\beta}^2 + \dot{\alpha}^2 \sin^2 \beta) + I_\zeta(\dot{\alpha} \cos \beta + \dot{\gamma})^2]. \quad (1.470)$$

Considering α, β, γ as Lagrange coordinates q^μ with $\mu = 1, 2, 3$, this can be written in the form (1.396) with the Hessian metric [recall (1.12) and (1.397)]:

$$g_{\mu\nu} = \begin{pmatrix} I_\xi \sin^2 \beta + I_\zeta \cos^2 \beta & 0 & I_\zeta \cos \beta \\ 0 & I_\xi & 0 \\ I_\zeta \cos \beta & 0 & I_\zeta \end{pmatrix}, \quad (1.471)$$

whose determinant is

$$g = I_\xi^2 I_\zeta \sin^2 \beta. \quad (1.472)$$

Hence the measure $\int d^3q \sqrt{g}$ in the scalar product (1.393) agrees, up to a trivial constant factor, with the rotation-invariant measure (1.464). Incidentally, this is also true for the asymmetric top with $I_\xi \neq I_\eta \neq I_\zeta$, where $g = I_\xi^2 I_\zeta \sin^2 \beta$, although the metric $g_{\mu\nu}$ is then much more complicated (see Appendix 1C).

The canonical momenta associated with the Lagrangian (1.466) are, according to (1.396),

$$\begin{aligned} p_\alpha &= \partial L / \partial \dot{\alpha} = I_\xi \dot{\alpha} \sin^2 \beta + I_\zeta \cos \beta (\dot{\alpha} \cos \beta + \dot{\gamma}), \\ p_\beta &= \partial L / \partial \dot{\beta} = I_\xi \dot{\beta}, \\ p_\gamma &= \partial L / \partial \dot{\gamma} = I_\zeta (\dot{\alpha} \cos \beta + \dot{\gamma}). \end{aligned} \quad (1.473)$$

After inverting the metric to

$$g^{\mu\nu} = \frac{1}{I_\xi \sin^2 \beta} \begin{pmatrix} 1 & 0 & -\cos \beta \\ 0 & \sin^2 \beta & 0 \\ -\cos \beta & 0 & \cos^2 \beta + I_\xi \sin^2 \beta / I_\zeta \end{pmatrix}^{\mu\nu}, \quad (1.474)$$

we find the classical Hamiltonian

$$H = \frac{1}{2} \left[\frac{1}{I_\xi} p_\beta^2 + \left(\frac{\cos^2 \beta}{I_\xi \sin^2 \beta} + \frac{1}{I_\zeta} \right) p_\gamma^2 + \frac{1}{I_\xi \sin^2 \beta} p_\alpha^2 - \frac{2 \cos \beta}{I_\xi \sin^2 \beta} p_\alpha p_\gamma \right]. \quad (1.475)$$

This Hamiltonian has no apparent ordering problem. One is therefore tempted to replace the momenta simply by the corresponding Hermitian operators which are, according to (1.400),

$$\begin{aligned} \hat{p}_\alpha &= -i\hbar \partial_\alpha, \\ \hat{p}_\beta &= -i\hbar (\sin \beta)^{-1/2} \partial_\beta (\sin \beta)^{1/2} = -i\hbar (\partial_\beta + \frac{1}{2} \cot \beta), \\ \hat{p}_\gamma &= -i\hbar \partial_\gamma. \end{aligned} \quad (1.476)$$

Inserting these into (1.475) gives the canonical Hamiltonian operator

$$\hat{H}_{\text{can}} = \hat{H} + \hat{H}_{\text{discr}}, \quad (1.477)$$

with

$$\begin{aligned} \hat{H} \equiv & -\frac{\hbar^2}{2I_\xi} \left[\partial_\beta^2 + \cot \beta \partial_\beta + \left(\frac{I_\xi}{I_\zeta} + \cot^2 \beta \right) \partial_\gamma^2 \right. \\ & \left. + \frac{1}{\sin^2 \beta} \partial_\alpha^2 - \frac{2 \cos \beta}{\sin^2 \beta} \partial_\alpha \partial_\gamma \right] \end{aligned} \quad (1.478)$$

and

$$\hat{H}_{\text{discr}} \equiv \frac{1}{2} (\partial_\beta \cot \beta) + \frac{1}{4} \cot^2 \beta = \frac{1}{4 \sin^2 \beta} - \frac{3}{4}. \quad (1.479)$$

The first term $\hat{H}$ agrees with the correct quantum-mechanical operator derived above. Indeed, inserting the differential operators for the body-fixed angular momenta (1.449) into the Hamiltonian (1.436), we find $\hat{H}$. The term $\hat{H}_{\text{discr}}$ is the discrepancy between the canonical and the correct Hamiltonian operator. It exists even though there is no apparent ordering problem, just as in the radial coordinate

expression (1.413). The correct Hamiltonian could be obtained by replacing the classical p_β^2 term in H by the operator $g^{-1/4}\hat{p}_\beta g^{1/2}\hat{p}_\beta g^{-1/4}$, as in the treatment of the radial coordinates in $\hat{H}$ of Eq. (1.407).

We also observe another similarity with the treatment of two-dimensional systems in radial coordinates. While canonical quantization fails, the Hamiltonian operator of the symmetric spinning top is correctly given by the Laplace-Beltrami operator (1.390), after inserting the metric (1.471) and the inverse (1.474). It is straightforward, although tedious, to verify that this is also true for the completely asymmetric top [which has quite a complicated dynamical metric given in Appendix 1C, see Eqs. (1C.2) and (1C.4)]. This is an important nontrivial result since, for a spinning top, the Lagrangian cannot be obtained by reparametrizing a particle in a euclidean space with curvilinear coordinates. The result suggests that a replacement

$$g_{\mu\nu}(q)p^\mu p^\nu \rightarrow -\hbar^2 \Delta \quad (1.480)$$

produces the correct Hamiltonian operator in any non-euclidean space.

What is the characteristic non-euclidean property of the α, β, γ space? It is the curvature scalar R . For the asymmetric spinning top we find (see Appendix 1C)

$$R = \frac{(I_\xi + I_\eta + I_\zeta)^2 - 2(I_\xi^2 + I_\eta^2 + I_\zeta^2)}{2I_\xi I_\eta I_\zeta}. \quad (1.481)$$

Thus, just like a particle on the surface of a sphere, the spinning top corresponds to a particle moving in a space with constant curvature. In this space, the correct correspondence principle can also be deduced from symmetry arguments. The geometry is most easily understood by observing that the α, β, γ space may be considered as the surface of a sphere in four dimensions, as was shown in detail in Chapter 8 of Ref. [1].

An important non-euclidean space of physical interest is encountered in the context of general relativity. Originally, gravitating matter was assumed to move in a spacetime with an arbitrary local curvature. In newer developments of the theory one also allows for the presence of a nonvanishing torsion. In such a general situation, where the group quantization rule is inapplicable, the correspondence principle has always been a matter of controversy [see the references after (1.414)]. It was solved in Ref. [1], where a natural and unique passage from classical to quantum mechanics in any coordinate frame was given.¹⁹ The configuration space may carry curvature and a certain class of torsions (gradient torsion). Several arguments suggest that our principle is correct. For the above systems with a Hamiltonian which can be expressed entirely in terms of generators of a group of motion in the underlying space, the new quantum equivalence principle will give the same results as the group quantization rule.

¹⁹H. Kleinert, Mod. Phys. Lett. A *4*, 2329 (1989) (<http://klnrt.de/199>); Phys. Lett. B *236*, 315 (1990) (<http://klnrt.de/202>).

1.16 Classical and Quantum Statistics

Consider a physical system with a constant number of particles N whose Hamiltonian has no explicit time dependence. If it is brought into contact with a thermal reservoir at a temperature T then, after having reached equilibrium, its thermodynamic properties can be obtained through the following rules: At the level of classical mechanics, each volume element in phase space

$$\frac{dp dq}{h} = \frac{dp dq}{2\pi\hbar} \quad (1.482)$$

is occupied with a probability proportional to the *Boltzmann factor*

$$e^{-H(p,q)/k_B T}, \quad (1.483)$$

where k_B is the *Boltzmann constant*,

$$k_B = 1.3806221(59) \times 10^{-16} \text{ erg/Kelvin}. \quad (1.484)$$

The number in parentheses indicates the experimental uncertainty of the two digits in front of it. The quantity $1/k_B T$ has the dimension of an inverse energy and is commonly denoted by β . It will be called the *inverse temperature*, forgetting about the factor k_B . In fact, we shall sometimes take T to be measured in energy units k_B times Kelvin rather than in Kelvin. Then we may drop k_B in all formulas.

The integral over the Boltzmann factors of all phase space elements,²⁰

$$Z_{\text{cl}}(T) \equiv \int \frac{dp dq}{2\pi\hbar} e^{-H(p,q)/k_B T}, \quad (1.485)$$

is called the *classical partition function*. It contains all classical thermodynamic information of the system. Of course, for a general Hamiltonian system with many degrees of freedom, the phase space integral is $\prod_n \int dp_n dq_n / 2\pi\hbar$. The normalized Boltzmann factor

$$w(p, q) = Z_{\text{cl}}^{-1}(T) e^{-H(p,q)/k_B T} \quad (1.486)$$

is called the *classical Gibbs distribution function*. The reader may wonder why an expression containing Planck's quantum $\hbar$ is called *classical*. The reason is that $\hbar$ can really be omitted in calculating any thermodynamic average. In classical statistics it merely supplies us with an irrelevant normalization factor which makes Z dimensionless.

1.16.1 Canonical Ensemble

In quantum statistics, the Hamiltonian is replaced by the operator $\hat{H}$ and the integral over phase space by the trace in Hilbert space. This leads to the *quantum-statistical partition function*

$$Z(T) \equiv \text{Tr} \left(e^{-\hat{H}/k_B T} \right) \equiv \text{Tr} \left(e^{-H(\hat{p}, \hat{x})/k_B T} \right), \quad (1.487)$$

²⁰In the sequel we shall always work at a fixed volume V and therefore suppress the argument V everywhere.

where $\text{Tr} \hat{O}$ denotes the trace of the operator $\hat{O}$. If $|n\rangle$ are eigenstates of the Hamiltonian with energy E_n , the partition function becomes a sum

$$Z(T) = \sum_n e^{-E_n/k_B T}. \quad (1.488)$$

The normalized Boltzmann factor

$$w_n = Z_{\text{cl}}^{-1}(T) e^{-E_n/k_B T} \quad (1.489)$$

defines the *quantum-statistical Gibbs distribution*.

If $\hat{H}$ is an N -particle Schrödinger Hamiltonian, the quantum-statistical system is referred to as a *canonical ensemble*.

The right-hand side of (1.487) contains the position operator $\hat{x}$ in Cartesian coordinates rather than $\hat{q}$ to ensure that the system can be quantized canonically. In cases such as the spinning top, the trace formula is also valid but the Hilbert space is spanned by the representation states of the angular momentum operators. In more general Lagrangian systems, the quantization has to be performed differently in the way described in Chapters 8 and 10 of the textbook [1].

At this point we make an important observation: The quantum partition function is related in a very simple way to the quantum-mechanical time evolution operator. To emphasize this relation we shall define the trace of this operator for time-independent Hamiltonians as the *quantum-mechanical partition function*:

$$Z_{\text{QM}}(t_b - t_a) \equiv \text{Tr} \left(\hat{U}(t_b, t_a) \right) = \text{Tr} \left(e^{-i(t_b - t_a)\hat{H}/\hbar} \right). \quad (1.490)$$

This may be considered as the partition function associated with a “quantum-mechanical Gibbs distribution”

$$w_n = Z_{\text{QM}}^{-1}(t_b - t_a) e^{iE_n(t_b - t_a)/\hbar}. \quad (1.491)$$

Obviously the quantum-statistical partition function $Z(T)$ may be obtained from the quantum-mechanical one by continuing the time interval $t_b - t_a$ to the negative imaginary value

$$t_b - t_a = -\frac{i\hbar}{k_B T} \equiv -i\hbar\beta. \quad (1.492)$$

This simple formal relation shows that the trace of the time evolution operator contains all information on the thermodynamic equilibrium properties of a quantum system.

1.16.2 Grand-Canonical Ensemble

For systems containing many bodies it is often convenient to study their equilibrium properties in contact with a particle reservoir characterized by a chemical potential μ . For this one defines what is called the *grand-canonical quantum-statistical partition function*

$$Z_G(T, \mu) = \text{Tr} \left(e^{-(\hat{H} - \mu\hat{N})/k_B T} \right). \quad (1.493)$$

Here $\hat{N}$ is the operator counting the number of particles in each state of the ensemble. The combination of operators in the exponent,

$$\hat{H}_G = \hat{H} - \mu\hat{N}, \quad (1.494)$$

is called the *grand-canonical Hamiltonian*.

Given a partition function $Z(T)$ at a fixed particle number N , the *free energy* is defined by

$$F(T) = -k_B T \log Z(T). \quad (1.495)$$

Its grand-canonical version at a fixed chemical potential is²¹

$$F_G(T, \mu) = -k_B T \log Z_G(T, \mu). \quad (1.496)$$

The *average energy* or *internal energy* is defined by

$$E = \text{Tr} \left(\hat{H} e^{-\hat{H}/k_B T} \right) / \text{Tr} \left(e^{-\hat{H}/k_B T} \right). \quad (1.497)$$

It may be obtained from the partition function $Z(T)$ by forming the temperature derivative

$$E = Z^{-1} k_B T^2 \frac{\partial}{\partial T} Z(T) = k_B T^2 \frac{\partial}{\partial T} \log Z(T). \quad (1.498)$$

In terms of the free energy (1.495), this becomes

$$E = T^2 \frac{\partial}{\partial T} (-F(T)/T) = \left(1 - T \frac{\partial}{\partial T} \right) F(T). \quad (1.499)$$

For a grand-canonical ensemble we may introduce an *average particle number* defined by

$$N = \text{Tr} \left(\hat{N} e^{-(\hat{H} - \mu\hat{N})/k_B T} \right) / \text{Tr} \left(e^{-(\hat{H} - \mu\hat{N})/k_B T} \right). \quad (1.500)$$

This can be derived from the grand-canonical partition function as

$$N = Z_G^{-1}(T, \mu) k_B T \frac{\partial}{\partial \mu} Z_G(T, \mu) = k_B T \frac{\partial}{\partial \mu} \log Z_G(T, \mu), \quad (1.501)$$

or, using the grand-canonical free energy, as

$$N = -\frac{\partial}{\partial \mu} F_G(T, \mu). \quad (1.502)$$

The average energy in a grand-canonical system,

$$E = \text{Tr} \left(\hat{H} e^{-(\hat{H} - \mu\hat{N})/k_B T} \right) / \text{Tr} \left(e^{-(\hat{H} - \mu\hat{N})/k_B T} \right), \quad (1.503)$$

²¹The grand-canonical free energy $F_G(T, \mu)$ is also known as the thermodynamic Gibbs potential, denoted by $\Omega(T, \mu)$. In Eq. (1.527) we shall see that it is also equal to $-pV$, where p is the pressure.

can be obtained by forming, similar to (1.498) and (1.499), the derivative

$$\begin{aligned} E - \mu N &= Z_G^{-1}(T, \mu) k_B T^2 \frac{\partial}{\partial T} Z_G(T, \mu) \\ &= \left(1 - T \frac{\partial}{\partial T} \right) F_G(T, \mu). \end{aligned} \quad (1.504)$$

For a large number of particles, the density is a rapidly growing function of energy. For a system of N free particles, for example, the number of states up to the energy E is given by

$$N(E) = \sum_{\mathbf{p}_i} \Theta(E - \sum_{i=1}^N \mathbf{p}_i^2 / 2M). \quad (1.505)$$

Here each of the particle momenta $\mathbf{p}_i$ is summed over all discrete momenta $\mathbf{p}^{\mathbf{m}}$ in (1.184) available to a single particle in a finite box of volume $V = L^3$. For a large V , the sum can be converted into an integral²²

$$N(E) = V^N \prod_{i=1}^N \left[\int \frac{d^3 p_i}{(2\pi\hbar)^3} \right] \Theta(E - \sum_{i=1}^N \mathbf{p}_i^2 / 2M), \quad (1.506)$$

which is simply $[V/(2\pi\hbar)^3]^N$ times the volume Ω_{3N} of a $3N$ -dimensional sphere of radius $\sqrt{2ME}$:

$$\begin{aligned} N(E) &= \left[\frac{V}{(2\pi\hbar)^3} \right]^N \Omega_{3N} \\ &\equiv \left[\frac{V}{(2\pi\hbar)^3} \right]^N \frac{(2\pi ME)^{3N/2}}{\Gamma(\frac{3}{2}N + 1)}. \end{aligned} \quad (1.507)$$

Recall the well-known formula for the volume of a unit sphere in D dimensions:

$$\Omega_D = \pi^{D/2} / \Gamma(D/2 + 1). \quad (1.508)$$

The surface is [see Subsection 8.5.2 in [1] for a derivation]

$$S_D = 2\pi^{D/2} / \Gamma(D/2). \quad (1.509)$$

This follows directly from the integral²³

$$S_D = \int d^D p \delta(p^2 - 1) = \int d^D p 2\delta(p^2 - 1) = \int d^D p \int_{-\infty}^{\infty} \frac{d\lambda}{\pi} e^{i\lambda(p^2 - 1)} \quad (1.510)$$

$$= \int_{-\infty}^{\infty} \frac{d\lambda}{\pi} \left(\frac{\pi}{-i\lambda} \right)^{D/2} e^{-i\lambda} = \frac{2\pi^{D/2}}{\Gamma(D/2)}. \quad (1.511)$$

²²Remember, however, the exception noted in the footnote to Eq. (1.189) for systems possessing a condensate.

²³I. S. Gradshteyn and I. M. Ryzhik, op. cit., Formula 3.382.7.

Therefore, the density per energy $\rho = \partial N / \partial E$ is given by

$$\rho(E) = \left[\frac{V}{(2\pi\hbar)^3} \right]^N 2\pi M \frac{(2\pi M E)^{3N/2-1}}{\Gamma(\frac{3}{2}N)}. \quad (1.512)$$

It grows with the very large power of the energy $E^{3N/2}$. Nevertheless, the integral for the partition function (1.533) is convergent, due to the overwhelming exponential falloff of the Boltzmann factor $e^{-E/k_B T}$. As the two functions $\rho(E)$ and $e^{-E/k_B T}$ are multiplied with each other, the product is a function that peaks very sharply at the average energy E of the system. The position of the peak depends on the temperature T . For the free N -particle system, for example, the product behaves like

$$\rho(E)e^{-E/k_B T} \sim e^{(3N/2-1)\log E - E/k_B T}, \quad (1.513)$$

and has a sharp peak at

$$E(T) = k_B T \left(\frac{3N}{2} - 1 \right) \approx k_B T \frac{3N}{2}. \quad (1.514)$$

The width of the peak is found by expanding the exponent of (1.513) around (1.514) in powers of $\delta E = E - E(T)$:

$$\exp \left\{ \frac{3N}{2} \log E(T) - \frac{E(T)}{k_B T} - \frac{1}{2E^2(T)} \frac{3N}{2} (\delta E)^2 + \dots \right\}. \quad (1.515)$$

Thus, as soon as E deviates from $E(T)$ by the tiny amount $E(T)/\sqrt{N}$, the exponential is reduced by a factor of two with respect to the peak $E(T) \approx k_B T 3N/2$. For large N , the width is extremely sharp, and the product (1.513) can be approximated by a δ -function, writing

$$\rho(E)e^{-E/k_B T} \approx \delta(E - E(T)) N(T) e^{-E(T)/k_B T}. \quad (1.516)$$

The quantity $N(T)$ measures the total number of states over which the system is distributed at the temperature T .

The entropy $S(T)$ is now defined in terms of $N(T)$ by setting

$$N(T) \equiv e^{S(T)/k_B}. \quad (1.517)$$

Inserting this with (1.516) into (1.533), we see that in the limit of a large number N of particles:

$$Z(T) = e^{-[E(T) - TS(T)]/k_B T}. \quad (1.518)$$

Using (1.495), the free energy can thus be expressed in the form

$$F(T) = E(T) - TS(T). \quad (1.519)$$

Comparison with (1.499) shows that the entropy may be calculated directly as the negative temperature derivative of the free energy:

$$S(T) = -\frac{\partial}{\partial T} F(T). \quad (1.520)$$

For grand-canonical ensembles, we may similarly consider

$$Z_G(T, \mu) = \int dE dn \rho(E, n) e^{-(E-\mu n)/k_B T}, \quad (1.521)$$

where

$$\rho(E, n) e^{-(E-\mu n)/k_B T} \quad (1.522)$$

is now strongly peaked at $E = E(T, \mu)$, $n = N(T, \mu)$ and can be written approximately as

$$\rho(E, n) e^{-(E-\mu n)/k_B T} \approx \delta(E - E(T, \mu)) \delta(n - N(T, \mu)) e^{S(T, \mu)/k_B} e^{-[E(T, \mu) - \mu N(T, \mu)]/k_B T}. \quad (1.523)$$

Inserting this back into (1.521) we find for large N

$$Z_G(T, \mu) = e^{-[E(T, \mu) - \mu N(T, \mu) - TS(T, \mu)]/k_B T}. \quad (1.524)$$

For the grand-canonical free energy (1.496), this implies the relation

$$F_G(T, \mu) = E(T, \mu) - \mu N(T, \mu) - TS(T, \mu). \quad (1.525)$$

By comparison with (1.504) we see that the entropy can be calculated directly from the derivative of the grand-canonical free energy

$$S(T, \mu) = -\frac{\partial}{\partial T} F_G(T, \mu). \quad (1.526)$$

The particle number is, of course, found from the derivative (1.502) with respect to the chemical potential, as follows directly from the definition (1.521).

The canonical free energy and the entropy appearing in the above equations depend on the particle number N and the volume V of the system, i.e., they are more explicitly written as $F(T, N, V)$ and $S(T, N, V)$, respectively.

In the arguments of the grand-canonical quantities, the particle number N is replaced by the chemical potential μ .

Among the arguments of the grand-canonical free energy $F_G(T, \mu, V)$, the volume V is the only one which grows with the system. Thus $F_G(T, \mu, V)$ must be directly proportional to V . The proportionality constant defines the *pressure* p of the system:

$$F_G(T, \mu, V) \equiv -p(T, \mu, V)V. \quad (1.527)$$

Under infinitesimal changes of the three variables, $F_G(T, \mu, V)$ changes as follows:

$$dF_G(T, \mu, V) = -SdT + \mu dN - pdV. \quad (1.528)$$

The first two terms on the right-hand side follow from varying Eq. (1.525) at a fixed volume. When varying the volume, the definition (1.527) renders the last term.

Inserting (1.527) into (1.525), we find *Euler's relation*:

$$E = TS + \mu N - pV. \quad (1.529)$$

The energy has S, N, V as natural variables. Equivalently, we may write

$$F = -\mu N - pV, \quad (1.530)$$

where T, N, V are the natural variables.

1.17 Density of States and Tracelog

In many thermodynamic calculations, a quantity of fundamental interest is the density of states. To define it, we express the canonical partition function

$$Z(T) = \text{Tr} \left(e^{-\hat{H}/k_B T} \right) \quad (1.531)$$

as a sum over the Boltzmann factors of all eigenstates $|n\rangle$ of the Hamiltonian:

$$Z(T) = \sum_n e^{-E_n/k_B T}. \quad (1.532)$$

This can be rewritten as an integral:

$$Z(T) = \int dE \rho(E) e^{-E/k_B T}. \quad (1.533)$$

The quantity

$$\rho(E) = \sum_n \delta(E - E_n) \quad (1.534)$$

specifies the *density of states* of the system in the energy interval $(E, E + dE)$. It may also be written formally as a trace $\text{Tr} \hat{\rho}(E)$ of an operator for the density of states:

$$\hat{\rho}(E) \equiv \delta(E - \hat{H}). \quad (1.535)$$

The density of states is obviously the Fourier transform of the canonical partition function (1.531):

$$\rho(E) = \int_{-i\infty}^{\infty} \frac{d\beta}{2\pi i} e^{\beta E} \text{Tr} \left(e^{-\beta \hat{H}} \right) = \int_{-i\infty}^{\infty} \frac{d\beta}{2\pi i} e^{\beta E} Z(1/k_B \beta). \quad (1.536)$$

The integral

$$N(E) = \int^E dE' \rho(E') \quad (1.537)$$

is the number of states up to the energy E . The integration may start anywhere below the ground state energy. The function $N(E)$ is a sum of Heaviside step functions (1.320):

$$N(E) = \sum_n \Theta(E - E_n). \quad (1.538)$$

This equation is correct only with the Heaviside function, which is equal to 1/2 at the origin, not with the one-sided version (1.313), as we shall see later. Indeed, if integrated to the energy of a certain level E_n , the result is

$$N(E_n) = (n + 1/2). \quad (1.539)$$

This formula may be used to determine the energies of bound states from approximations to $\omega(E)$, the classical approximation leading to the well-known Bohr-Sommerfeld condition. In order to apply this relation one must be sure that all

levels have different energies. Otherwise $N(E)$ jumps at E_n by half the degeneracy of this level.

An important quantity related to $\rho(E)$ is frequently used in this text: the trace of the logarithm, short *tracelog*, of the operator $\hat{H} - E$.

$$\text{Tr log}(\hat{H} - E) = \sum_n \log(E_n - E). \quad (1.540)$$

It may be expressed in terms of the density of states (1.535) as

$$\text{Tr log}(\hat{H} - E) = \text{Tr} \int_{-\infty}^{\infty} dE' \delta(E' - \hat{H}) \log(E' - E) = \int_{-\infty}^{\infty} dE' \rho(E') \log(E' - E). \quad (1.541)$$

The tracelog of the Hamiltonian operator itself can be viewed as a limit of an *operator zeta function* associated with $\hat{H}$:

$$\hat{\zeta}_{\hat{H}}(\nu) = \text{Tr} \hat{H}^{-\nu}, \quad (1.542)$$

whose trace is the generalized zeta function

$$\zeta_{\hat{H}}(\nu) \equiv \text{Tr} [\hat{\zeta}_{\hat{H}}(\nu)] = \text{Tr}(\hat{H}^{-\nu}) = \sum_n E_n^{-\nu}. \quad (1.543)$$

For a linearly spaced spectrum $E_n = n$ with $n = 1, 2, 3, \dots$, this reduces to Riemann's zeta function (2.277).

From the generalized zeta function we can obtain the tracelog by forming the derivative

$$\text{Tr log} \hat{H} = -\partial_{\nu} \zeta_{\hat{H}}(\nu)|_{\nu=0}. \quad (1.544)$$

By differentiating (1.540) with respect to E , we find the trace of the resolvent (11.8):

$$\partial_E \text{Tr log}(\hat{H} - E) = \text{Tr} \frac{1}{E - \hat{H}} = \sum_n \frac{1}{E - E_n} = \frac{1}{i\hbar} \sum_n R_n(E) = \frac{1}{i\hbar} \text{Tr} \hat{R}(E). \quad (1.545)$$

Recalling Eq. (1.338) we see that the imaginary part of this quantity slightly above the real E -axis yields the density of states

$$-\frac{1}{\pi} \text{Im} \partial_E \text{Tr log}(\hat{H} - E - i\eta) = \sum_n \delta(E - E_n) = \rho(E). \quad (1.546)$$

An integrating over the energy yields the function $N(E)$ of Eq. (1.537):

$$-\frac{1}{\pi} \text{Im} \text{Tr log}(E - \hat{H}) = \sum_n \Theta(E - E_n) = N(E). \quad (1.547)$$

Appendix 1A Simple Time Evolution Operator

Consider the simplest nontrivial time evolution operator of a spin-1/2 particle in a magnetic field $\mathbf{B}$. The reduced Hamiltonian operator is $\hat{H}_0 = -\mathbf{B} \cdot \boldsymbol{\sigma}/2$, so that the time evolution operator reads, in natural units with $\hbar = 1$,

$$e^{-i\hat{H}_0(t_b-t_a)} = e^{i(t_b-t_a)\mathbf{B} \cdot \boldsymbol{\sigma}/2}. \quad (1A.1)$$

Expanding this as in (1.301) and using the fact that $(\mathbf{B} \cdot \boldsymbol{\sigma})^{2n} = B^{2n}$ and $(\mathbf{B} \cdot \boldsymbol{\sigma})^{2n+1} = B^{2n}(\mathbf{B} \cdot \boldsymbol{\sigma})$, we obtain

$$e^{-i\hat{H}_0(t_b-t_a)} = \cos B(t_b-t_a)/2 + i\hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \sin B(t_b-t_a)/2, \quad (1A.2)$$

where $\hat{\mathbf{B}} \equiv \mathbf{B}/|\mathbf{B}|$. Suppose now that the magnetic field is not constant but has a small time-dependent variation $\delta\mathbf{B}(t)$. Then we obtain from (1.261) [or from the lowest expansion term in (1.301)]

$$\delta e^{-i\hat{H}_0(t_b-t_a)} = \int_{t_a}^{t_b} dt e^{-i\hat{H}_0(t_b-t)} \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} e^{-i\hat{H}_0(t-t_a)}. \quad (1A.3)$$

Using (1A.2), the integrand on the right-hand side becomes

$$\left[\cos B(t_b-t)/2 + i\hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \sin B(t_b-t)/2 \right] \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} \left[\cos B(t-t_a)/2 + i\hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \sin B(t-t_a)/2 \right]. \quad (1A.4)$$

We simplify this with the help of the formula [recall (23.56)]

$$\sigma^i \sigma^j = \delta_{ij} + i\epsilon_{ijk} \sigma^k, \quad (1A.5)$$

so that

$$\hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} = \hat{\mathbf{B}} \cdot \delta\mathbf{B}(t) + i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \boldsymbol{\sigma}, \quad \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} \hat{\mathbf{B}} \cdot \boldsymbol{\sigma} = \hat{\mathbf{B}} \cdot \delta\mathbf{B}(t) - i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \boldsymbol{\sigma}, \quad (1A.6)$$

and

$$\begin{aligned} \hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} \hat{\mathbf{B}} \cdot \boldsymbol{\sigma} &= [\hat{\mathbf{B}} \cdot \delta\mathbf{B}(t)] \hat{\mathbf{B}} \cdot \boldsymbol{\sigma} + i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \boldsymbol{\sigma} \hat{\mathbf{B}} \cdot \boldsymbol{\sigma} \\ &= i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \hat{\mathbf{B}} + \left\{ [\hat{\mathbf{B}} \cdot \delta\mathbf{B}(t)] \hat{\mathbf{B}} - [\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \times \hat{\mathbf{B}} \right\} \cdot \boldsymbol{\sigma}. \end{aligned} \quad (1A.7)$$

The first term on the right-hand side vanishes, the second term is equal to $\delta\mathbf{B}$, since $\hat{\mathbf{B}}^2 = 1$. Thus we find for the integrand in (1A.4):

$$\begin{aligned} &\cos B(t_b-t)/2 \cos B(t-t_a)/2 \delta\mathbf{B}(t) \cdot \boldsymbol{\sigma} + i \sin B(t_b-t)/2 \cos B(t-t_a)/2 \{ \hat{\mathbf{B}} \cdot \delta\mathbf{B}(t) + i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \boldsymbol{\sigma} \} \\ &+ i \cos B(t_b-t)/2 \sin B(t-t_a)/2 \{ \hat{\mathbf{B}} \cdot \delta\mathbf{B}(t) - i[\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \cdot \boldsymbol{\sigma} \} + \sin B(t_b-t)/2 \sin B(t-t_a)/2 \delta\mathbf{B} \cdot \boldsymbol{\sigma} \end{aligned}$$

which can be combined to give

$$\left\{ \cos B[(t_b+t_a)/2-t] \delta\mathbf{B}(t) - \sin B[(t_b+t_a)/2-t] [\hat{\mathbf{B}} \times \delta\mathbf{B}(t)] \right\} \cdot \boldsymbol{\sigma} + i \sin B(t_b-t_a)/2 \hat{\mathbf{B}} \cdot \delta\mathbf{B}(t). \quad (1A.8)$$

Integrating this from t_a to t_b we obtain the variation (1A.3).

Appendix 1B Convergence of the Fresnel Integral

Here we prove the convergence of the Fresnel integral (1.346) by relating it to the Gauss integral. According to Cauchy's integral theorem, the sum of the three pieces of integrals that run along the closed contour in Fig. 1.4 vanishes, since the integrand e^{-z^2} is analytic in the triangular domain:

$$\oint dz e^{-z^2} = \int_0^A dz e^{-z^2} + \int_A^B dz e^{-z^2} + \int_B^O dz e^{-z^2} = 0. \quad (1B.1)$$

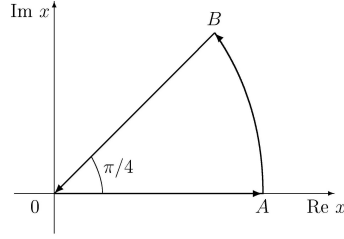


FIGURE 1.4 Triangular closed contour for a Cauchy integral (1B.1).

Let R be the radius of the arc. Then we substitute in the three integrals the variable z as follows:

$$\begin{aligned} 0A: \quad z &= p, & dz &= dp, & z^2 &= p^2, \\ B0: \quad z &= pe^{i\pi/4}, & dz &= dp e^{i\pi/4}, & z^2 &= ip^2, \\ AB: \quad z &= R e^{i\varphi}, & dz &= i R dp, & z^2 &= p^2, \end{aligned}$$

and obtain the equation

$$\int_0^R dp e^{-p^2} + e^{i\pi/4} \int_R^0 dp e^{-ip^2} + \int_0^{\pi/4} d\varphi i R e^{-R^2(\cos 2\varphi + i \sin 2\varphi) + i\varphi} = 0. \quad (1B.2)$$

The first integral converges rapidly to $\sqrt{\pi}/2$ for $R \rightarrow \infty$. The last term goes to zero in this limit. To see this we estimate its absolute value as follows:

$$\left| \int_0^{\pi/4} d\varphi i R e^{-R^2(\cos 2\varphi + i \sin 2\varphi) + i\varphi} \right| < R \int_0^{\pi/4} d\varphi e^{-R^2 \cos 2\varphi}. \quad (1B.3)$$

The right-hand side goes to zero exponentially fast, except for angles φ close to $\pi/4$ where the cosine in the exponent vanishes. In the dangerous regime $\alpha \in (\pi/4 - \epsilon, \pi/4)$ with small $\epsilon > 0$, one certainly has $\sin 2\varphi > \sin 2\alpha$, so that

$$R \int_{\alpha}^{\pi/4} d\varphi e^{-R^2 \cos 2\varphi} < R \int_{\alpha}^{\pi/4} d\varphi \frac{\sin 2\varphi}{\sin 2\alpha} e^{-R^2 \cos 2\varphi}. \quad (1B.4)$$

The right-hand integral can be performed by parts and yields

$$\alpha R e^{-R^2 \cos 2\alpha} + \frac{1}{R \sin 2\alpha} \left[e^{-R^2 \cos 2\varphi} \right]_{\varphi=\alpha}^{\varphi=\pi/4}, \quad (1B.5)$$

which goes to zero like $1/R$ for large R . Thus we find from (1B.2) the limiting formula $\int_{\infty}^0 dp e^{-ip^2} = -e^{-i\pi/4} \sqrt{\pi}/2$, or

$$\int_{\infty}^0 dp e^{-ip^2} = e^{-i\pi/4} \sqrt{\pi}, \quad (1B.6)$$

which goes into Fresnel's integral formula (1.346) by substituting $p \rightarrow p\sqrt{a/2}$.

Appendix 1C The Asymmetric Top

The Lagrangian of the asymmetric top with three different moments of inertia reads

$$L = \frac{1}{2} [I_{\xi} \omega_{\xi}^2 + I_{\eta} \omega_{\eta}^2 + I_{\zeta} \omega_{\zeta}^2]. \quad (1C.1)$$

It has the Hessian metric [recall (1.12) and (1.397)]

$$g_{11} = I_{\xi} \sin^2 \beta + I_{\zeta} \cos^2 \beta - (I_{\xi} - I_{\eta}) \sin^2 \beta \sin^2 \gamma,$$

$$\begin{aligned}
g_{21} &= -(I_\xi - I_\eta) \sin \beta \sin \gamma \cos \gamma, \\
g_{31} &= I_\zeta \cos \beta, \\
g_{22} &= I_\eta + (I_\xi - I_\eta) \sin^2 \gamma, \\
g_{32} &= 0, \\
g_{33} &= I_\zeta,
\end{aligned} \tag{1C.2}$$

rather than (1.471). The determinant is

$$g = I_\xi I_\eta I_\zeta \sin^2 \beta, \tag{1C.3}$$

and the inverse metric has the components

$$\begin{aligned}
g^{11} &= \frac{1}{g} \{I_\eta + (I_\xi - I_\eta) \sin^2 \gamma\} I_\zeta, \\
g^{21} &= \frac{1}{g} \sin \beta \sin \gamma \cos \gamma (I_\xi - I_\eta) I_\zeta, \\
g^{31} &= \frac{1}{g} \{\cos \beta [-\sin^2 \gamma (I_\xi - I_\eta) - I_\eta]\} I_\zeta, \\
g^{22} &= \frac{1}{g} \{\sin^2 \beta [I_\xi - \sin^2 \gamma (I_\xi - I_\eta)]\} I_\zeta, \\
g^{32} &= \frac{1}{g} \{\sin \beta \cos \beta \sin \gamma \cos \gamma (I_\eta - I_\xi)\} I_\zeta, \\
g^{33} &= \frac{1}{g} \{\sin^2 \beta I_\xi I_\eta + \cos^2 \beta I_\eta I_\zeta + \cos^2 \beta \sin^2 \gamma (I_\xi - I_\eta) I_\zeta\}.
\end{aligned} \tag{1C.4}$$

From this we find the components of the Riemann connection, the Christoffel symbol defined in Eq. (1.71):

$$\begin{aligned}
\bar{\Gamma}_{11}^1 &= [\cos \beta \cos \gamma \sin \gamma (I_\eta^2 - I_\eta I_\zeta - I_\xi^2 + I_\xi I_\zeta)] / I_\xi I_\eta, \\
\bar{\Gamma}_{21}^1 &= \{\cos \beta [\sin^2 \gamma (I_\xi^2 - I_\eta^2 - (I_\xi - I_\eta) I_\zeta) \\
&\quad + I_\eta (I_\xi + I_\eta - I_\zeta)]\} / 2 \sin \beta I_\xi I_\eta, \\
\bar{\Gamma}_{31}^1 &= \{\cos \gamma \sin \gamma [I_\eta^2 - I_\xi^2 + (I_\xi - I_\eta) I_\zeta]\} / 2 I_\xi I_\eta, \\
\bar{\Gamma}_{22}^1 &= 0, \\
\bar{\Gamma}_{32}^1 &= [\sin^2 \gamma (I_\xi^2 - I_\eta^2 - (I_\xi - I_\eta) I_\zeta) - I_\eta (I_\xi - I_\eta + I_\zeta)] / 2 \sin \beta I_\xi I_\eta, \\
\bar{\Gamma}_{33}^1 &= 0, \\
\bar{\Gamma}_{11}^2 &= \{\cos \beta \sin \beta [\sin^2 \gamma (I_\xi^2 - I_\eta^2 - I_\zeta (I_\xi - I_\eta)) - I_\xi (I_\xi - I_\zeta)]\} / I_\xi I_\eta, \\
\bar{\Gamma}_{21}^2 &= \{\cos \beta \cos \gamma \sin \gamma [I_\xi^2 - I_\eta^2 - I_\zeta (I_\xi - I_\eta)]\} / 2 I_\xi I_\eta, \\
\bar{\Gamma}_{31}^2 &= \{\sin \beta [\sin^2 \gamma (I_\xi^2 - I_\eta^2 - I_\zeta (I_\xi - I_\eta)) - I_\xi (I_\xi - I_\eta - I_\zeta)]\} / 2 I_\xi I_\eta, \\
\bar{\Gamma}_{22}^2 &= 0, \\
\bar{\Gamma}_{32}^2 &= [\cos \gamma \sin \gamma (I_\xi^2 - I_\eta^2 - I_\zeta (I_\xi - I_\eta))] / 2 I_\xi I_\eta, \\
\bar{\Gamma}_{33}^2 &= 0, \\
\bar{\Gamma}_{11}^3 &= \{\cos \gamma \sin \gamma [\sin^2 \beta (I_\xi I_\eta (I_\xi - I_\eta) - I_\zeta (I_\xi^2 - I_\eta^2) + I_\zeta^2 (I_\xi - I_\eta)) \\
&\quad + (I_\xi^2 - I_\eta^2) I_\zeta - I_\zeta^2 (I_\xi - I_\eta)]\} / I_\xi I_\eta I_\zeta, \\
\bar{\Gamma}_{21}^3 &= \{\sin^2 \beta [\sin^2 \gamma (2 I_\xi I_\eta (I_\eta - I_\xi) + I_\zeta (I_\xi^2 - I_\eta^2) - I_\zeta^2 (I_\xi - I_\eta)) \\
&\quad + I_\xi I_\eta (I_\xi - I_\eta) + I_\eta I_\zeta (I_\eta - I_\zeta)] - \sin^2 \gamma [(I_\xi^2 - I_\eta^2) I_\zeta - I_\zeta^2 (I_\xi - I_\eta)) \\
&\quad - I_\eta I_\zeta (I_\xi + I_\eta - I_\zeta)]\} / 2 \sin \beta I_\xi I_\eta I_\zeta, \\
\bar{\Gamma}_{31}^3 &= [\cos \beta \cos \gamma \sin \gamma (I_\xi^2 - I_\eta^2 - I_\zeta (I_\xi - I_\eta))] / 2 I_\xi I_\eta,
\end{aligned}$$

$$\begin{aligned}
\bar{\Gamma}_{22}^3 &= \cos \gamma \sin \gamma (I_\eta - I_\xi) / I_\zeta, \\
\bar{\Gamma}_{32}^3 &= \{\cos \beta [\sin^2 \gamma (I_\eta^2 - I_\xi^2 + (I_\xi - I_\eta) I_\zeta) + I_\eta (I_\xi - I_\eta + I_\zeta)]\} / 2 \sin \beta I_\eta I_\xi, \\
\bar{\Gamma}_{33}^3 &= 0.
\end{aligned} \tag{1C.5}$$

The other components follow from the symmetry in the first two indices $\bar{\Gamma}_{\mu\nu}^\lambda = \bar{\Gamma}_{\nu\mu}^\lambda$. From this Christoffel symbol we calculate the Ricci tensor (see Eq. (10.8) in [1]):

$$\begin{aligned}
\bar{R}_{11} &= \{\sin^2 \beta [\sin^2 \gamma (I_\eta^3 - I_\xi^3 - (I_\xi I_\eta - I_\zeta^2)(I_\xi - I_\eta)) \\
&\quad + ((I_\xi + I_\zeta)^2 - I_\eta^2)(I_\xi - I_\zeta)] + I_\zeta^3 - I_\zeta (I_\xi - I_\eta)^2\} / 2 I_\xi I_\eta I_\zeta, \\
\bar{R}_{21} &= \{\sin \beta \sin \gamma \cos \gamma [I_\eta^3 - I_\xi^3 + (I_\xi I_\eta - I_\zeta^2)(I_\eta - I_\xi)]\} / 2 I_\xi I_\eta I_\zeta, \\
\bar{R}_{31} &= -\{\cos \beta [(I_\xi - I_\eta)^2 - I_\zeta^2]\} / 2 I_\xi I_\eta, \\
\bar{R}_{22} &= \{\sin^2 \gamma [I_\xi^3 - I_\eta^3 + (I_\xi I_\eta - I_\zeta^2)(I_\xi - I_\eta)] + I_\eta^3 - (I_\xi - I_\zeta)^2 I_\eta\} / 2 I_\xi I_\eta I_\zeta, \\
\bar{R}_{32} &= 0, \\
\bar{R}_{33} &= -[(I_\xi - I_\eta)^2 - I_\zeta^2] / 2 I_\xi I_\eta.
\end{aligned} \tag{1C.6}$$

Contraction with $g^{\mu\nu}$ gives the curvature scalar

$$\bar{R} = [2(I_\xi I_\eta + I_\eta I_\zeta + I_\zeta I_\xi) - I_\xi^2 - I_\eta^2 - I_\zeta^2] / 2 I_\xi I_\eta I_\zeta. \tag{1C.7}$$

Since the space under consideration is free of torsion, the Christoffel symbol $\bar{\Gamma}_{\mu\nu}^\lambda$ is equal to the full affine connection $\Gamma_{\mu\nu}^\lambda$. The same thing is true for the curvature scalars $\bar{R}$ and R calculated from $\bar{\Gamma}_{\mu\nu}^\lambda$ and $\Gamma_{\mu\nu}^\lambda$, respectively.

Notes and References

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or the textbook [5].
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*A common mistake that people make
when trying to design something completely foolproof
is to underestimate the ingenuity of complete fools.*
DOUGLAS ADAMS (1952-2001)

2

Field Formulation of Many-Body Quantum Physics

A piece of matter composed of a large number of microscopic particles is called a *many-body system*. The microscopic particles may either be all identical or of different species. Examples are crystal lattices, liquids, and gases, all of these being aggregates of molecules and atoms. Molecules are composed of atoms which, in turn, consist of an atomic nucleus and electrons, held together by electromagnetic forces, or more precisely their quanta, the photons. The mass of an atom is mostly due to the nucleus, only a small fraction being due to the electrons and an even smaller fraction due to the electromagnetic binding energy. Atomic nuclei are themselves bound states of nucleons, held together by mesonic forces, or more precisely their quanta, the mesons. The nucleons and mesons, finally, consist of the presently most fundamental objects of nuclear material, called quarks, held together by gluonic forces. Quarks and gluons are apparently as fundamental as electrons and photons. It is a wonderful miracle of nature that this deep hierarchy of increasingly fundamental particles allows a common description with the help of a single theoretical structure called quantum field theory.

As a first step towards developing this powerful theory we shall start from the well-founded Schrödinger theory of nonrelativistic spinless particles. We show that there exists a completely equivalent formulation of this theory in terms of quantum fields. This formulation will serve as a basis for setting up various quantum field theoretical models which can eventually explain the physics of the entire particle hierarchy described above.

2.1 Mechanics and Quantum Mechanics for n Distinguishable Nonrelativistic Particles

For a many-body system with only one type of nonrelativistic spinless particles of mass M , which may be spherical atoms or molecules, the classical Lagrangian has the form

$$L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t) = \sum_{\nu=1}^n \frac{M}{2} \dot{\mathbf{x}}_\nu^2 - V(\mathbf{x}_1, \dots, \mathbf{x}_n; t), \quad (2.1)$$

where the arguments $\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu$ in $L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t)$ stand, *pars pro toto*, for all positions $\mathbf{x}_\nu$ and velocities $\dot{\mathbf{x}}_\nu$, $\nu = 1, \dots, n$. The general n -body potential $V(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ can usually be assumed to consist of a sum of an *external potential* $V_1(\mathbf{x}_\nu; t)$ and a *pair potential* $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$, also called *one-* and *two-body-potentials*, respectively:

$$V(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = \sum_{\nu} V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu, \mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \quad (2.2)$$

The second sum is symmetric in μ and ν , so that $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ may be taken as a symmetric function of the two spatial arguments — any asymmetric part would not contribute. The symmetry ensures the validity of *Newton's third law* “*actio est reactio*”. The two-body potential is initially defined only for $\mu \neq \nu$, and the sum is restricted accordingly, but for the development to come it will be useful to include also the $\mu = \nu$ -terms into the second sum (2.2), and compensate this by an appropriate modification of the one-body potential $V_1(\mathbf{x}_\nu; t)$, so that the total potential remains the same. Such a rearrangement excludes pair potentials $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ which are singular at the origin, such as the Coulomb potential between point charges $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) = e^2/4\pi|\mathbf{x}_\nu - \mathbf{x}_\mu|$. Physically, this is not a serious obstacle since all charges in nature really have a finite charge radius. Even the light fundamental particles electrons and muons possess a finite charge radius, as will be seen in Chapter 12.

At first we shall consider all particles to be distinguishable. This assumption is often unphysical and will be removed later. For the particle at $\mathbf{x}_\nu$, the Euler-Lagrange equation of motion that extremizes the above Lagrangian (2.1) reads [recall Eq. (1.8)]

$$M\ddot{\mathbf{x}}_\nu = -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_{\mu} \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \quad (2.3)$$

The transition to the Hamiltonian formalism proceeds by introducing the canonical momenta [see (1.10)]

$$\mathbf{p}_\nu = \frac{\partial L}{\partial \dot{\mathbf{x}}_\nu} = M\dot{\mathbf{x}}_\nu, \quad (2.4)$$

and forming the Legendre transform [see (1.9)]

$$\begin{aligned} H(\mathbf{p}_\nu, \mathbf{x}_\nu; t) &= \left[\sum_{\nu} \mathbf{p}_\nu \dot{\mathbf{x}}_\nu - L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t) \right]_{\dot{\mathbf{x}}_\nu = \mathbf{p}_\nu / M} \\ &= \sum_{\nu} \frac{\mathbf{p}_\nu^2}{2M} + \sum_{\nu} V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu, \mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \end{aligned} \quad (2.5)$$

From this, the Hamilton equations of motions are derived as [see (1.17)]

$$\dot{\mathbf{p}}_\nu = \{H, \mathbf{p}_\nu\} = -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_{\mu} \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t), \quad (2.6)$$

$$\dot{\mathbf{x}}_\nu = \{H, \mathbf{x}_\nu\} = \frac{\partial H}{\partial \mathbf{p}_\nu} = \frac{\mathbf{p}_\nu}{M}, \quad (2.7)$$

with $\{A, B\}$ denoting the Poisson brackets defined in Eq. (1.20):

$$\{A, B\} = \sum_{\nu=1}^n \left(\frac{\partial A}{\partial \mathbf{p}_\nu} \frac{\partial B}{\partial \mathbf{x}_\nu} - \frac{\partial B}{\partial \mathbf{p}_\nu} \frac{\partial A}{\partial \mathbf{x}_\nu} \right). \quad (2.8)$$

An arbitrary observable $F(\mathbf{p}_\nu, \mathbf{x}_\nu; t)$ changes as a function of time according to the equation of motion (1.19):

$$\frac{dF}{dt} = \{H, F\} + \frac{\partial F}{\partial t}. \quad (2.9)$$

It is now straightforward to write down the laws of quantum mechanics for the system. We follow the rules in Eqs. (1.236)–(1.238), and take the local basis

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \quad (2.10)$$

as eigenstates of the position operators $\hat{\mathbf{x}}_\nu$:

$$\hat{\mathbf{x}}_\nu |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle = \mathbf{x}_\nu |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle, \quad \nu = 1, \dots, n. \quad (2.11)$$

They are orthonormal to each other:

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \mathbf{x}'_1, \dots, \mathbf{x}'_n \rangle = \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_n), \quad (2.12)$$

and form a complete basis in the space of localized n -particle states:

$$\int d^3x_1 \cdots d^3x_n |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \langle \mathbf{x}_1, \dots, \mathbf{x}_n| = 1. \quad (2.13)$$

An arbitrary state is denoted by a ket vector and can be expanded in this basis by multiplying the state formally with the unit operator (14.245), yielding the expansion

$$|\psi(t)\rangle \equiv 1 \times |\psi(t)\rangle = \int d^3x_1 \cdots d^3x_n |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \langle \mathbf{x}_1, \dots, \mathbf{x}_n | \psi(t)\rangle. \quad (2.14)$$

The scalar products

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \psi(t)\rangle \equiv \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \quad (2.15)$$

are the wave functions of the n -body system. They are the probability amplitudes for the particle 1 to be found at $\mathbf{x}_1$, particle 2 at $\mathbf{x}_2$, etc..

The Schrödinger equation reads, in operator form,

$$\hat{H}|\psi(t)\rangle = H(\hat{\mathbf{p}}_\nu, \hat{\mathbf{x}}_\nu; t)|\psi(t)\rangle = i\hbar \partial_t |\psi(t)\rangle, \quad (2.16)$$

where $\hat{\mathbf{p}}_\nu$ are Schrödinger's momentum operators, whose action upon the wave functions is specified by the rule

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \hat{\mathbf{p}}_\nu = -i\hbar \partial_{\mathbf{x}_\nu} \langle \mathbf{x}_1, \dots, \mathbf{x}_n|. \quad (2.17)$$

Multiplication of (14.247) from the left with the bra vectors $\langle \mathbf{x}_1, \dots, \mathbf{x}_n |$ yields via (14.248) the Schrödinger differential equation for the wave functions:

$$\begin{aligned} & H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \\ &= \left[-\sum_{\nu} \frac{\hbar^2}{2M} \partial_{\mathbf{x}_\nu}^2 + \sum_{\nu} V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu, \mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) \right] \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \\ &= i\hbar\partial_t\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \end{aligned} \quad (2.18)$$

In many physical systems, the potentials $V_1(\mathbf{x}_\nu; t)$ and $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ are independent of time. Then we can factor out the time dependence of the wave functions with fixed energy as

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = e^{-iEt/\hbar} \psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n), \quad (2.19)$$

and find for $\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n)$ the time-independent Schrödinger equation

$$H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n) = E\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n). \quad (2.20)$$

2.2 Identical Particles: Bosons and Fermions

The quantum mechanical rules in the last section were written down in the previous section under the assumption that all particles are distinguishable. For most realistic n -body systems, however, this is an unphysical assumption. For example, there is no way of distinguishing the electrons in an atom. Thus not all of the solutions $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ of the Schrödinger equation (2.18) can be physically permissible. Consider the case where the system contains only one species of identical particles, for example electrons. The Hamilton operator in Eq. (2.18) is invariant under all permutations of the particle labels ν . In addition, all probability amplitudes $\langle \psi_1 | \psi_2 \rangle$ must reflect this invariance. They must form a representation space of all permutations. Let T_{ij} be an operator which interchanges the variables $\mathbf{x}_i$ and $\mathbf{x}_j$.

$$T_{ij}\psi(\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_n; t) \equiv \psi(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots, \mathbf{x}_n; t). \quad (2.21)$$

It is called a *transposition*. The invariance may then be expressed as $\langle T_{ij}\psi_1 | T_{ij}\psi_2 \rangle = \langle \psi_1 | \psi_2 \rangle$, implying that the wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ can change at most by a phase:

$$T_{ij}\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = e^{i\alpha_{ij}} \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \quad (2.22)$$

But from the definition (2.21) we see that T_{ij} satisfies

$$T_{ij}^2 = 1. \quad (2.23)$$

Thus $e^{i\alpha_{ij}}$ can only have the values $+1$ or -1 . Moreover, due to the identity of all particles, the sign must be the same for any pair ij .

The set of all multiparticle wave functions can be decomposed into wave functions transforming in specific ways under arbitrary permutations P of the coordinates.

It will be shown in Appendix 2A that each permutation P can be decomposed into products of transpositions. Of special importance are wave functions which are completely symmetric, i.e., which are obtained by applying, to an arbitrary n -particle wave function, the operation

$$S = \frac{1}{n!} \sum_P P. \quad (2.24)$$

The sum runs over all $n!$ permutations of the particle indices. Another important type of wave function is obtained by applying the antisymmetrizing operator

$$A = \frac{1}{n!} \sum_P \epsilon_P P \quad (2.25)$$

to the arbitrary n -particle wave function. The symbol ϵ_P is unity for even permutations and -1 for odd permutations. It is called the *parity* of the permutation.

By applying S or A to an arbitrary n -particle wave function one obtains completely symmetric or completely antisymmetric n -particle wave functions. In nature, both signs can occur. Particles with symmetric wave functions are called *bosons*, the others *fermions*. Examples for bosons are photons, mesons, α -particles, or any nuclei with an even atomic number. Examples for fermions are electrons, neutrinos, muons, protons, neutrons, or any nuclei with an odd atomic number.

In two-dimensional multi-electron systems in very strong magnetic fields, an interesting new situation has been discovered. These systems have wave functions which look like those of free quasiparticles on which transpositions T_{ij} yield a phase factor $e^{i\alpha_{ij}}$ which is not equal to ± 1 : These quasiparticles are neither bosons nor fermions. They have therefore been called *anyons*. Their existence in two dimensions is made possible by imagining each particle to introduce a singularity in the plane, which makes the plane multisheeted. A second particle moving by 360° around this singularity does not arrive at the initial point but at a point lying in a second sheet below the initial point. For this reason, the equation (2.23) needs no longer to be fulfilled.

Distinguishing the symmetry properties of the wave functions provides us with an important tool to classify the various solutions of the Schrödinger equation (2.18). Let us illustrate this by looking at the simplest nontrivial case in which the particles have only a common time-independent external potential $V_1(\mathbf{x}_\nu)$ but are otherwise noninteracting, i.e., their time-independent Schrödinger equation (2.20) reads

$$\sum_\nu \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu) \right] \psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n) = E \psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n). \quad (2.26)$$

It can be solved by the factorizing ansatz in terms of single-particle states $\psi_{E_{\alpha_\nu}}$ of energy E_{α_ν} ,

$$\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n) = \prod_{\nu=1}^n \psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu), \quad (2.27)$$

with the total energy being the sum of the individual energies:

$$E = \sum_{\nu=1}^n E_{\alpha_\nu}. \quad (2.28)$$

The single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are the solutions of the one-particle Schrödinger equation

$$\left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + V_1(\mathbf{x}) \right] \psi_{E_\alpha}(\mathbf{x}) = E_\alpha \psi_{E_\alpha}(\mathbf{x}). \quad (2.29)$$

If the wave functions $\psi_{E_\alpha}(\mathbf{x})$ form a complete set of states, they satisfy the one-particle completeness relation

$$\sum_{\alpha} \psi_{E_\alpha}(\mathbf{x}) \psi_{E_\alpha}^*(\mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.30)$$

The sum over the labels α may, of course, involve an integral over a continuous part of the spectrum. It is trivial to verify that the set of all products (14.266) is complete in the space of n -particle wave functions:

$$\begin{aligned} \sum_{\alpha_1, \dots, \alpha_n} \psi_{E_{\alpha_1}}(\mathbf{x}_1) \cdots \psi_{E_{\alpha_n}}(\mathbf{x}_n) \psi_{E_{\alpha_n}}^*(\mathbf{x}'_n) \cdots \psi_{E_{\alpha_1}}^*(\mathbf{x}'_1) \\ = \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_n). \end{aligned} \quad (2.31)$$

For identical particles, this Hilbert space is greatly reduced. In the case of bosons, only the fully symmetrized products correspond to physical energy eigenstates. We apply the symmetrizing operation S of Eq. (2.24) to the product of single-particle wave functions $\prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu)$ and normalize the result to find

$$\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \dots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^S S \prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu) = \mathcal{N}_{\{E_\alpha\}}^S \frac{1}{n!} \sum_P \prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu). \quad (2.32)$$

The sum runs over $n!$ permutations of the indices $\nu = 1, \dots, n$, the permuted indices being denoted by $p(\nu)$.

Note that $\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \dots, \mathbf{x}_n)$ no longer depends on the order of labels of the energies $E_{\alpha_1}, \dots, E_{\alpha_n}$. This is a manifestation of the indistinguishability of the particles in the corresponding one-particle states indicated by the curly-bracket notation $\psi_{\{E_\alpha\}}^S$. Also the normalization factor is independent of the order and has been denoted by $\mathcal{N}_{\{E_\alpha\}}^S$.

For fermions, the wave functions are

$$\psi_{\{E_\alpha\}}^A(\mathbf{x}_1, \dots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^A A \prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu) = \mathcal{N}_{\{E_\alpha\}}^A \frac{1}{n!} \sum_P \epsilon_P \prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu), \quad (2.33)$$

where ϵ_P has the values $\epsilon_P = \pm 1$ for even or odd permutations, respectively.

Instead of the indices on the labels α_ν of the energies, we may just as well symmetrize or antisymmetrize the labels of the position variables:

$$\psi_{\{E_\alpha\}}^{S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^{S,A} \frac{1}{n!} \sum_P \left\{ \begin{matrix} 1 \\ \epsilon_P \end{matrix} \right\} \prod_{\nu=1}^n \psi_{E_{\alpha_\nu}}(\mathbf{x}_{p(\nu)}). \quad (2.34)$$

See Appendix 2A for more details.

The completely antisymmetrized products (2.33) can also be written in the form of a determinant first introduced by Slater:

$$\psi_{\{E_\alpha\}}^A(\mathbf{x}_1, \dots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^A \frac{1}{n!} \begin{vmatrix} \psi_{E_{\alpha_1}}(\mathbf{x}_1) & \psi_{E_{\alpha_1}}(\mathbf{x}_2) & \dots & \psi_{E_{\alpha_1}}(\mathbf{x}_n) \\ \vdots & \vdots & & \vdots \\ \psi_{E_{\alpha_n}}(\mathbf{x}_1) & \psi_{E_{\alpha_n}}(\mathbf{x}_2) & \dots & \psi_{E_{\alpha_n}}(\mathbf{x}_n) \end{vmatrix}. \quad (2.35)$$

To determine the normalization factors in (2.32)–(2.35), we calculate the integral

$$\begin{aligned} & \int d^3x_1 \cdots d^3x_n \psi_{\{E_\alpha\}}^{S*}(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \dots, \mathbf{x}_n) \\ &= \mathcal{N}_{\{E_\alpha\}}^{S\ 2} \frac{1}{n!} \sum_{P,Q} \prod_{\nu=1}^n \int d^3x_\nu \psi_{E_{\alpha_{p(\nu)}}}^*(\mathbf{x}_\nu) \psi_{E_{\alpha_{q(\nu)}}}(\mathbf{x}_\nu). \end{aligned} \quad (2.36)$$

Due to the group property of permutations, the double-sum contains $n!$ identical terms with $P = Q$ and can be rewritten as

$$\begin{aligned} & \int d^3x_1 \cdots d^3x_n \psi_{\{E_\alpha\}}^{S*}(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \dots, \mathbf{x}_n) \\ &= \mathcal{N}_{\{E_\alpha\}}^{S\ 2} \frac{1}{n!} \sum_P \prod_{\nu=1}^n \int d^3x_\nu \psi_{E_{\alpha_\nu}}^*(\mathbf{x}_\nu) \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu). \end{aligned} \quad (2.37)$$

If all single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are different from each other, then only the identity permutation $P = 1$ with $p(\nu) = \nu$ survives, and the normalization integral (2.37) fixes

$$\mathcal{N}_{\{E_\alpha\}}^{S\ 2} = n!. \quad (2.38)$$

Suppose now that two of the single-particle wave functions $\psi_{E_{\alpha_\nu}}$, say $\psi_{E_{\alpha_1}}$ and $\psi_{E_{\alpha_2}}$, coincide, while all others are different from these and each other. Then only two permutations survive in (2.37): those with $p(\nu) = \nu$, and those in which P is a transposition T_{ij} of two elements (see Appendix 2A). The right-hand side of (2.38) is then reduced by a factor of 2:

$$\mathcal{N}_{\{E_\alpha\}}^{S\ 2} = \frac{n!}{2}. \quad (2.39)$$

Extending this consideration to n_1 identical states $\psi_{E_{\alpha_1}}, \dots, \psi_{E_{\alpha_{n_1}}}$, all $n_1!$ permutations among these give equal contributions to the normalization integral (2.37) and lead to

$$\mathcal{N}_{\{E_\alpha\}}^{S\ 2} = \frac{n!}{n_1!} = 1. \quad (2.40)$$

Finally it is easy to see that, if there are groups of $n_1, n_2, \dots, n_k$ identical states, the normalization factor is

$$\mathcal{N}_{\{E_\alpha\}}^{S^2} = \frac{n!}{n_1! n_2! \dots n_k!}. \quad (2.41)$$

For the antisymmetric states of fermion systems, the situation is much simpler. Here, no two states can be identical as is obvious from the Slater determinant (2.35). Similar considerations as in (2.36), (2.37) for the wave functions (2.33) lead to

$$\mathcal{N}_{\{E_\alpha\}}^{A^2} = n!. \quad (2.42)$$

The projection into the symmetric and antisymmetric subspaces has the following effect upon the completeness relation (2.31): Multiplying it by the symmetrization or antisymmetrization operators

$$\hat{P}^{S,A} = \frac{1}{n!} \sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\}, \quad (2.43)$$

which may be applied upon the particle positions $\mathbf{x}_1, \dots, \mathbf{x}_n$ as in (2.34), we calculate

$$\sum_{\alpha_1, \dots, \alpha_n} \left[\mathcal{N}_{\{E_\alpha\}}^{S,A} \right]^2 \psi_{\{E_\alpha\}}^{S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^{S,A*}(\mathbf{x}'_1, \dots, \mathbf{x}'_n) = \delta^{(3)S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n), \quad (2.44)$$

where the symmetrized or antisymmetrized δ -function is defined by

$$\delta^{(3)S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n) \equiv \frac{1}{n!} \sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_{p(1)}) \dots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_{p(n)}). \quad (2.45)$$

Since the left-hand side of (2.44) is independent of the order of $E_{\alpha_1}, \dots, E_{\alpha_n}$, we may sum only over a certain order among the labels

$$\sum_{\alpha_1, \dots, \alpha_n} \longrightarrow n! \sum_{\alpha_1 > \dots > \alpha_n}. \quad (2.46)$$

If there are degeneracy labels in addition to the energy, these have to be ordered in the same way.

For antisymmetric states, the labels $\alpha_1, \dots, \alpha_n$ are necessarily different from each other. Inserting (2.42) and (2.46) into (2.45), this gives directly

$$\sum_{\alpha_1 > \dots > \alpha_n} \psi_{\{E_\alpha\}}^A(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^{A*}(\mathbf{x}'_1, \dots, \mathbf{x}'_n) = \delta^{(3)A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n). \quad (2.47)$$

For the symmetric case we can order the different groups of identical states and denote their common labels by $\alpha_{n_1}, \alpha_{n_2}, \dots, \alpha_{n_k}$, with the numbers n_ν indicating how often the corresponding label α is present. Obviously, there are $n!/n_1! n_2! \dots n_k!$ permutations in the completeness sum (2.44) for each set of labels $\alpha_{n_1} > \alpha_{n_2} >$

$\dots > \alpha_{n_k}$, the divisions by $n_\nu!$ coming from the permutations *within* each group of $n_1, \dots, n_k$ identical states. This combinatorial factor cancels precisely the normalization factor (2.41), so that the completeness relation for symmetric n -particle states reads

$$\sum_{n_1, \dots, n_k} \sum_{\alpha_{n_1} > \dots > \alpha_{n_k}} \psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^{S*}(\mathbf{x}'_1, \dots, \mathbf{x}'_n) = \delta^{(3)S}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n). \quad (2.48)$$

The first sum runs over the different breakups of the total number n of states into identical groups so that $n = n_1 + \dots + n_k$.

It is useful to describe the symmetrization or antisymmetrization procedure directly in terms of Dirac's bra and ket formalism. The n -particle states are direct products of single-particle states multiplied by the operator $\hat{P}^{S,A}$, and can be written as

$$|\psi^{S,A}\rangle = \hat{P}^{S,A} |E_{\alpha_1}\rangle \dots |E_{\alpha_n}\rangle = \mathcal{N}^{S,A} \frac{1}{n!} \sum_P \left\{ \frac{1}{\epsilon_P} \right\} |E_{\alpha_{p(1)}}\rangle \dots |E_{\alpha_{p(n)}}\rangle. \quad (2.49)$$

The wave functions (2.32) and (2.33) consist of scalar products of these states with the localized boson states $|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle$, which may be written as direct products

$$|\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\rangle = |\mathbf{x}_1\rangle \otimes |\mathbf{x}_2\rangle \otimes \dots \otimes |\mathbf{x}_n\rangle. \quad (2.50)$$

In this state, the particle with number 1 sits at $\mathbf{x}_1$, the particle with number 2 at $\mathbf{x}_2$, $\dots$, etc. The symmetrization process wipes out the distinction between the particles 1, 2, $\dots$, n .

Let us adapt the symbolic completeness relation to the symmetry of the wave functions. The general relation

$$\int d^3x_1 \dots d^3x_n |\mathbf{x}_1\rangle \langle \mathbf{x}_1| \otimes \dots \otimes |\mathbf{x}_n\rangle \langle \mathbf{x}_n| = 1 \quad (2.51)$$

covers *all* square integrable wave functions in the product space. As far as the physical Hilbert space is concerned, it can be restricted as follows:

$$\int d^3x_1 \dots d^3x_n |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^{S,A} {}^{S,A}\langle \mathbf{x}_1, \dots, \mathbf{x}_n| = \hat{P}^{S,A}, \quad (2.52)$$

where

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^{S,A} = \frac{1}{n!} \sum_P \left\{ \frac{1}{\epsilon_P} \right\} |\mathbf{x}_{p(1)}, \dots, \mathbf{x}_{p(n)}\rangle. \quad (2.53)$$

The states are orthonormal in the sense

$${}^{S,A}\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \mathbf{x}'_1, \dots, \mathbf{x}'_n \rangle^{S,A} = \delta^{(3)S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n). \quad (2.54)$$

This basis will play an essential role for the introduction of quantum fields.

While the formalism presented so far is applicable to any number of particles, practical calculations usually present a tremendous task. The number of particles is often so large, of the order 10^{23} , that no existing computer could even list the wave functions. On the other hand, macroscopic many-body systems containing such a large number of microscopic particles make up our normal environment, and our experience teaches us that many global phenomena can be predicted quite reliably. They should therefore also be calculable in simple terms. For example, for most purposes a crystal follows the laws of a rigid body, and nothing in these laws records the immense number of degrees of freedom inherent in a microscopic description. If the solid is excited, there are sound waves in which all the many atoms in the lattice vibrate around their equilibrium positions. Their description requires only a few bulk parameters such as elastic constants and mass density. Phenomena of this type are called *collective phenomena*.

To describe such phenomena, an economic way had to be found which does not require the solution of the Schrödinger differential equation with $3n \sim 10^{23}$ coordinates. We shall later see that field theory provides us with an elegant and efficient access to such phenomena. After a suitable choice of field variables, simple mean-field approximations will often give a rough explanation of many collective phenomena. In the subsequent sections we shall demonstrate how the Schrödinger theory of any number of particles can be transformed into the quantum field theory of a single field.

There is further motivation at a more fundamental level for introducing fields. They offer a natural way of accounting for the symmetry properties of the wave functions, as we shall now see.

2.3 Creation and Annihilation Operators for Bosons

When dealing with n -particle Schrödinger equations, the imposition of symmetry upon the Schrödinger wave functions $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ seems to be a rather artificial procedure. There exists an alternative formulation of the quantum mechanics of n particles in which the Hilbert space *automatically* carries the correct symmetry. This formulation may therefore be viewed as a more “natural” description of such quantum systems. The basic mathematical structure which will serve this purpose was first encountered in a particular quantum mechanical description of harmonic oscillators which we now recall. It is well-known that the Hamilton operator of an oscillator of unit mass

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{q}^2 \quad (2.55)$$

can be rewritten in the form

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right), \quad (2.56)$$

where

$$\hat{a}^\dagger = \frac{\sqrt{\omega}\hat{q} - i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}}, \quad \hat{a} = \frac{\sqrt{\omega}\hat{q} + i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}} \quad (2.57)$$

are the so-called *raising* and *lowering* operators. The canonical quantization rules

$$\begin{aligned} [\hat{p}, \hat{p}] &= [\hat{x}, \hat{x}] = 0, \\ [\hat{p}, \hat{x}] &= -i\hbar \end{aligned} \quad (2.58)$$

imply that $\hat{a}, \hat{a}^\dagger$ satisfy

$$\begin{aligned} [\hat{a}, \hat{a}] &= [\hat{a}^\dagger, \hat{a}^\dagger] = 0, \\ [\hat{a}, \hat{a}^\dagger] &= 1. \end{aligned} \quad (2.59)$$

The energy spectrum of the oscillator follows directly from these commutation rules. We introduce the *number operator*

$$\hat{N} = \hat{a}^\dagger \hat{a}, \quad (2.60)$$

which satisfies the equations

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger, \quad (2.61)$$

$$[\hat{N}, \hat{a}] = -\hat{a}. \quad (2.62)$$

These imply that $\hat{a}^\dagger$ and $\hat{a}$ raise and lower the eigenvalues of the number operator $\hat{N}$ by one unit, respectively. Indeed, if $|\nu\rangle$ is an eigenstate with eigenvalue ν ,

$$\hat{N}|\nu\rangle = \nu|\nu\rangle, \quad (2.63)$$

we see that

$$\hat{N}\hat{a}^\dagger|\nu\rangle = (\hat{a}^\dagger\hat{N} + \hat{a}^\dagger)|\nu\rangle = (\nu + 1)\hat{a}^\dagger|\nu\rangle, \quad (2.64)$$

$$\hat{N}\hat{a}|\nu\rangle = (\hat{a}\hat{N} - \hat{a})|\nu\rangle = (\nu - 1)\hat{a}|\nu\rangle. \quad (2.65)$$

Moreover, the eigenvalues ν must all be integer numbers n which are larger or equal to zero. To see this, we observe that $\hat{a}^\dagger\hat{a}$ is a positive operator. It satisfies for every state $|\psi\rangle$ in Hilbert space the inequality

$$\langle\psi|\hat{a}^\dagger\hat{a}|\psi\rangle = \|\hat{a}|\psi\rangle\|^2 \geq 0. \quad (2.66)$$

Hence there exists a state, usually denoted by $|0\rangle$, whose energy cannot be lowered by one more application of $\hat{a}$. This state will satisfy

$$\hat{a}|0\rangle = 0. \quad (2.67)$$

As a consequence, the operator $\hat{N}$ applied to $|0\rangle$ must be zero. Applying the raising operator $\hat{a}^\dagger$ any number of times, the eigenvalues ν of $\hat{N}$ will cover all integer numbers $\nu = n$ with $n = 0, 1, 2, 3, \dots$. The corresponding states are denoted by $|n\rangle$:

$$\hat{N}|n\rangle = n|n\rangle, \quad n = 0, 1, 2, 3, \dots \quad (2.68)$$

Explicitly, these states are given by

$$|n\rangle = \mathcal{N}_n (\hat{a}^\dagger)^n |0\rangle, \quad (2.69)$$

with some normalization factor $\mathcal{N}_n$, that can be calculated using the commutation rules (2.59) to be

$$\mathcal{N}_n = \frac{1}{\sqrt{n!}}. \quad (2.70)$$

By considering the commutation rules (2.59) between different states $|n\rangle$ and inserting intermediate states, we derive the matrix elements of the operators $\hat{a}, \hat{a}^\dagger$:

$$\langle n' | \hat{a} | n \rangle = \sqrt{n} \delta_{n', n-1}, \quad (2.71)$$

$$\langle n' | \hat{a}^\dagger | n \rangle = \sqrt{n+1} \delta_{n', n+1}. \quad (2.72)$$

In this way, all properties of the harmonic oscillator are recovered by purely algebraic manipulations, using (2.59) with the condition (2.67) to define the ground state.

This mathematical structure can be used to describe the complete set of symmetric localized states (2.32). All we need to do is reinterpret the eigenvalue n of the operator $\hat{N}$. In the case of the oscillator, n is the principal quantum number of the single-particle state that counts the number of zeros in the Schrödinger wave function. In quantum field theory, the operator changes its role and its eigenvalues n count the number of particles contained in the many-body wave function. The operators $\hat{a}^\dagger$ and $\hat{a}$ which raise and lower n are renamed *creation* and *annihilation operators*, which add or take away a single particle in the state $|n\rangle$. The ground state $|0\rangle$ contains no particle. It constitutes the vacuum state of the n -body system. In the states (2.32), there are n particles at places $\mathbf{x}_1, \dots, \mathbf{x}_n$. We therefore introduce the spatial degree of freedom by giving $\hat{a}^\dagger, \hat{a}$ a spatial label and defining the operators

$$\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}},$$

which permit the creation and annihilation of a particle localized at the position $\mathbf{x}$.¹

The operators at different locations are taken to be independent, i.e., they commute as

$$[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}] = [\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}'}^\dagger] = 0, \quad (2.73)$$

$$[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}^\dagger] = 0, \quad \mathbf{x} \neq \mathbf{x}'. \quad (2.74)$$

The commutation rule between $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}'}$ for coinciding space variables $\mathbf{x}$ and $\mathbf{x}'$ is specified with the help of a Dirac δ -function as follows:

$$[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}^\dagger] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.75)$$

We shall refer to these $\mathbf{x}$ -dependent commutation rules as the *local oscillator algebra*.

The δ -function singularity in (2.75) is dictated by the fact that we want to preserve the raising and lowering commutation rules (2.61) and (2.62) for the particle number at each point $\mathbf{x}$, i.e., we want that

$$[\hat{N}, \hat{a}_{\mathbf{x}}^\dagger] = \hat{a}_{\mathbf{x}}^\dagger, \quad (2.76)$$

¹The label $\mathbf{x}$ in configuration space of the particles bears no relation to the operator $\hat{q}$ in the Hamiltonian (2.55), which here denotes an operator in field space, as we shall better understand in Section 2.8.

$$[\hat{N}, \hat{a}_{\mathbf{x}}] = -\hat{a}_{\mathbf{x}}. \quad (2.77)$$

The total particle number operator is then given by the integral

$$\hat{N} = \int d^3x \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}. \quad (2.78)$$

Due to (2.74), all parts in the integral (2.78) with $\mathbf{x}'$ different from the $\mathbf{x}$ in (2.76) and (2.77) do not contribute. If the integral is supposed to give the right-hand sides in (2.76) and (2.77), the commutator between $\hat{a}_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}^\dagger$ has to be equal to a δ -function.

The use of the δ -function is of course completely analogous to that in Subsection 1.4. [recall the limiting process in Eq. (1.160)]. In fact, we could have introduced local creation and annihilation operators with ordinary unit commutation rules at each point by discretizing the space into a fine-grained point-lattice of a tiny lattice spacing ϵ , with discrete lattice points at

$$\mathbf{x}_{\mathbf{n}} = (n_1, n_2, n_3)\epsilon, \quad n_\nu = 0, \pm 1, \pm 2, \dots \quad (2.79)$$

And for the creation or annihilation of a particle in the small cubic box around $\mathbf{x}_{\mathbf{n}}$ we could have introduced the operators $\hat{a}_{\mathbf{n}}^\dagger$ or $\hat{a}_{\mathbf{n}}$, which satisfy the discrete commutation rules

$$[\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}] = [\hat{a}_{\mathbf{n}}^\dagger, \hat{a}_{\mathbf{n}'}^\dagger] = 0, \quad (2.80)$$

$$[\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}^\dagger] = \delta_{\mathbf{n}\mathbf{n}'}^{(3)}. \quad (2.81)$$

For these the total particle number operator is

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}}. \quad (2.82)$$

This would amount to identifying $\hat{a}_{\mathbf{n}}$ with a discrete subset of the continuous set of operators $\hat{a}_{\mathbf{x}}$ as follows:

$$\hat{a}_{\mathbf{n}} = \sqrt{\epsilon^3} \hat{a}_{\mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}_{\mathbf{n}}}. \quad (2.83)$$

Then the discrete and continuous formulations of the particle number operator would be related by

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}} \equiv \epsilon^3 \sum_{\mathbf{x}_{\mathbf{n}}} \hat{a}_{\mathbf{x}_{\mathbf{n}}}^\dagger \hat{a}_{\mathbf{x}_{\mathbf{n}}} \xrightarrow{\epsilon \rightarrow 0} \int d^3x \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}. \quad (2.84)$$

In the same limit, the commutator

$$\frac{1}{\epsilon^3} [\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}^\dagger] \equiv [\hat{a}_{\mathbf{x}_{\mathbf{n}}}, \hat{a}_{\mathbf{x}_{\mathbf{n}'}}^\dagger] = \frac{1}{\epsilon^3} \delta_{\mathbf{n}\mathbf{n}'}^{(3)} \quad (2.85)$$

would tend to $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$, which can be seen in the same way as in Eq. (1.160).

We are now ready to define the vacuum state of the many-particle system. It is given by the unique state $|0\rangle$ of the local oscillator algebra (2.73) and (2.74), which contains no particle at *all* places $\mathbf{x}$, thus satisfying

$$\hat{a}_{\mathbf{x}}|0\rangle \equiv 0, \quad \langle 0|\hat{a}_{\mathbf{x}}^\dagger \equiv 0. \quad (2.86)$$

It will always be normalized to unity:

$$\langle 0|0\rangle = 1. \quad (2.87)$$

We can now convince ourselves that the fully symmetrized Hilbert space of all localized states of n particles may be identified with the states created by repeated application of the local creation operators $\hat{a}_{\mathbf{x}}^\dagger$:

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^S \equiv \frac{1}{\sqrt{n!}} \hat{a}_{\mathbf{x}_1}^\dagger \cdots \hat{a}_{\mathbf{x}_n}^\dagger |0\rangle. \quad (2.88)$$

The such-generated Hilbert space will be referred to as the *second-quantized Hilbert space* for reasons to be seen below. It decomposes into a direct sum of n -particle sectors. The symmetry of these states in the position variables is obvious, due to the commutativity (2.73) of all $\hat{a}_{\mathbf{x}_\nu}^\dagger, \hat{a}_{\mathbf{x}_\mu}^\dagger$ among each other.

Let us verify that the generalized orthonormality relation is indeed fulfilled by the single-particle states. Using the local commutation rules (2.73), (2.74), and the definition of the vacuum state (2.86), we calculate for a single particle

$$\begin{aligned} {}^S\langle \mathbf{x}|\mathbf{x}'\rangle^S &= \langle 0|\hat{a}_{\mathbf{x}}\hat{a}_{\mathbf{x}'}^\dagger|0\rangle \\ &= \langle 0|\delta^{(3)}(\mathbf{x} - \mathbf{x}') + \hat{a}_{\mathbf{x}'}^\dagger\hat{a}_{\mathbf{x}}|0\rangle \\ &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (2.89)$$

For two particles we find

$$\begin{aligned} {}^S\langle \mathbf{x}_1, \mathbf{x}_2|\mathbf{x}'_1, \mathbf{x}'_2\rangle^S &= \frac{1}{2!} \langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{x}'_1}^\dagger\hat{a}_{\mathbf{x}'_2}^\dagger|0\rangle \\ &= \frac{1}{2!} \left[\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}'_2}^\dagger|0\rangle + \langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}'_1}^\dagger\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{x}'_2}^\dagger|0\rangle \right] \\ &= \frac{1}{2!} \left[\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1)\delta^{(3)}(\mathbf{x}_2 - \mathbf{x}'_2) + \delta^{(3)}(\mathbf{x}_2 - \mathbf{x}'_1)\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_2) \right] \\ &= \delta^{(3)S}(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}'_1, \mathbf{x}'_2). \end{aligned} \quad (2.90)$$

The generalization to n particles is straightforward, although somewhat tedious. It is left to the reader as an exercise. Later in Section 7.17.1, rules will be derived in a different context by a procedure due to Wick, which greatly simplifies calculations of this type.

2.4 Schrödinger Equation for Noninteracting Bosons in Terms of Creation and Annihilation Operators

Expressing the localized states in terms of the local creation and annihilation operators $\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}}$ does not only lead to an automatic symmetrization of the states. It also brings about an extremely simple unified form of the Schrödinger equation, which does not require the initial specification of the particle number n , as in Eq. (2.18).

This will now be shown for the case of identical particles with no two-body interactions $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$.

In order to exhibit the unified Schrödinger equation for any number of particles, let us first neglect interactions and consider only the motion of the particles in an external potential with the Schrödinger equation:

$$\left\{ \sum_\nu \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu; t) \right] \right\} \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = i\hbar \partial_t \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \quad (2.91)$$

We shall now demonstrate that the $\hat{a}^\dagger, \hat{a}$ -form of this equation, which is valid for any particle number n , reads

$$\hat{H}(t)|\psi(t)\rangle = i\hbar \partial_t |\psi(t)\rangle, \quad (2.92)$$

where $\hat{H}(t)$ is simply the one-particle Hamiltonian sandwiched between creation and annihilation operators $\hat{a}_\mathbf{x}^\dagger$ and $\hat{a}_\mathbf{x}$ and integrated over $\mathbf{x}$, i.e.,

$$\hat{H}(t) = \int d^3x \hat{a}_\mathbf{x}^\dagger \left[-\frac{\hbar^2}{2M} \partial_\mathbf{x}^2 + V_1(\mathbf{x}; t) \right] \hat{a}_\mathbf{x}. \quad (2.93)$$

The operator (2.93) is called the *second-quantized Hamiltonian*, equation (2.92) the *second-quantized Schrödinger equation*, and the state $|\psi(t)\rangle$ is an arbitrary n -particle state in the second-quantized Hilbert space, generated by multiple application of $\hat{a}_\mathbf{x}^\dagger$ upon the vacuum state $|0\rangle$, as described in the last section. The operator nature of $\hat{a}_\mathbf{x}, \hat{a}_\mathbf{x}^\dagger$ accounts automatically for the many-body content of Eq. (2.92).

This statement is proved by multiplying Eq. (2.92) from the left with

$${}^S\langle \mathbf{x}_1, \dots, \mathbf{x}_n | = \frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1},$$

which leads to

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \hat{H}(t) |\psi(t)\rangle = i\hbar \partial_t \frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} |\psi(t)\rangle. \quad (2.94)$$

Here we make use of the property (2.86) of the vacuum state to satisfy $\langle 0 | \hat{a}_\mathbf{x}^\dagger = 0$. As a consequence, we may rewrite the left-hand side of (2.94) with the help of a commutator as

$$\frac{1}{\sqrt{n!}} \langle 0 | [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{H}] |\psi(t)\rangle.$$

This commutator is easily calculated using the *operator chain rules*

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}, \quad [\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}. \quad (2.95)$$

These rules can easily be memorized, noting that their structure is exactly the same as in the Leibnitz rule for derivatives. In the first rule we may imagine A to be a differential operator applied to the product BC , which is evaluated by first

differentiating B , leaving C untouched, and then C , leaving B untouched. In the second rule we imagine C to be a differential operator acting similarly to the left upon the product AB . Generalizing this rule to products of more than two operators we derive

$$\begin{aligned} [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger \hat{a}_{\mathbf{z}}] &= [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger] \hat{a}_{\mathbf{z}} + \hat{a}_{\mathbf{y}}^\dagger [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{z}}] \\ &= \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_3} \hat{a}_{\mathbf{x}_2} [\hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger] \hat{a}_{\mathbf{z}} + [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_3} \hat{a}_{\mathbf{x}_2}, \hat{a}_{\mathbf{y}}^\dagger] \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{z}} + \cdots \\ &= \sum_{\nu} \delta^{(3)}(\mathbf{x}_{\nu} - \mathbf{y}) \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{z}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1}. \end{aligned}$$

Multiplying both sides by

$$\delta^{(3)}(\mathbf{y} - \mathbf{z}) \left[-\hbar^2 \partial_{\mathbf{z}}^2 / 2M + V_1(\mathbf{z}; t) \right],$$

and integrating over $d^3y d^3z$ using (2.93) and (2.75) we find

$$[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{H}(t)] = \sum_{\nu} \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_{\nu}}^2 + V_1(\mathbf{x}_{\nu}; t) \right] \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1}, \quad (2.96)$$

so that (2.94) becomes

$$\sum_{\nu} \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_{\nu}}^2 + V_1(\mathbf{x}_{\nu}; t) \right] \frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} | \psi(t) \rangle = i\hbar \partial_t \frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} | \psi(t) \rangle, \quad (2.97)$$

which is precisely the n -body Schrödinger equation (2.91) for the wave function

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \equiv \frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} | \psi(t) \rangle. \quad (2.98)$$

2.5 Second Quantization and Symmetrized Product Representation

It is worth pointing out that the mathematical structure exploited in the process of second quantization is of a very general nature.

Consider a set of matrices M_i with indices α', α

$$(M_i)_{\alpha' \alpha}$$

which satisfy some matrix commutation rules, say

$$[M_i, M_j] = if_{ijk} M_k. \quad (2.99)$$

Let us sandwich these matrices between creation and annihilation operators which satisfy

$$\begin{aligned} [\hat{a}_{\alpha}, \hat{a}_{\alpha'}] &= [\hat{a}_{\alpha}^\dagger, \hat{a}_{\alpha'}^\dagger] = 0, \\ [\hat{a}_{\alpha}, \hat{a}_{\alpha'}^\dagger] &= \delta_{\alpha\alpha'}, \end{aligned} \quad (2.100)$$

and form the analogs of “second-quantized operators” (2.93) by defining

$$\hat{M}_i \equiv \hat{a}_{\alpha'}^\dagger (M_i)_{\alpha'\alpha} \hat{a}_\alpha = \hat{a}^\dagger M_i \hat{a}. \quad (2.101)$$

In expressions of this type, repeated indices α, α' imply a summation over all α, α' . This is commonly referred to as *Einstein's summation convention*. On the right-hand side of (2.101) we have suppressed the indices α, α' completely, for brevity. It is now easy to verify, using the operator chain rules (2.95), that the operators $\hat{M}_i$ satisfy the same commutation rules as the matrices M_i :

$$\begin{aligned} [\hat{M}_i, \hat{M}_j] &= [\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger M_j \hat{a}] \\ &= [\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger] M_j \hat{a} + \hat{a}^\dagger M_j [\hat{a}^\dagger M_i \hat{a}, \hat{a}] \\ &= \hat{a}^\dagger M_i M_j \hat{a} - \hat{a}^\dagger M_j M_i \hat{a} \\ &= \hat{a}^\dagger [M_i, M_j] \hat{a} = i f_{ijk} \hat{a}^\dagger M_k \hat{a} = i f_{ijk} \hat{M}_k. \end{aligned} \quad (2.102)$$

Thus the “second-quantized” operators $\hat{M}_i$ generate an *operator representation* of the matrices M_i . They can be sandwiched between states in the “second-quantized” Hilbert space generated by applying products of creation operators $\hat{a}_n^\dagger$ upon the vacuum state $|0\rangle$. Thereby they are mapped into an infinite-dimensional matrix representation. On each subspace spanned by the products of a fixed number of creation operators, they generate the symmetrized part of the direct product representation.

The action of the “second-quantized” operators $\hat{M}_i$ upon the large Hilbert space is very simple to calculate. The only commutation rules required are

$$\begin{aligned} [\hat{M}_i, \hat{a}_\alpha^\dagger] &= \hat{a}_{\alpha'}^\dagger (M_i)_{\alpha'\alpha}, \\ [\hat{a}_{\alpha'}^\dagger, \hat{M}_i] &= (M_i)_{\alpha'\alpha} \hat{a}_\alpha. \end{aligned} \quad (2.103)$$

From this property we calculate directly the action upon “single-particle states”:

$$\begin{aligned} \hat{M}_i \hat{a}_\alpha^\dagger |0\rangle &= [\hat{M}_i, \hat{a}_\alpha^\dagger] |0\rangle = \hat{a}_{\alpha'}^\dagger |0\rangle (M_i)_{\alpha'\alpha}, \\ \langle 0 | \hat{a}_{\alpha'} \hat{M}_i &= \langle 0 | [\hat{a}_{\alpha'}, \hat{M}_i] = (M_i)_{\alpha'\alpha} \langle 0 | \hat{a}_\alpha. \end{aligned} \quad (2.104)$$

Thus the states $\hat{a}_\alpha^\dagger |0\rangle$ span an invariant subspace and are transformed into each other via the matrix $(M_i)_{\alpha'\alpha}$.

Consider now a state with two particles:

$$\hat{a}_{\alpha_1}^\dagger \hat{a}_{\alpha_2}^\dagger |0\rangle. \quad (2.105)$$

Applying $\hat{M}_i$ to this state yields

$$\begin{aligned} [\hat{M}_i, \hat{a}_{\alpha_1}^\dagger \hat{a}_{\alpha_2}^\dagger] &= [\hat{M}_i, \hat{a}_{\alpha_1}^\dagger] \hat{a}_{\alpha_2}^\dagger + \hat{a}_{\alpha_1}^\dagger [\hat{M}_i, \hat{a}_{\alpha_2}^\dagger] \\ &= \hat{a}_{\alpha_1'}^\dagger \hat{a}_{\alpha_2}^\dagger [(M_i)_{\alpha_1'\alpha_1} \delta_{\alpha_2'\alpha_2} + \delta_{\alpha_1'\alpha_1} (M_i)_{\alpha_2'\alpha_2}]. \end{aligned} \quad (2.106)$$

Multiplying Eq. (2.106) by $|0\rangle$ from the right, we find the transformation law for the two-particle states $\hat{a}_{\alpha_1}^\dagger \hat{a}_{\alpha_2}^\dagger |0\rangle$. They are transformed via the representation matrices

$$(M_i)_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2} = (M_i)_{\alpha'_1 \alpha_1} \delta_{\alpha'_2 \alpha_2} + \delta_{\alpha'_1 \alpha_1} (M_i)_{\alpha'_2 \alpha_2}. \quad (2.107)$$

Omitting the indices, we may also write the matrices as

$$M_i^{(2)} = M_i \times 1 + 1 \times M_i, \quad (2.108)$$

which is the well-known way of forming representations of a matrix algebra in a direct product space.

Since $a_{\alpha_1}^\dagger$ and $a_{\alpha_2}^\dagger$ commute with each other, the invariant space constructed in this way contains only symmetric tensors, and only the symmetrized part of the matrices $(M_i)_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}$ contribute.

The alert reader will have realized that the same operator structure can be obtained for the *antisymmetrized* parts of the matrices $(M_i)_{\alpha'_1 \alpha'_2, \alpha_1 \alpha_2}$ by using creation and annihilation operators $a_{\alpha_1}^\dagger$ and a_{α_2} which satisfy the fermionic version of the algebraic rules (2.100):

$$\begin{aligned} \{\hat{a}_\alpha, \hat{a}_{\alpha'}\} &= \{\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger\} = 0, \\ \{\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger\} &= \delta_{\alpha\alpha'}. \end{aligned} \quad (2.109)$$

In these, curly brackets are used to abbreviate *anticommutators*

$$\{A, B\} \equiv AB + BA. \quad (2.110)$$

The first two lines in (2.102) are unchanged since the operator chain rules (2.95) hold for both Bose and Fermi operators. To derive the third line we must use the additional rules

$$\begin{aligned} [\hat{A}, \hat{B}\hat{C}] &= \{\hat{A}, \hat{B}\}\hat{C} - \hat{B}\{\hat{A}, \hat{C}\}, \\ [\hat{A}\hat{B}, \hat{C}] &= \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B}. \end{aligned} \quad (2.111)$$

This fermionic version of the commutation relation (2.102) will form, in Section 2.10, the basis for constructing a second-quantized representation for the n -particle wave functions and Schrödinger operators of fermions.

If M_i are chosen to be representation matrices L_i of the generators of the rotation group (to be discussed in detail in Section 4.1), the law (2.108) represents the quantum mechanical law of addition of two angular momenta:

$$L_i^{(2)} = L_i \times 1 + 1 \times L_i.$$

The generalization to any number of angular momenta is obvious.

Incidentally, any operator which satisfies the same commutation rules with $\hat{M}_i$, as $\hat{a}_\alpha$ in (2.103), i.e., satisfies the commutation rules

$$\begin{aligned} [\hat{M}_i, \hat{O}_\alpha^\dagger] &= \hat{O}_{\alpha'}^\dagger (M_i)_{\alpha'\alpha}, \\ [\hat{O}_{\alpha'}, \hat{M}_i] &= (M_i)_{\alpha'\alpha} \hat{O}_\alpha, \end{aligned} \quad (2.112)$$

will be referred to as a *spinor operator*. Generalizing this definition, an operator $\hat{O}_{\alpha_1\alpha_2\ldots\alpha_n}$ which commutes with $\hat{M}_i$ like a product $\hat{O}_{\alpha_1}\hat{O}_{\alpha_2}\cdots\hat{O}_{\alpha_n}$, generalizing Eq. (2.106), is called a *multispinor operator* of rank n .

Another type of operators which frequently occurs in quantum mechanics and quantum field theory is a *vector operator*. This is any operator $\hat{O}_j$ which commutes with $\hat{M}_i$ in the same way as $\hat{M}_j$ does in (2.102), i.e.,

$$[\hat{M}_i, \hat{O}_j] = if_{ijk}\hat{O}_k. \quad (2.113)$$

Its generalization $\hat{O}_{j_1j_2\ldots j_n}$, which commutes with $\hat{M}_i$ as the product of operators $\hat{M}_{j_1}\hat{M}_{j_2}\ldots\hat{M}_{j_n}$, is called a *tensor operator* of rank n .

The many-particle version of the Schrödinger theory is obtained if we view the one-particle Schrödinger equation

$$H(-i\hbar\partial_{\mathbf{x}}, \mathbf{x})\psi(\mathbf{x}, t) = i\hbar\partial_t\psi(\mathbf{x}, t) \quad (2.114)$$

as a matrix equation in the discretized $\mathbf{x}$ -space with the lattice positions $\mathbf{x} = (n_1, n_2, n_3)\epsilon$, so that the wave functions $\psi(\mathbf{x}, t)$ correspond to vectors $\psi_{\mathbf{n}}(t)$. Then the differential operator $\partial_i\psi(\mathbf{x})$ becomes simply $\nabla_i\psi(\mathbf{x}) = [\psi(\mathbf{x} + \mathbf{i}\epsilon) - \psi(\mathbf{x})]/\epsilon = [\psi_{\mathbf{n}+\mathbf{i}} - \psi_{\mathbf{n}}]/\epsilon$ where $\mathbf{i}$ is the unit vector in the i th direction, and ϵ the lattice spacing. The Laplacian may be viewed as the continuum limit of the matrix

$$\begin{aligned} \bar{\nabla}_i\nabla_i\psi(\mathbf{x}) &= \frac{1}{\epsilon^2} \sum_{i=1}^3 [\psi(\mathbf{x} + \mathbf{i}\epsilon) - 2\psi(\mathbf{x}) + \psi(\mathbf{x} - \mathbf{i}\epsilon)] \\ &= \frac{1}{\epsilon^2} \sum_{i=1}^3 [\psi_{\mathbf{n}+\mathbf{i}} - 2\psi_{\mathbf{n}} + \psi_{\mathbf{n}-\mathbf{i}}]. \end{aligned} \quad (2.115)$$

The Schrödinger equation (2.114) is then the $\epsilon \rightarrow 0$ -limit of the matrix equation

$$H_{\mathbf{nn}'}\psi_{\mathbf{n}'}(t) = i\hbar\partial_t\psi_{\mathbf{n}}(t). \quad (2.116)$$

The many-particle Schrödinger equation in second quantization form reads

$$\hat{H}|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \quad (2.117)$$

with the Hamiltonian operator

$$\hat{H} = \hat{a}_{\mathbf{n}'}^\dagger H_{\mathbf{n}'\mathbf{n}} \hat{a}_{\mathbf{n}}. \quad (2.118)$$

It can be used to find the eigenstates in the symmetrized multispinor representation space spanned by

$$\hat{a}_{\mathbf{n}_1}^\dagger \ldots \hat{a}_{\mathbf{n}_N}^\dagger |0\rangle. \quad (2.119)$$

Applying $\hat{H}$ to it we see that this state is multiplied from the right by a direct-product matrix

$$H \times 1 \times \ldots \times 1 + 1 \times H \times \ldots \times 1 + \ldots 1 \times 1 \times \ldots \times H. \quad (2.120)$$

Due to this very general relation, the Schrödinger energy of a many-body system without two- or higher-body interactions is the sum of the one-particle energies.

2.6 Bosons with Two-Body Interactions

We now include two-body interactions. For simplicity, we neglect the one-body potential $V_1(\mathbf{x}; t)$ which can be added at the end and search for the second-quantized form of the Schrödinger equation

$$\left[-\sum_{\nu} \frac{\hbar^2}{2M} \partial_{\mathbf{x}_{\nu}}^2 + \frac{1}{2} \sum_{\mu, \nu} V_2(\mathbf{x}_{\nu} - \mathbf{x}_{\mu}; t) \right] \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = i\hbar \partial_t \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \quad (2.121)$$

It is easy to see that such a two-body potential can be introduced into the second-quantized Schrödinger equation (2.92) by adding to the Hamilton operator in (2.93) the interaction term

$$\hat{H}_{\text{int}}(t) = \frac{1}{2} \int d^3x d^3x' \hat{a}_{\mathbf{x}}^{\dagger} \hat{a}_{\mathbf{x}'}^{\dagger} V_2(\mathbf{x} - \mathbf{x}'; t) \hat{a}_{\mathbf{x}'} \hat{a}_{\mathbf{x}}. \quad (2.122)$$

To prove this we work out the expectation value

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} \hat{H}_{\text{int}}(t) | \psi(t) \rangle = \frac{1}{\sqrt{n!}} \langle 0 | [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{H}_{\text{int}}(t)] | \psi(t) \rangle. \quad (2.123)$$

We do this by using the local commutation rules (2.73), (2.75), and the vacuum property (2.86). First we generalize Eq. (2.96) to

$$\begin{aligned} & [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}_2}^{\dagger} \hat{a}_{\mathbf{y}_1}^{\dagger} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}] \\ &= [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}_2}^{\dagger} \hat{a}_{\mathbf{y}_1}^{\dagger}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} + \hat{a}_{\mathbf{y}_2}^{\dagger} \hat{a}_{\mathbf{y}_1}^{\dagger} [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}] \\ &= [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}_2}^{\dagger}] \hat{a}_{\mathbf{y}_1}^{\dagger} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} + \hat{a}_{\mathbf{y}_2}^{\dagger} [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}_1}^{\dagger}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \\ &= \sum_{\nu} \delta^{(3)}(\mathbf{x}_{\nu} - \mathbf{y}_2) \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \dots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{y}_1}^{\dagger} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \\ &\quad + \hat{a}_{\mathbf{y}_2}^{\dagger} \sum_{\nu} \delta^{(3)}(\mathbf{x}_{\nu} - \mathbf{y}_1) \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \dots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}. \end{aligned} \quad (2.124)$$

The second piece does not contribute to Eq. (2.123) since $\hat{a}_{\mathbf{y}_2}^{\dagger}$ annihilates the vacuum on the left. For the same reason, the first piece can be written as

$$\sum_{\nu} \delta^{(3)}(\mathbf{x}_{\nu} - \mathbf{y}_2) [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \dots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}_1}^{\dagger}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}, \quad (2.125)$$

as long as it stands to the right of the vacuum. Using the commutation rule (2.96), this leads to

$$\begin{aligned} \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{y}_2}^{\dagger} \hat{a}_{\mathbf{y}_1}^{\dagger} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} | \psi(t) \rangle &= \sum_{\mu, \nu} \delta^{(3)}(\mathbf{x}_{\mu} - \mathbf{y}_1) \delta^{(3)}(\mathbf{x}_{\nu} - \mathbf{y}_2) \\ &\quad \times \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \dots \hat{a}_{\mathbf{x}_{\mu+1}} \hat{a}_{\mathbf{x}_{\mu-1}} \dots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} | \psi(t) \rangle. \end{aligned} \quad (2.126)$$

After multiplying this relation by $V_2(\mathbf{y}_2 - \mathbf{y}_1; t) \delta^{(3)}(\mathbf{y}_1 - \mathbf{z}_1) \delta^{(3)}(\mathbf{y}_2 - \mathbf{z}_2)/2$, and integrating over $d^3y_1 d^3y_2 d^3z_1 d^3z_2$, we find

$$\langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} \hat{H}_{\text{int}} | \psi(t) \rangle = \frac{1}{2} \sum_{\mu, \nu} V_2(\mathbf{x}_{\nu} - \mathbf{x}_{\mu}; t) \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} | \psi(t) \rangle, \quad (2.127)$$

which is precisely the two-body interaction in the Schrödinger equation (2.121).

Adding now the one-body interactions, we see that an n -body Schrödinger equation with arbitrary one- and two-body potentials can be written in the form of a single operator Schrödinger equation

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \quad (2.128)$$

with the second-quantized Hamilton operator

$$\hat{H}(t) = \int d^3x \hat{a}_{\mathbf{x}}^\dagger \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + V_1(\mathbf{x}; t) \right] \hat{a}_{\mathbf{x}} + \frac{1}{2} \int d^3x d^3x' \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}'}^\dagger V_2(\mathbf{x} - \mathbf{x}'; t) \hat{a}_{\mathbf{x}'} \hat{a}_{\mathbf{x}}. \quad (2.129)$$

The second-quantized Hilbert space of the states $|\psi(t)\rangle$ is constructed by repeated multiplication of the vacuum vector $|0\rangle$ with particle creation operators $\hat{a}_{\mathbf{x}}^\dagger$. The order of the creation and annihilation operators in this Hamiltonian is such that the vacuum, as a zero-particle state, has zero energy:

$$\hat{H}(t)|0\rangle = 0, \quad \langle 0|\hat{H}(t) = 0, \quad (2.130)$$

as in the original Schrödinger equation.

A Hamiltonian which is a spatial integral over a *Hamiltonian density* $\mathcal{H}(\mathbf{x})$ as

$$H = \int d^3x \mathcal{H}(\mathbf{x}), \quad (2.131)$$

is called a *local Hamiltonian*. In (2.129), the free part is local, but the interacting part is not. It consists of an integral over two spatial variables, thus forming a *bilocal* operator.

2.7 Quantum Field Formulation of Many-Body Schrödinger Equations for Bosons

The annihilation operator $\hat{a}_{\mathbf{x}}$ can now be used to define a time-dependent quantum field $\hat{\psi}(\mathbf{x}, t)$ as being the Heisenberg picture of the operator $\hat{a}_{\mathbf{x}}$ (which itself is also referred to as the Schrödinger picture of the annihilation operator). According to Eq. (1.285), the Heisenberg operator associated with $\hat{a}_{\mathbf{x}}$ is

$$a_{\mathbf{xH}}(t) \equiv [\hat{U}(t, t_a)]^{-1} \hat{a}_{\mathbf{x}} \hat{U}(t, t_a). \quad (2.132)$$

Thus we define

$$\hat{\psi}(\mathbf{x}, t) \equiv a_{\mathbf{xH}}(t). \quad (2.133)$$

Choosing the time variable $t_a = 0$, the quantum field $\hat{\psi}(\mathbf{x}, t)$ coincides with $\hat{a}_{\mathbf{x}}$ at $t = 0$:

$$\hat{\psi}(\mathbf{x}, 0) \equiv \hat{a}_{\mathbf{x}}. \quad (2.134)$$

The time dependence of $\hat{\psi}(\mathbf{x}, t)$ is ruled by Heisenberg's equation of motion (1.280):

$$\partial_t \hat{\psi}(\mathbf{x}, t) = \frac{i}{\hbar} [\hat{H}_H(t), \hat{\psi}(\mathbf{x}, t)]. \quad (2.135)$$

For simplicity, we shall at first assume the potentials to have no explicit time dependence, an assumption to be removed later. Then Eq. (2.135) is solved by

$$\hat{\psi}(\mathbf{x}, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(\mathbf{x}, 0) e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{x}} e^{-i\hat{H}t/\hbar}. \quad (2.136)$$

The Hermitian conjugate of this determines the time dependence of the Heisenberg picture of the creation operator:

$$\hat{\psi}^\dagger(\mathbf{x}, t) = e^{i\hat{H}t/\hbar} \hat{\psi}^\dagger(\mathbf{x}, 0) e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{x}}^\dagger e^{-i\hat{H}t/\hbar}. \quad (2.137)$$

At each given time t , the field $\hat{\psi}(\mathbf{x}, t)$ fulfills the same commutation rules (2.73) and (2.74) as $\hat{a}_{\mathbf{x}}$:

$$\begin{aligned} [\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)] &= 0, \\ [\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] &= 0, \\ [\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (2.138)$$

Consider now the Hamiltonian operator (2.129) in the Heisenberg representation. Under the assumption of no explicit time dependence in the potentials we may simply multiply it by $e^{i\hat{H}t/\hbar}$ and $e^{-i\hat{H}t/\hbar}$ from the left and right, respectively, and see that

$$\begin{aligned} \hat{H}_H(t) &= \int d^3x \hat{\psi}^\dagger(\mathbf{x}, t) \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + V_1(\mathbf{x}) \right] \hat{\psi}(\mathbf{x}, t) \\ &\quad + \frac{1}{2} \int d^3x d^3x' \hat{\psi}^\dagger(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t) V_2(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}', t) \hat{\psi}(\mathbf{x}, t). \end{aligned} \quad (2.139)$$

Since $\hat{H}$ commutes with itself, the operator $\hat{H}_H(t)$ is time independent, so that

$$\hat{H}_H(t) \equiv \hat{H}. \quad (2.140)$$

The important point about the expression (2.139) for $\hat{H}$ is now that by containing the time-dependent fields $\hat{\psi}(\mathbf{x}, t)$, it can be viewed as the Hamilton operator of a canonically quantized Heisenberg field. This is completely analogous to the Hamiltonian operator $\hat{H} \equiv H(\hat{p}_H(t), \hat{x}_H(t), t)$ in (1.278). Instead of $p_H(t)$ and $q_H(t)$, we are dealing here with generalized coordinates and their canonically conjugate momenta of the field system. They consist of the Hermitian and anti-Hermitian parts of the field, $\hat{\psi}_R(\mathbf{x}, t)$ and $\hat{\psi}_I(\mathbf{x}, t)$, defined by

$$\hat{\psi}_R \equiv \frac{(\hat{\psi} + \hat{\psi}^\dagger)}{\sqrt{2}}, \quad \hat{\psi}_I \equiv \frac{(\hat{\psi} - \hat{\psi}^\dagger)}{\sqrt{2}i}. \quad (2.141)$$

They commute like

$$\begin{aligned} [\hat{\psi}_I(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\hat{\psi}_I(\mathbf{x}, t), \hat{\psi}_I(\mathbf{x}', t)] &= 0, \\ [\hat{\psi}_R(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)] &= 0. \end{aligned} \quad (2.142)$$

These commutation rules are structurally identical to those between the quasi-Cartesian generalized canonical coordinates $\hat{q}_{iH}(t)$ and $\hat{p}_{iH}(t)$ in Eq. (1.97).

In fact, the formalism developed there can be generalized to an infinite set of canonical variables labeled by the space points $\mathbf{x}$ rather than i , i.e., to canonical variables $p_{\mathbf{x}}(t)$ and $q_{\mathbf{x}}(t)$. Then the quantization rules (1.97) take the form

$$\begin{aligned} [\hat{p}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)] &= -i\hbar\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\hat{p}_{\mathbf{x}}(t), \hat{p}_{\mathbf{x}'}(t)] &= 0, \\ [\hat{q}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)] &= 0, \end{aligned} \quad (2.143)$$

which is a local version of the algebra (2.58). The replacement $i \rightarrow \mathbf{x}$ can of course be done on a lattice with a subsequent continuum limit as in Eqs. (2.79)–(2.85). When going from the index i to the continuous spatial variable $\mathbf{x}$, the Kronecker δ_{ij} turns into Dirac's $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$, and sums become integrals.

By identifying

$$\hat{p}_{\mathbf{x}}(t) \equiv \hbar\hat{\psi}_I(\mathbf{x}, t), \quad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x}, t), \quad (2.144)$$

we now obtain the commutation relations (2.142). In quantum field theory it is customary to denote the canonical momentum variable $p_{\mathbf{x}}(t)$ by the symbol $\pi_{\mathbf{x}}(t)$, and write

$$\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x}, t) \equiv \hat{\pi}(\mathbf{x}, t). \quad (2.145)$$

Thus the many-body nature of the system may be considered as a consequence of *quantizing the fields* $q_{\mathbf{x}}(t) = \hat{\psi}_R(\mathbf{x}, t)$ and $\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x}, t)$ canonically via Eq. (2.143).

2.8 Canonical Formalism in Quantum Field Theory

So far, the commutation rules have been imposed upon the fields $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}', t)$ by the particle nature of the n -body Schrödinger theory. It is, however, possible to *derive* these rules by applying the standard canonical formalism to the fields $\psi_R(\mathbf{x}, t)$ and $\psi_I(\mathbf{x}, t)$, treating them as generalized Lagrange coordinates. To see this, let us recall once more the general procedure for finding the quantization rules and the Schrödinger equation for a general Lagrangian system with an action

$$\mathcal{A} = \int dt L(q(t), \dot{q}(t)), \quad (2.146)$$

where the Lagrangian L is some function of the independent variables $q(t) = (q_1(t), \dots, q_N(t))$ and their velocities $\dot{q}(t) = (\dot{q}_1(t), \dots, \dot{q}_N(t))$. The conjugate momenta are defined, as usual, by the derivatives

$$p_i(t) = \frac{\partial L}{\partial \dot{q}_i(t)}. \quad (2.147)$$

The Hamiltonian is given by the Legendre transformation

$$H(p(t), q(t)) = \sum_i p_i(t) \dot{q}_i(t) - L(q(t), \dot{q}(t)). \quad (2.148)$$

If $q(t)$ are Cartesian or quasi-Cartesian coordinates, quantum physics is imposed in the Heisenberg picture by letting $p_i(t)$, $q_i(t)$ become operators $\hat{p}_{iH}(t)$, $\hat{q}_{iH}(t)$ which satisfy the canonical equal time commutation rules

$$\begin{aligned} [\hat{p}_{iH}(t), \hat{q}_{jH}(t)] &= -i\hbar \delta_{ij}, \\ [\hat{p}_{iH}(t), \hat{p}_{jH}(t)] &= [\hat{q}_{iH}(t), \hat{q}_{jH}(t)] = 0, \end{aligned} \quad (2.149)$$

and postulating the Heisenberg equation of motion

$$\frac{d}{dt} \hat{O}_H = \frac{i}{\hbar} [\hat{H}_H, \hat{O}_H] + \frac{\partial}{\partial t} \hat{O}_H \quad (2.150)$$

for any observable

$$\hat{O}_H(t) \equiv O(\hat{p}_H(t), \hat{q}_H(t), t). \quad (2.151)$$

This formalism holds for any number of Cartesian or quasi-Cartesian variables. It can therefore be generalized to functions of space variables $\mathbf{x}_n$ lying on a lattice with a tiny width ϵ [see (2.79)]. Suppressing the subscripts of $\mathbf{x}_n$, the canonical momenta (2.147) read

$$p_{\mathbf{x}}(t) = \frac{\partial L}{\partial \dot{q}_{\mathbf{x}}(t)}, \quad (2.152)$$

and the Hamiltonian becomes

$$H = \sum_{\mathbf{x}} p_{\mathbf{x}}(t) \dot{q}_{\mathbf{x}}(t) - L(q_{\mathbf{x}}, \dot{q}_{\mathbf{x}}). \quad (2.153)$$

The canonical commutation rules (2.149) become the commutation rules (2.143) of second quantization.

In quantum field theory, the formalism must be generalized to continuous space variables $\mathbf{x}$. For a Hamiltonian (2.153), the action (2.146) is

$$\mathcal{A} = \int dt L(t) = \int dt \int d^3x \psi_I(\mathbf{x}, t) \hbar \partial_t \psi_R(\mathbf{x}, t) - \int dt H[\psi_I, \psi_R], \quad (2.154)$$

where $H[\psi_I, \psi_R]$ denotes the classical Hamiltonian associated with the operator $H_H(t)$ in Eq. (2.139). The derivative term can be written as an integral over a kinetic Lagrangian $L^{\text{kin}}(t)$ as

$$\mathcal{A}^{\text{kin}} = \int dt L^{\text{kin}}(t) = \int dt \int d^3x \mathcal{L}^{\text{kin}}(\mathbf{x}, t) \equiv \int dt \int d^3x \psi_I(\mathbf{x}, t) \hbar \partial_t \psi_R(\mathbf{x}, t). \quad (2.155)$$

Then the lattice rule (2.152) for finding the canonical momentum has the following functional generalization to find the canonical field momentum:

$$p_{\mathbf{x}}(t) = \frac{\partial L}{\partial \dot{q}_{\mathbf{x}}(t)} \rightarrow \pi(\mathbf{x}, t) \equiv \frac{\partial \mathcal{L}^{\text{kin}}}{\partial \partial_t \psi_R(\mathbf{x}, t)} = \hbar \psi_I(\mathbf{x}, t), \quad (2.156)$$

in agreement with the identification (2.152) and the action (2.155). The canonical quantization rules

$$\begin{aligned} [\pi(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] &= 0, \\ [\hat{\psi}_R(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)] &= 0 \end{aligned} \quad (2.157)$$

coincide with the commutation rules (2.142) of second quantization. Obviously, the Legendre transformation (2.153) turns L into the correct Hamiltonian H .

More conveniently, one expresses the classical action in terms of complex fields

$$\mathcal{A} = \int dt L(t) = \int dt \int d^3x \psi^*(\mathbf{x}, t) i\hbar \partial_t \psi(\mathbf{x}, t) - \int dt H[\psi, \psi^*], \quad (2.158)$$

and defines the canonical field momentum as

$$\pi(\mathbf{x}, t) \equiv \frac{\partial \mathcal{L}^{\text{kin}}}{\partial \partial_t \psi(\mathbf{x}, t)} = \hbar \psi^*(\mathbf{x}, t). \quad (2.159)$$

Then the canonical quantization rules become

$$\begin{aligned} [\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\psi(\mathbf{x}, t), \psi(\mathbf{x}', t)] &= 0, \\ [\psi^\dagger(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)] &= 0. \end{aligned} \quad (2.160)$$

We have emphasized before that the canonical quantization rules are applicable only if the field space is quasi-Cartesian (see the remark on page 15). For this, the dynamical metric (1.94) has to be q -independent. This condition is violated by the interaction in the Hamiltonian (2.139). There are ambiguities in ordering the field operators in this interaction. These are, however, removed by the requirement that, after quantizing the field system, one wants to reproduce the n -body Schrödinger equation, which requires that the zero-body state has zero energy and thus satisfies Eq. (2.130).

The equivalence of the n -body Schrödinger theory with the above-derived canonically quantized field theory requires specification of the ordering of the field operators after having imposed the canonical commutation rules upon the fields.

By analogy with the definition of a local Hamiltonian we call an action $\mathcal{A}$ *local* if it can be written as a spacetime integral over a *Lagrangian density* $\mathcal{L}(\mathbf{x}, t)$:

$$\mathcal{A} = \int dt \int d^3x \mathcal{L}(\mathbf{x}, t), \quad (2.161)$$

where $\mathcal{L}(\mathbf{x}, t)$ depends only on the fields $\psi(\mathbf{x}, t)$ and their first derivatives. The kinetic part in (2.158) is obviously local, the interacting part is bilocal [recall (2.139)].

For a local theory, the canonical field momentum (2.162) becomes

$$\pi(\mathbf{x}, t) \equiv \frac{\partial \mathcal{L}}{\partial \partial_t \psi(\mathbf{x}, t)} = \hbar \psi^*(\mathbf{x}, t). \quad (2.162)$$

The formal application of the rules (2.143) leads again directly to the commutation rules (2.138) without prior splitting into kinetic part and remainder.

In the complex-field formulation, only $\psi(\mathbf{x}, t)$ has a canonical momentum, not $\psi^*(\mathbf{x}, t)$. This, however, is an artifact of the use of complex field variables. Later, in Section 7.5.1 we shall encounter a more severe problem, where the canonical momentum of a component of the real electromagnetic vector field vanishes as a consequence of gauge invariance, requiring an essential modification of the quantization procedure.

Let us calculate the classical equations of motion for the continuous field theory. They are obtained by extremizing the action with respect to $\psi(x)$ and $\psi^*(x)$. To do this we need the rules of functional differentiation. These rules are derived as follows: we take the obvious differentiation rules stating the independence of generalized Lagrange variables $q_i(t)$, which read

$$\frac{\partial q_i(t)}{\partial q_j(t)} = \delta_{ij}, \quad (2.163)$$

and generalize them to lattice variables

$$\frac{\partial q_{\mathbf{x}}(t)}{\partial q_{\mathbf{x}'}(t)} = \delta_{\mathbf{x}\mathbf{x}'}. \quad (2.164)$$

For continuous field variables, these become

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial \psi(\mathbf{x}', t)} = \delta(\mathbf{x} - \mathbf{x}'). \quad (2.165)$$

The entire formalism can be generalized, thus considering the action as a local functional of fields living in continuous four-dimensional *spacetime*. Then the derivative rules must be generalized further to functional derivatives whose variations satisfy the basic rules

$$\frac{\delta \psi(\mathbf{x}, t)}{\delta \psi(\mathbf{x}', t')} = \delta^{(3)}(\mathbf{x} - \mathbf{x}') \delta(t - t') = \delta^{(4)}(x - x'). \quad (2.166)$$

The functional derivatives of actions which depend on spacetime-dependent fields $\psi(\mathbf{x}, t)$ are obtained by using the chain rule of differentiation together with (2.166). The formalism of functional differentiation and integration will be treated in detail in Chapter 14.

For a local theory, where the action has the form (2.161), and the fields and their canonical momenta (2.162) are time-dependent Lagrange coordinates with differentiation rules (2.165), the extremality conditions lead to the Euler-Lagrange equations

$$\frac{\partial \mathcal{A}}{\partial \psi(\mathbf{x}, t)} = \frac{\partial \mathcal{L}}{\partial \psi(\mathbf{x}, t)} - \partial_t \frac{\delta \mathcal{L}}{\partial \partial_t \psi(\mathbf{x}, t)} = 0, \quad (2.167)$$

$$\frac{\partial \mathcal{A}}{\partial \psi^*(\mathbf{x}, t)} = \frac{\partial \mathcal{L}}{\partial \psi^*(\mathbf{x}, t)} - \partial_t \frac{\delta \mathcal{L}}{\partial \partial_t^* \psi(\mathbf{x}, t)} = 0. \quad (2.168)$$

The second equation is simply the complex-conjugate of the first.

Note that these equations are insensitive to surface terms. This is why, in spite of the asymmetric appearance of ψ and ψ^* in the action (2.158), the two equations (2.167) and (2.168) are complex conjugate to each other. Indeed, the latter reads explicitly

$$\left[i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 - V_1(\mathbf{x}) \right] \psi(\mathbf{x}, t) = \int d\mathbf{x}' \psi^*(\mathbf{x}', t) V_2(\mathbf{x} - \mathbf{x}'; t) \psi(\mathbf{x}', t) \psi(\mathbf{x}, t), \quad (2.169)$$

and it is easy to verify that (2.167) produces the complex conjugate of this.

After field quantization, the above Euler-Lagrange equation becomes an equation for the field operator $\psi(\mathbf{x}', t)$ and its conjugate $\psi^*(\mathbf{x}', t)$ must be replaced by the Hermitian conjugate field operator $\psi^\dagger(\mathbf{x}', t)$.

Let us also remark that the equation of motion (2.168) can be used directly to derive the n -body Schrödinger equation (2.91) once more in another way, by working with time-dependent field operators. As a function of time, an arbitrary state vector evolves as follows:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle. \quad (2.170)$$

Multiplying this by the basis bra-vectors

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \quad (2.171)$$

we obtain the time-dependent Schrödinger wave function

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \quad (2.172)$$

Inserting between each pair of $\hat{a}_{\mathbf{x}_\nu}$ -operators in (2.171) the trivial unit factors $\mathbf{1} = e^{-i\hat{H}t/\hbar} e^{i\hat{H}t/\hbar}$, each of these operators is transformed into the time-dependent field operators $\hat{\psi}(\mathbf{x}_\nu, t)$, and one has

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = \frac{1}{\sqrt{n!}} \langle 0 | e^{-i\hat{H}t/\hbar} \hat{\psi}(\mathbf{x}_n, t) \cdots \hat{\psi}(\mathbf{x}_1, t) | \psi(0) \rangle. \quad (2.173)$$

Using the zero-energy property (2.130) of the vacuum state, this becomes

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = \langle \mathbf{x}_1, \dots, \mathbf{x}_n; t | \psi(0) \rangle. \quad (2.174)$$

The bra-states arising from the application of the time-dependent field operators $\hat{\psi}(\mathbf{x}_i, t)$ to the vacuum state on the left

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, t) \cdots \hat{\psi}(\mathbf{x}_1, t), \quad (2.175)$$

define a new time-dependent basis

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n; t |, \quad (2.176)$$

with the property

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n; t | \psi(0) \rangle \equiv \langle \mathbf{x}_1, \dots, \mathbf{x}_n | \psi(t) \rangle. \quad (2.177)$$

If we apply to the states (2.175) the differential operator (2.169) and use the canonical equal-time commutation rules (2.138), we may derive once more that $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ obeys the Schrödinger equation (2.18).

The difference between the earlier way (2.98) of defining the wave function and the formula (2.174) is, of course, the second-quantized version of the difference between the Schrödinger and the Heisenberg picture for the ordinary quantum mechanical wave functions. In Eq. (2.98), the states $|\psi(t)\rangle$ are *time-dependent* but the basis ket vectors $\langle \mathbf{x}_1, \dots, \mathbf{x}_n |$ are not, and with them also the field operators $\hat{\psi}(\mathbf{x}, 0) = \hat{a}_{\mathbf{x}}$ generating them. In Eq. (2.174), on the contrary, the states $\langle \psi(0) |$ are *time-independent* (and may be called Heisenberg states), but the local basis bra states $\langle \mathbf{x}_1, \dots, \mathbf{x}_n; t |$ are not, and with them the field operators $\hat{\psi}(\mathbf{x}, t)$ generating them. Whatever representation we use, the n -body wave function $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n, t)$ remains the same and obeys the Schrödinger equation (2.18). The change of picture is relevant only for the operator properties of the many-particle description.

Certainly, there is also the possibility of changing the picture in the Schrödinger wave function $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$. But the associated unitary transformation would take place in another Hilbert space, namely in the space of square integrable functions of n arguments, where $\hat{p}$ and $\hat{x}$ are the differential operators $-i\hbar\partial_{\mathbf{x}}$ and $\mathbf{x}$.

When going through the proof that (2.174) satisfies the n -body Schrödinger equation (2.18), we realize that at no place do we need the assumption of time-independent potentials. Thus we can conclude that the canonical quantization scheme for the action (2.158) is valid for an arbitrary explicit time dependence of the potentials in the Hamiltonian operator $\hat{H}$ [see (2.5)]. It is always equivalent to the Schrödinger description for an arbitrary number of particles.

2.9 More General Creation and Annihilation Operators

In many applications it is possible to solve exactly the Schrödinger equation with only the one-body potential $V_1(\mathbf{x}; t)$. In these cases it is useful to employ, instead of the creation and annihilation operators of particles at a point, another equivalent set of such operators which refers, right away, to the corresponding eigenstates. We

do this by expanding the field operator into the complete set of solutions of the one-particle Schrödinger equation

$$\hat{\psi}(\mathbf{x}, t) = \sum_{\alpha} \psi_{E_{\alpha}}(\mathbf{x}, t) \hat{a}_{\alpha}. \quad (2.178)$$

If the one-body potential is time-independent and there is no two-body potential, the states have the time dependence

$$\psi_{E_{\alpha}}(\mathbf{x}, t) = \psi_{E_{\alpha}}(\mathbf{x}) e^{-iE_{\alpha}t/\hbar}. \quad (2.179)$$

The expansion (2.178) is inverted to give

$$\hat{a}_{\alpha} = \int d^3x \psi_{E_{\alpha}}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t), \quad (2.180)$$

which we shall write shorter in a scalar-product notation as

$$\hat{a}_{\alpha} = (\psi_{E_{\alpha}}(t), \hat{\psi}(t)). \quad (2.181)$$

As opposed to the Dirac bracket notation to denote basis-independent scalar products, the parentheses indicate more specifically a scalar product between spatial wave functions.

From the commutation rules (2.138) we find that the new operators $\hat{a}_{\alpha}, \hat{a}_{\alpha}^{\dagger}$ satisfy the commutation rules

$$\begin{aligned} [\hat{a}_{\alpha}, \hat{a}_{\alpha'}] &= [\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha'}^{\dagger}] = 0, \\ [\hat{a}_{\alpha}, \hat{a}_{\alpha'}^{\dagger}] &= \delta_{\alpha, \alpha'}. \end{aligned} \quad (2.182)$$

Inserting (2.178) into (2.139) with $V_2 = 0$, we may use the orthonormality relation among the one-particle states $\psi_{E_{\alpha}}(\mathbf{x})$ to find the field operator representation for the Hamilton operator

$$\hat{H} = \sum_{\alpha} E_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}. \quad (2.183)$$

The eigenstates of the time-independent Schrödinger equation

$$\hat{H}|\psi(t)\rangle = E|\psi(t)\rangle \quad (2.184)$$

are now

$$|n_1, \dots, n_n\rangle = \frac{1}{\sqrt{n_1! \dots n_n!}} (\hat{a}_{\alpha_1}^{\dagger})^{n_1} \dots (\hat{a}_{\alpha_k}^{\dagger})^{n_k} |0\rangle, \quad (2.185)$$

where the prefactor ensures the proper normalization. The energy is

$$E = \sum_{i=1}^k E_{\alpha_i} n_i. \quad (2.186)$$

Finally, by forming the scalar products

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} (\hat{a}_{\alpha_1}^{\dagger})^{n_1} \dots (\hat{a}_{\alpha_k}^{\dagger})^{n_k} | 0 \rangle \frac{1}{\sqrt{n_1! \dots n_k!}}, \quad (2.187)$$

we recover precisely the symmetrized wave functions (2.32) with the normalization factors (2.41).

Similar considerations are, of course, possible in the Heisenberg picture of the operators $\hat{a}_\alpha^\dagger, \hat{a}_\alpha$ which can be obtained from

$$\hat{a}_\alpha(t) = \int d^3x \psi_{E_\alpha}^*(\mathbf{x}) \hat{\psi}(\mathbf{x}, t). \quad (2.188)$$

In the field operator description of many-body systems, the Schrödinger wave function $\psi(\mathbf{x}, t)$ has become a canonically quantized field object. Observe that the field $\psi(\mathbf{x}, t)$ by itself contains all relevant quantum mechanical information of the system via the derivative terms of the action (2.158),

$$\hat{\psi}^\dagger(\mathbf{x}, t) i\hbar \partial_t \hat{\psi}(\mathbf{x}, t) + \frac{\hbar^2}{2M} \hat{\psi}^\dagger(\mathbf{x}, t) \partial_{\mathbf{x}}^2 \hat{\psi}(\mathbf{x}, t). \quad (2.189)$$

This fixes the relation between wavelength and momentum, and between frequency and energy. The field quantization which introduces the additional processes of particle creation and annihilation is distinguished from this and often referred to as *second quantization*.

It should be kept in mind that, for a given n -body system, second quantization is completely equivalent and does not go beyond the usual n -body Schrödinger theory. It merely introduces the technical advantage of collecting the wave equations for any particle number n in a single operator representation. This advantage is, nevertheless, of great use in treating systems with many identical particles. In the limit of large particle densities, it gives rise to approximations which would be very difficult to formulate in the Schrödinger formulation. In particular, collective excitations of many-particle systems find their easiest explanation in terms of a quantum field formulation.

The full power of quantum fields, however, will unfold itself when trying to explain the physics of relativistic particles, where the number of particles is no longer conserved. Since the second-quantized Hilbert space contains any number of particles, the second-quantized formulation allows naturally for the description of the emission and absorption of fundamental particles, processes which the Schrödinger equation is unable to deal with.

2.10 Quantum Field Formulation of Many-Fermion Schrödinger Equations

The question arises whether an equally simple formalism can be found which automatically leads to the correct antisymmetric many-particle states

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}} \sum_P \epsilon_P |\mathbf{x}_{p(1)}\rangle \otimes \dots \otimes |\mathbf{x}_{p(n)}\rangle. \quad (2.190)$$

This is indeed possible. Let us remember that the symmetry of the wave functions was a consequence of the commutativity of the operators $\hat{\psi}(\mathbf{x}, t)$ for different position

values $\mathbf{x}$. Obviously, we can achieve an antisymmetry in the coordinates by forming product states

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}} \hat{a}_{\mathbf{x}_1}^\dagger \cdots \hat{a}_{\mathbf{x}_n}^\dagger |0\rangle \quad (2.191)$$

and requiring anticommutativity of the particle creation and annihilation operators:

$$\{\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}'}^\dagger\} = 0, \quad \{\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\} = 0. \quad (2.192)$$

The curly brackets denote the anticommutator defined in Eq. (2.110). To define a closed algebra, we require in addition, by analogy with the third commutation rule (2.75) for bosons, the anticommutation rule

$$\{\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}^\dagger\} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.193)$$

As in the bosonic case we introduce a vacuum state $|0\rangle$ which is normalized as in (2.87) and contains no particle [cf. (2.86)]:

$$\hat{a}_{\mathbf{x}}|0\rangle = 0, \quad \langle 0|\hat{a}_{\mathbf{x}}^\dagger = 0. \quad (2.194)$$

The anticommutation rules (2.192) have the consequence that each point can at most be occupied by a single particle. Indeed, applying the creation operator twice to the vacuum state yields zero:

$$\hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}^\dagger |0\rangle = \{\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}}^\dagger\} |0\rangle - \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}^\dagger |0\rangle = 0. \quad (2.195)$$

This guarantees the validity of the *Pauli exclusion principle*.

The properties (2.192), (2.193), and (2.194) are sufficient to derive the many-body Schrödinger equations with two-body interactions for an arbitrary number of fermionic particles. It is easy to verify that the second-quantized Hamiltonian has the same form as in Eq. (2.129). The proof proceeds along the same line as in the symmetric case, Eqs. (2.94)–(2.129). A crucial tool is the operator chain rule (2.111) derived for anticommutators. The minus sign, by which anticommutators differ from commutators, cancels out in all relevant equations.

As for bosons we define a time-dependent quantum field for fermions in the Heisenberg picture as

$$\begin{aligned} \hat{\psi}(\mathbf{x}, t) &= e^{i\hat{H}t/\hbar} \hat{\psi}(\mathbf{x}, 0) e^{-i\hat{H}t/\hbar} \\ &= e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{x}} e^{-i\hat{H}t/\hbar}, \end{aligned} \quad (2.196)$$

and find equal-time anticommutation rules of the same type as the commutation relations (2.138):

$$\begin{aligned} \{\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)\} &= 0, \\ \{\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)\} &= 0, \\ \{\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)\} &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (2.197)$$

The Hamiltonian has again the form Eq. (2.139).

There is only one place where the fermionic case is not completely analogous to the bosonic one: The second-quantized formulation cannot be derived from a standard canonical formalism of an infinite number of generalized coordinates. The standard formalism of quantum mechanics applies only to true physical canonical coordinates $p(t)$ and $q(t)$, and these can never account for anticommuting properties of field variables.² Thus an identification analogous to (2.144),

$$\hat{p}_{\mathbf{x}}(t) \equiv \hat{\psi}_I(\mathbf{x}, t), \quad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x}, t), \quad (2.198)$$

is at first impossible.

The canonical formalism may nevertheless be generalized appropriately. We may start out with exactly the same classical Lagrangian as in the boson case, Eq. (2.158), but treat the fields formally as anticommuting objects, i.e.,

$$\psi(\mathbf{x}, t)\psi(\mathbf{x}', t') = -\psi(\mathbf{x}', t')\psi(\mathbf{x}, t). \quad (2.199)$$

In mathematics, such objects are called *Grassmann variables*. Using these, we define again classical canonical momenta

$$p_{\mathbf{x}}(t) \equiv \frac{\delta L}{\delta \dot{\psi}(\mathbf{x}, t)} = -i\hbar\psi^\dagger(\mathbf{x}, t) \equiv \pi(\mathbf{x}, t). \quad (2.200)$$

Together with the field variable $q_{\mathbf{x}}(t) = \psi^\dagger(\mathbf{x}, t)$, this is postulated to satisfy the canonical anticommutation rule

$$\{p_{\mathbf{x}}(t), q_{\mathbf{x}'}(t)\} = -i\hbar\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.201)$$

2.11 Free Nonrelativistic Particles and Fields

An important way to approach interacting theories is based on perturbative methods. Usually, these begin with the free theory and prescribe how to calculate successive corrections due to the interaction energies. A detailed discussion of how and when this works will be given later. It seems intuitively obvious, however, that at least for weak interactions, the free theory may be a good starting point for an approximation scheme. It is therefore worthwhile to study a few properties of the free theory in detail.

The free-field action is, according to Eqs. (2.158) and (2.139) for $V_1(\mathbf{x}) = 0$ and $V_2(\mathbf{x} - \mathbf{x}') = 0$:

$$\mathcal{A} = \int dt d^3x \psi^*(\mathbf{x}, t) \left[i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 \right] \psi(\mathbf{x}, t). \quad (2.202)$$

²For a detailed discussion of classical mechanics with supersymmetric Lagrange coordinates see A. Kapka, *Supersymmetrie*, Teubner, 1997.

The quantum field $\hat{\psi}(\mathbf{x}, t)$ satisfies the field operator equation

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)\hat{\psi}(\mathbf{x}, t) = 0, \quad (2.203)$$

with the conjugate field satisfying

$$\hat{\psi}^\dagger(x, t) \left(-i\hbar \overleftarrow{\partial}_t + \frac{\hbar^2}{2M} \overleftarrow{\partial}_{\mathbf{x}}^2\right) = 0. \quad (2.204)$$

The equal-time commutation rules for bosons and fermions are

$$\begin{aligned} [\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)]_{\mp} &= 0, \\ [\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp} &= 0, \\ [\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp} &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \end{aligned} \quad (2.205)$$

where we have denoted commutator and anticommutator collectively by $[\dots, \dots]_{\mp}$, respectively.

In a finite volume V , the solutions of the free one-particle Schrödinger equation are given by the time-dependent version of the plane wave functions (1.185) [compare (2.179)]:

$$\psi_{\mathbf{p}^m}(\mathbf{x}, t) = \langle \mathbf{x}, t | \mathbf{p}^m \rangle = \langle \mathbf{x}, t | \hat{a}_{\mathbf{p}^m}^\dagger \rangle = \frac{1}{\sqrt{V}} \exp \left\{ \frac{i}{\hbar} \left(\mathbf{p}^m \mathbf{x} - \frac{\mathbf{p}^{m2}}{2M} t \right) \right\}. \quad (2.206)$$

These are orthonormal in the sense

$$\int d^3x \psi_{\mathbf{p}^m}^*(\mathbf{x}, t) \psi_{\mathbf{p}^{m'}}(\mathbf{x}, t) = \delta_{\mathbf{p}^m, \mathbf{p}^{m'}}, \quad (2.207)$$

and complete, implying that

$$\sum_{\mathbf{p}^m} \psi_{\mathbf{p}^m}(\mathbf{x}, t) \psi_{\mathbf{p}^m}^*(\mathbf{x}', t) = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.208)$$

As in Eq. (2.178), we now expand the field operator in terms of these solutions as

$$\hat{\psi}(\mathbf{x}, t) = \sum_{\mathbf{p}^m} \psi_{\mathbf{p}^m}(\mathbf{x}, t) \hat{a}_{\mathbf{p}^m}. \quad (2.209)$$

This expansion is inverted with the help of the scalar product (2.181) as

$$\hat{a}_{\mathbf{p}^m} = (\psi_{\mathbf{p}^m}(t), \hat{\psi}(t)) = \int d^3x \psi_{\mathbf{p}^m}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t). \quad (2.210)$$

In the sequel we shall usually omit the superscript of the momenta $\mathbf{p}^m$ if their discrete nature is evident from the context. The operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$, obey the canonical commutation rules corresponding to Eq. (2.182):

$$\begin{aligned} [\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}]_{\mp} &= 0, \\ [\hat{a}_{\mathbf{p}}^\dagger, \hat{a}_{\mathbf{p}'}^\dagger]_{\mp} &= 0, \\ [\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}^\dagger]_{\mp} &= \delta_{\mathbf{p}\mathbf{p}'}, \end{aligned} \quad (2.211)$$

where we have used the modified δ -functions introduced in Eq. (1.196).

In an infinite volume, we use the time-dependent version of the continuous wave functions (1.195)

$$\psi_{\mathbf{p}}(\mathbf{x}, t) = \langle \mathbf{x}, t | \mathbf{p} \rangle = \langle \mathbf{x}, t | \hat{a}_{\mathbf{p}}^\dagger \rangle = \frac{1}{\sqrt{V}} \exp \left\{ \frac{i}{\hbar} \left(\mathbf{p}^m \mathbf{x} - \frac{\mathbf{p}^{m2}}{2M} t \right) \right\}, \quad (2.212)$$

which are orthonormal in the sense

$$\begin{aligned} \int d^3x \psi_{\mathbf{p}}^*(\mathbf{x}, t) \psi_{\mathbf{p}'}(\mathbf{x}, t) &= (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}') \\ &\equiv \delta^{(3)}(\mathbf{p} - \mathbf{p}'), \end{aligned} \quad (2.213)$$

and complete, as expressed by

$$\int \frac{d^3p}{(2\pi\hbar)^3} \psi_{\mathbf{p}}(\mathbf{x}, t) \psi_{\mathbf{p}}^*(\mathbf{x}', t) \equiv \int d^3p \psi_{\mathbf{p}}(\mathbf{x}, t) \psi_{\mathbf{p}}^*(\mathbf{x}', t) = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (2.214)$$

In terms of these continuum wave functions, we expand the field operator as

$$\hat{\psi}(\mathbf{x}, t) = \int d^3p \psi_{\mathbf{p}}(\mathbf{x}, t) \hat{a}(\mathbf{p}), \quad (2.215)$$

and have the inverse

$$\hat{a}(\mathbf{p}) = (\psi_{\mathbf{p}}(t), \hat{\psi}(t)) = \int d^3x \psi_{\mathbf{p}}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t). \quad (2.216)$$

The discrete-momentum operators $\hat{a}_{\mathbf{p}}$, and $\hat{a}_{\mathbf{p}}^\dagger$ and the continuous ones $\hat{a}(\mathbf{p})$ and $\hat{a}^\dagger(\mathbf{p})$, are related by [recall Eq. (1.190)]

$$\hat{a}(\mathbf{p}) = \sqrt{V} \hat{a}_{\mathbf{p}}, \quad \hat{a}^\dagger(\mathbf{p}) = \sqrt{V} \hat{a}_{\mathbf{p}}^\dagger. \quad (2.217)$$

For the continuous-momentum operators $\hat{a}(\mathbf{p})$ and $\hat{a}(\mathbf{p})^\dagger$, the canonical commutation rules in Eq. (2.182) take the form

$$\begin{aligned} [\hat{a}(\mathbf{p}), \hat{a}(\mathbf{p}')]_{\mp} &= [\hat{a}^\dagger(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')]_{\mp} = 0, \\ [\hat{a}(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')]_{\mp} &= \delta^{(3)}(\mathbf{p} - \mathbf{p}'). \end{aligned} \quad (2.218)$$

The time-independent many-particle states are obtained, as in (2.185), by repeatedly applying any number of creation operators $\hat{a}_{\mathbf{p}}^\dagger$ [or $\hat{a}^\dagger(\mathbf{p})$] to the vacuum state $|0\rangle$, thus creating states

$$|n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \dots, n_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A} (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \dots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} |0\rangle, \quad (2.219)$$

where the normalization factor is determined as in Eq. (2.185). For bosons with $n_{\mathbf{p}_1}$ identical states of momentum $\mathbf{p}_1$, with $n_{\mathbf{p}_2}$ identical states of momentum $\mathbf{p}_2$, etc., the normalization factor is

$$\mathcal{N}^S = \frac{1}{\sqrt{n_{\mathbf{p}_1}! \dots n_{\mathbf{p}_k}!}}. \quad (2.220)$$

The same formula can be used for fermions, only that then the values of $n_{\mathbf{p}_i}$ are restricted to 0 or 1, and the normalization constant $\mathcal{N}^A$ is equal to 1. The time-independent wave functions are obtained as

$$\begin{aligned} \langle \mathbf{x}_1, \dots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \dots, n_{\mathbf{p}_k} \rangle^{S,A} &= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \\ &\times \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \cdots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} | 0 \rangle, \end{aligned} \quad (2.221)$$

and the time-dependent ones as

$$\begin{aligned} \langle \mathbf{x}_1, \dots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \dots, n_{\mathbf{p}_k}; t \rangle^{S,A} &= \langle \mathbf{x}_1, \dots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \dots, n_{\mathbf{p}_k} \rangle^{S,A} e^{-iEt/\hbar} \\ &= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) e^{-i\hat{H}t/\hbar} (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \cdots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} | 0 \rangle \\ &= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) [\hat{a}_{\mathbf{p}_1}^\dagger(t)]^{n_{\mathbf{p}_1}} \cdots [\hat{a}_{\mathbf{p}_k}^\dagger(t)]^{n_{\mathbf{p}_k}} | 0 \rangle, \end{aligned}$$

with the time-dependent creation operators being defined by

$$\hat{a}_{\mathbf{p}}^\dagger(t) \equiv e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{p}}^\dagger e^{-i\hat{H}t/\hbar}. \quad (2.222)$$

The energy of these states is

$$E = \sum_{i=1}^k n_i \varepsilon_{\mathbf{p}_i}, \quad (2.223)$$

where $\varepsilon_{\mathbf{p}} \equiv \mathbf{p}^2/2M$ are the energies of the single-particle wave functions (2.212). The many-body states (2.219) form the so-called *occupation number basis* of the Hilbert space. For fermions, n_i can only be 0 or 1, due to the anticommutativity of the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ among themselves. The basis states are properly normalized:

$$\langle n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \cdots n_{\mathbf{p}_k} | n'_{\mathbf{p}_1} n'_{\mathbf{p}_2} n'_{\mathbf{p}_3} \cdots n'_{\mathbf{p}_k} \rangle = \delta_{n_{\mathbf{p}_1} n'_{\mathbf{p}_1}} \delta_{n_{\mathbf{p}_2} n'_{\mathbf{p}_2}} \delta_{n_{\mathbf{p}_3} n'_{\mathbf{p}_3}} \cdots \delta_{n_{\mathbf{p}_k} n'_{\mathbf{p}_k}}. \quad (2.224)$$

They satisfy the completeness relation:

$$\sum_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3 \cdots} \sum_{n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \cdots n_{\mathbf{p}_k}} | n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \cdots n_{\mathbf{p}_k} \rangle \langle n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \cdots n_{\mathbf{p}_k} | = 1^{S,A}, \quad (2.225)$$

where the unit operator on the right-hand side covers only the physical Hilbert space of symmetric or antisymmetric n -body wave functions.

2.12 Second-Quantized Current Conservation Law

In Subsection 1.3.4 of Chapter 1 we have observed an essential property for the probability interpretation of the Schrödinger wave functions: The probability current density (1.107) and the probability density (1.108) are related by the *local conservation law* (1.109):

$$\partial_t \rho(\mathbf{x}, t) = -\nabla \cdot \mathbf{j}(\mathbf{x}, t). \quad (2.226)$$

This followed directly from the Schrödinger equation (2.169). Since the same equation holds for the field operators, i.e., with $\psi^*(\mathbf{x}', t)$ replaced by $\hat{\psi}^\dagger(\mathbf{x}', t)$, the field operators of charge and current density,

$$\begin{aligned}\hat{\rho}(\mathbf{x}, t) &= \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t), \\ \hat{\mathbf{j}}(\mathbf{x}, t) &= -i\frac{\hbar}{2M}\hat{\psi}^\dagger(\mathbf{x}, t)\overleftrightarrow{\nabla}\hat{\psi}(\mathbf{x}, t)\end{aligned}\quad (2.227)$$

satisfy the same relation. When integrating (2.226) over all $\mathbf{x}$, and using Green's theorem as done in Eq. (1.110), we obtain a *global conservation law* that ensures the time independence of the particle number operator

$$\hat{N} = \int d^3x \hat{\rho}(\mathbf{x}, t) = \int d^3x \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t). \quad (2.228)$$

Since this is time-independent, we can use (2.134) to rewrite

$$\hat{N} = \int d^3x \hat{\rho}(\mathbf{x}, 0) = \int d^3x \hat{\psi}^\dagger(\mathbf{x}, 0)\hat{\psi}(\mathbf{x}, 0) = \int d^3x \hat{a}_\mathbf{x}^\dagger \hat{a}_\mathbf{x}, \quad (2.229)$$

so that $\hat{N}$ coincides with the particle number operator (2.78). The original form (2.228) is the Heisenberg picture of the particle number operator, which coincides with (2.229), since the particle number is conserved.

2.13 Free-Particle Propagator

The perturbation theory of interacting fields to be developed later in Chapter 10 requires knowledge of an important free-field quantity called the *free-particle propagator*. It is the vacuum expectation of the time-ordered product of two free field operators. As we shall see, the calculation of any observable quantities can be reduced to the calculation of some linear combination of products of free propagators [see Section 7.17.1]. Let us first extend the definition (1.249) of the time-ordered product of n time-dependent operators to allow for fermion field operators. Suppose that the times in an operator product $\hat{A}_n(t_n) \cdots \hat{A}_1(t_1)$ have an order

$$t_{i_n} > t_{i_{n-1}} > \cdots > t_{i_1}. \quad (2.230)$$

Then the time-ordered product of the operators is defined by

$$\hat{T}\hat{A}_n(t_n) \cdots \hat{A}_1(t_1) \equiv \epsilon_P \hat{A}_{i_n}(t_{i_n}) \cdots \hat{A}_{i_1}(t_{i_1}). \quad (2.231)$$

With respect to the definition (1.250), the right hand side carries a sign factor $\epsilon_P = \pm 1$ depending on whether an even or an odd permutation P of the fermion field operators is necessary to reach the time-ordered form. For bosons, $\epsilon_P \equiv 1$.

The definition of the time-ordered products can be given more concisely using the Heaviside function $\Theta(t)$ of Eq. (1.313).

For two operators, we have

$$\hat{T}\hat{A}(t_1)\hat{B}(t_2) = \Theta(t_1 - t_2)\hat{A}(t_1)\hat{B}(t_2) \pm \Theta(t_2 - t_1)\hat{B}(t_2)\hat{A}(t_1), \quad (2.232)$$

with the upper and lower sign applying to bosons and fermions, respectively. The free-particle propagator can now be constructed from the field operators as the vacuum expectation value

$$G(\mathbf{x}, t; \mathbf{x}', t') = \langle 0 | \hat{T} \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle. \quad (2.233)$$

Applying the free-field operator equations (2.203) and (2.204), we notice a remarkable property: The free-particle propagator $G(\mathbf{x}, t; \mathbf{x}', t')$ coincides with the *Green function* of the Schrödinger differential operator. Recall that a Green function of a homogeneous differential equation is defined by being the solution of the inhomogeneous equation with a δ -function source (see Section 1.6). This property may easily be verified for the free-particle propagator, which satisfies the differential equations

$$\left(i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right) G(\mathbf{x}, t; \mathbf{x}', t') = i\hbar \delta(t - t') \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (2.234)$$

$$G(\mathbf{x}, t; \mathbf{x}', t') \left(-i\hbar \overleftarrow{\partial}_{t'} + \frac{\hbar^2}{2M} \overleftarrow{\partial}_{\mathbf{x}'}^2 \right) = i\hbar \delta(t - t') \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (2.235)$$

thus being a Green function of the free-particle Schrödinger equation: The right-hand side follows directly from the fact that the field $\hat{\psi}(\mathbf{x}, t)$ satisfies the Schrödinger equation and the obvious formula

$$\partial_t \Theta(t - t') = \delta(t - t'). \quad (2.236)$$

With the help of the chain rule of differentiation and Eq. (2.232), we see that

$$\begin{aligned} & \left(i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right) \langle 0 | \hat{T} \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle \\ &= i\hbar \left[\partial_t \Theta(t - t') \langle 0 | \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle \pm \partial_t \Theta(t' - t) \langle 0 | \hat{\psi}^\dagger(\mathbf{x}', t') \hat{\psi}(\mathbf{x}, t) | 0 \rangle \right] \\ &= i\hbar \delta(t - t') \langle 0 | [\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp} | 0 \rangle = i\hbar \delta(t - t') \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \end{aligned} \quad (2.237)$$

where the commutation and anticommutation rules (2.138) and (2.197) have been used, together with the unit normalization (2.87) of the vacuum state.

In the theory of differential equations, Green functions are introduced to find solutions for arbitrary inhomogeneous terms. These solutions may be derived from superpositions of δ -function sources. In quantum field theory, the same Green functions serve as propagators to solve inhomogeneous differential equations that involve *field operators*.

Explicitly, the free field propagator is calculated as follows: Since $\hat{\psi}(\mathbf{x}, t)$ annihilates the vacuum, only the first term in the defining Eq. (2.232) contributes, so that we can write

$$G(\mathbf{x}, t; \mathbf{x}', t') = \Theta(t - t') \langle 0 | \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle. \quad (2.238)$$

Inserting the expansion Eq. (2.215) with the wave functions (2.212), and using (2.218), the right-hand side becomes

$$\begin{aligned} \Theta(t-t') \int \tilde{d}^3p \, \tilde{d}^3p' \, e^{i[(\mathbf{p}\mathbf{x}-\mathbf{p}'\mathbf{x}')-(\mathbf{p}^2t/2M-\mathbf{p}'^2t'/2M)]/\hbar} \langle 0|\hat{a}(\mathbf{p})\hat{a}^\dagger(\mathbf{p}')|0\rangle \\ = \Theta(t-t') \int \tilde{d}^3p \, e^{i[\mathbf{p}(\mathbf{x}-\mathbf{x}')-\mathbf{p}^2(t-t')/2M]/\hbar}. \end{aligned} \quad (2.239)$$

By completing the square and using the Gaussian integral

$$\int \tilde{d}^3p \, e^{-ap^2/2\hbar} = \frac{1}{\sqrt{2\pi\hbar a}}^3, \quad (2.240)$$

we find

$$\begin{aligned} G(\mathbf{x}, t; \mathbf{x}', t') &= \Theta(t-t') \frac{1}{\sqrt{2\pi i\hbar(t-t')/M}}^3 e^{iM(\mathbf{x}-\mathbf{x}')^2/2\hbar(t-t')} \\ &= G(\mathbf{x}-\mathbf{x}', t-t'). \end{aligned} \quad (2.241)$$

The right-hand side is recognized as the usual quantum-mechanical Green function of the free-particle Schrödinger equation of Eq. (1.350). Indeed, the factor after $\Theta(t-t')$ is simply the one-particle matrix element of the time evolution operator

$$\begin{aligned} \langle 0|\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle &= \langle 0|\hat{\psi}(\mathbf{x})e^{-i\hat{H}(t-t')/\hbar}\hat{\psi}^\dagger(\mathbf{x}')|0\rangle \\ &= \langle \mathbf{x}|\hat{U}(t, t')|\mathbf{x}'\rangle. \end{aligned} \quad (2.242)$$

This is precisely the expression discussed in Eqs. (1.310)–(1.312). It describes the probability amplitude that a single free particle has propagated from $\mathbf{x}$ to $\mathbf{x}'$ in the time $t-t' > 0$. For $t-t' < 0$, G vanishes.

There exists a more useful way of writing the Fourier representation of the propagator than that in Eq. (2.239). It is based on the integral representation (1.319) of the Heaviside function:

$$\Theta(t-t') = \int_{-\infty}^{\infty} dE \, e^{-iE(t-t')/\hbar} \frac{i\hbar}{E+i\eta}. \quad (2.243)$$

As discussed in general in Eqs. (1.317)–(1.319), the $i\eta$ in the denominator ensures the causality. For $t > t'$, the contour of integration can be closed by an infinite semicircle below the energy axis, thereby picking up the pole at $E = -i\eta$, so that we obtain by the residue theorem

$$\Theta(t-t') = 1, \quad t > t'. \quad (2.244)$$

For $t < t'$, on the other hand, the contour may be closed above the energy axis and, since there is no pole in the upper half-plane, we have

$$\Theta(t-t') = 0, \quad t < t'. \quad (2.245)$$

Relation (2.243) can be generalized to

$$\Theta(t - t')e^{-iE_0(t-t')/\hbar} = \int_{-\infty}^{\infty} dE e^{-iE(t-t')/\hbar} \frac{i\hbar}{E - E_0 + i\eta}. \quad (2.246)$$

Using this with $E_0 = \mathbf{p}^2/2M$ we find from (2.239) the integral representation

$$G(\mathbf{x} - \mathbf{x}', t - t') = \int d^3p \int_{-\infty}^{\infty} dE e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar - iE(t-t')/\hbar} \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta}. \quad (2.247)$$

In this form we can trivially verify the equations of motion (2.234) and (2.235). This expression agrees, of course, with the quantum mechanical time evolution amplitude (1.344).

The Fourier-transformed propagator

$$\begin{aligned} G(\mathbf{p}, E) &= \int d^3x \int_{-\infty}^{\infty} dt e^{-i(\mathbf{p}\mathbf{x} - Et)/\hbar} G(\mathbf{x}, t) \\ &= \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta} \end{aligned} \quad (2.248)$$

has the property of being singular when the variable E is equal to a physical particle energy $E = \mathbf{p}^2/2M$. This condition is often called the *energy shell* condition. It is a general property of Green functions that their singularities in the energy-momentum variables display the spectra of the particles of the system.

2.14 Collapse of Wave Function

A related Green function can be used to illustrate the much discussed phenomenon of the *collapse of the wave function* in quantum mechanics [10]. If we create a particle at some time t' , we create a Schrödinger wave function that fills immediately the entire space. If we annihilate the particle at some later time t , the wave function disappears instantaneously from the entire space. This phenomenon which is hard to comprehend physically is obviously an artifact of the nonrelativistic Schrödinger theory. Let us see how it comes about in the formalism. If we measure the particle density at a time t'' that lies only slightly later than the later time t in the above Green function, we find

$$\begin{aligned} G(\mathbf{z}, t''; \mathbf{x}, t; \mathbf{x}', t') &= \langle 0 | \hat{T} \hat{\rho}(\mathbf{z}, t'') \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle \\ &= \langle 0 | \hat{T} \hat{\psi}^\dagger(\mathbf{z}, t'') \hat{\psi}(\mathbf{z}, t'') \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') | 0 \rangle. \end{aligned} \quad (2.249)$$

The second and the fourth field operators yield a time-ordered Green function $\langle \hat{T} \hat{\psi}(\mathbf{z}, t'') \hat{\psi}^\dagger(\mathbf{x}', t') \rangle = \Theta(t'' - t') G(\mathbf{z}, t''; \mathbf{x}', t')$, which is zero for $t'' > t'$. This is multiplied by the time-ordered Green function of the first and the third field operators which is $\langle \hat{T} \hat{\psi}^\dagger(\mathbf{z}, t'') \hat{\psi}(\mathbf{x}, t) \rangle = \Theta(t - t'') G(\mathbf{z}, t''; \mathbf{x}, t)$, and thus vanishes for $t'' > t$. Applying Wick's theorem to (2.249) shows that by the time t'' that is later than t and t' , the wave function created at the initial time t' has completely collapsed.

2.15 Quantum Statistics of Free Nonrelativistic Fields

2.15.1 Thermodynamic Quantities

Consider the grand-canonical partition function introduced in Eq. (1.493):

$$Z_G(T, \mu) = \text{Tr}(e^{-(\hat{H} - \mu \hat{N})/k_B T}). \quad (2.250)$$

The trace has to be taken over the complete set of basis states (2.219):

$$\sum_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3 \dots} \sum_{n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \dots n_{\mathbf{p}_k}} \langle n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \dots | e^{-(E_{n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \dots} - \mu \sum_i n_{\mathbf{p}_i})/k_B T} | n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \dots \rangle.$$

Using the additivity of the energies of all single-particle states found in Eq. (2.223), this can be written as an infinite product

$$Z_G(T, \mu) = \sum_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3 \dots} \sum_{n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \dots n_{\mathbf{p}_k}} e^{-(\frac{\mathbf{p}_1^2}{2M} - \mu)n_{\mathbf{p}_1}/k_B T} e^{-(\frac{\mathbf{p}_2^2}{2M} - \mu)n_{\mathbf{p}_2}/k_B T} e^{-(\frac{\mathbf{p}_3^2}{2M} - \mu)n_{\mathbf{p}_3}/k_B T} \dots \quad (2.251)$$

Each Boltzmann factor leads to the partition function associated with the available single-particle momentum $\mathbf{p}_1, \mathbf{p}_2, \dots$. The product is turned into a sum by taking the logarithm of this and considering the grand-canonical free energy

$$F_G(T, \mu) \equiv -k_B T \log Z_G(T, \mu) = -k_B T \sum_{\mathbf{p}} \log \sum_n e^{-(\frac{\mathbf{p}^2}{2M} - \mu)n/k_B T}. \quad (2.252)$$

We now distinguish between Bose and Fermi particles. In the first case, the occupation numbers n_i run over all integers 0, 1, 2, ... up to infinity:

$$\sum_{n=0}^{\infty} e^{-(\frac{\mathbf{p}^2}{2M} - \mu)n/k_B T} = \frac{1}{1 - e^{-(\frac{\mathbf{p}^2}{2M} - \mu)/k_B T}}. \quad (2.253)$$

In the second case, n_i can be only zero or one, so that

$$\sum_{n=0}^1 e^{-(\frac{\mathbf{p}^2}{2M} - \mu)n/k_B T} = 1 + e^{-(\frac{\mathbf{p}^2}{2M} - \mu)/k_B T}. \quad (2.254)$$

Thus we obtain

$$F_G(T, \mu) = \pm k_B T \sum_{\mathbf{p}} \log[1 \mp e^{-(\frac{\mathbf{p}^2}{2M} - \mu)/k_B T}]. \quad (2.255)$$

Because of the frequent appearance of the energy combination $\mathbf{p}^2/2M - \mu$, it will often be useful to define the quantity

$$\xi_{\mathbf{p}} = \frac{\mathbf{p}^2}{2M} - \mu = \varepsilon_{\mathbf{p}} - \mu. \quad (2.256)$$

This will abbreviate calculations in grand-canonical ensembles.

In a large volume, momentum states lie so close to each other that the sum may be approximately evaluated as an integral with the help of the limiting formula

$$\sum_{\mathbf{p}} \xrightarrow{V \rightarrow \infty} gV \int \frac{d^3p}{(2\pi\hbar)^3} = gV \int d^3p. \quad (2.257)$$

In writing this we have allowed for a degeneracy number g for each momentum state $\mathbf{p}$. It accounts for extra degrees of freedom of the particles in each momentum state. In the absence of internal quantum numbers, g counts the different spin polarization states. If s denotes the spin, then its third component can run from $-s$ to s so that

$$g = 2s + 1. \quad (2.258)$$

Moreover, the limit (2.257) is certainly valid only for sums over sufficiently smooth functions. We shall see in Section 2.15.3 that the limit fails for a Bose gas near $T = 0$, where the limit requires the more careful treatment in Eq. (2.337).

As an alternative to the momentum integral (2.257), we may integrate over the single-particle energies. With the energy $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/2M$, the relation between the integration measures is

$$\begin{aligned} \int d^3p &= \frac{4\pi}{(2\pi)^3\hbar^3} \int_0^\infty dp p^2 \\ &= \frac{1}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \int_0^\infty d\varepsilon \sqrt{\varepsilon} \equiv \int g_\varepsilon d\varepsilon. \end{aligned} \quad (2.259)$$

In the last expression we have introduced the quantity

$$g_\varepsilon \equiv \frac{1}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \sqrt{\varepsilon}, \quad (2.260)$$

which is the *density of states* per unit energy interval and volume. With the help of this quantity we may write (2.255) as an energy integral

$$F_G(T, \mu, V) = gV \int_0^\infty d\varepsilon g_\varepsilon F_\varepsilon(T, \mu), \quad (2.261)$$

where

$$F_\varepsilon(T, \mu) \equiv \pm k_B T \log[1 \mp e^{-(\varepsilon - \mu)/k_B T}] \quad (2.262)$$

is the grand-canonical free energy of an individual single-particle energy state.

According to the thermodynamic rule (1.502), the average particle number is found from the derivative of $F_G(T, \mu, V)$ with respect to the chemical potential. Using (2.255) or the integral representation (2.261), we find

$$\begin{aligned} N &= gV \sum_{\mathbf{p}} \frac{1}{e^{(\mathbf{p}^2/2M - \mu)/k_B T} \mp 1} = -gV \int_0^\infty d\varepsilon g_\varepsilon \frac{\partial}{\partial \mu} F_\varepsilon(T, \mu) \\ &\equiv gV \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon, \end{aligned} \quad (2.263)$$

where

$$f_\varepsilon \equiv -\frac{\partial}{\partial \mu} F_\varepsilon(T, \mu) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} \mp 1} \quad (2.264)$$

are the average Bose and Fermi occupation numbers of a level of energy ε , respectively. They are plotted in Figs. 2.1 and 2.2.

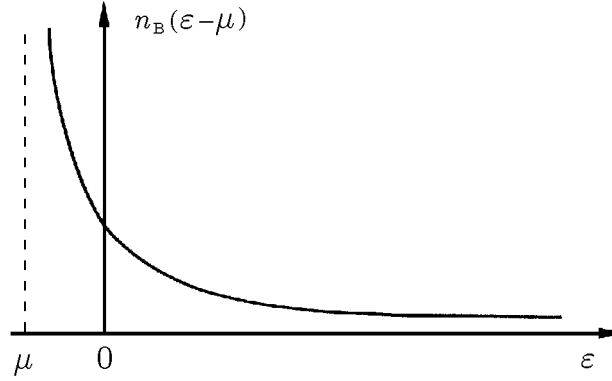


FIGURE 2.1 Average Bose occupation number $n_B(\varepsilon - \mu)$. Note that free bosons have a negative chemical potential μ .

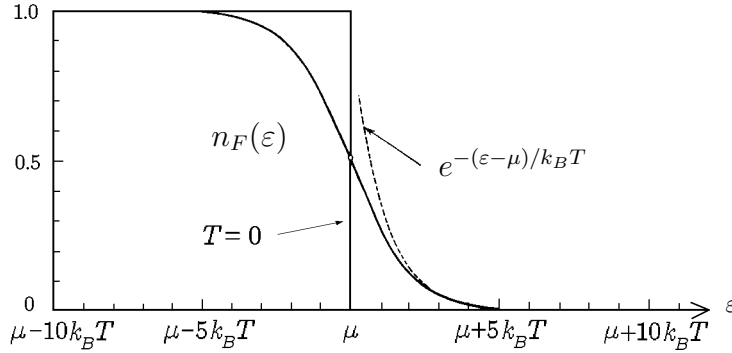


FIGURE 2.2 Average Fermi occupation number $n_F(\varepsilon)$. Fermions have a positive chemical potential μ .

The internal energy of the system can be calculated from the integral

$$\begin{aligned} E &= g \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon \varepsilon \\ &= g \frac{V}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{d\varepsilon \sqrt{\varepsilon} \varepsilon}{e^{(\varepsilon-\mu)/k_B T} \mp 1}. \end{aligned} \quad (2.265)$$

On the other hand, we find by a partial integration of the integral in (2.261):

$$\int_0^\infty d\varepsilon \varepsilon^{1/2} \log[e^{(\varepsilon-\mu)/k_B T} \mp 1] = -\frac{2}{3} \int_0^\infty \frac{d\varepsilon \varepsilon^{3/2}}{e^{(\varepsilon-\mu)/k_B T} \mp 1}, \quad (2.266)$$

so that the grand-canonical partition function can be rewritten as

$$F_G(T, \mu, V) = g \int_0^\infty d\varepsilon g_\varepsilon F_\varepsilon = -\frac{2}{3} g \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon \varepsilon. \quad (2.267)$$

This implies the general thermodynamic relation for a free Bose or Fermi gas:

$$F_G = -\frac{2}{3} E. \quad (2.268)$$

Recalling the definition of the pressure (1.527), we have thus found the *equation of state* for a free Bose or Fermi gas:

$$pV = \frac{2}{3} E. \quad (2.269)$$

To evaluate the energy integral, we introduce the variable $z \equiv \varepsilon/k_B T$ and write (2.263) as

$$N = N(T, \mu) \equiv g \frac{V}{\lambda^3(T)} \frac{1}{\Gamma(3/2)} I_{3/2}^\mp \left(\frac{\mu}{k_B T} \right), \quad (2.270)$$

where

$$\lambda(T) \equiv \frac{1}{\sqrt{2\pi\hbar^2/Mk_B T}} \quad (2.271)$$

is the *thermal length* associated with mass M and temperature T , and $I_n^\mp(\mu/k_B T)$ denotes the function

$$I_n^\mp(\alpha) \equiv \int_0^\infty dz \frac{z^{n-1}}{e^{z-\alpha} \mp 1}. \quad (2.272)$$

After expanding the denominator in a power series, each term can be integrated and leads for bosons to a series representation

$$I_n^-(\alpha) = \Gamma(n) \sum_{k=1}^\infty \frac{e^{k\alpha}}{k^n}. \quad (2.273)$$

The sum can be expressed in terms of the *polylogarithmic function* [8]³

$$\zeta_n(z) \equiv \sum_{k=1}^\infty \frac{z^k}{k^n} \quad (2.274)$$

as

$$I_n^-(\alpha) = \Gamma(n) \zeta_n(e^\alpha). \quad (2.275)$$

³A frequently used notation for $\zeta_n(z)$ is $\text{Li}_n(z)$.

The sum in (2.273) converges only for $\alpha < 0$. In the limit $\alpha \rightarrow -0$, it has the limit

$$I_n^-(0) = \Gamma(n)\zeta(n), \quad n > 1, \quad (2.276)$$

where $\zeta(n)$ is *Riemann's zeta function*

$$\zeta(\nu) \equiv \sum_{k=1}^{\infty} \frac{1}{k^\nu}. \quad (2.277)$$

For $n \leq 1$, the function $I_n^-(\alpha)$ diverges like $(-\alpha)^{n-1}$ in the limit $\alpha \rightarrow -0$. In the opposite limit $\alpha \rightarrow -\infty$, it goes to a constant:

$$I_n^-(\alpha) \rightarrow e^\alpha \Gamma(n). \quad (2.278)$$

This limit is needed to find the high-temperature behavior of the free Bose gas at a fixed average particle number N , as we see from Eq. (2.270). For large T , the ratio $\mu/k_B T$ diverges to $-\infty$.

In the case of fermions, the expansions (2.273), (2.275) read

$$I_n^+(\alpha) = \Gamma(n) \sum_{k=1}^{\infty} (-1)^{k-1} \frac{e^{k\alpha}}{k^n} = -\Gamma(n)\zeta_n(-e^\alpha), \quad (2.279)$$

the only difference with respect to bosons being the alternating signs in the sum. For $\alpha = 0$, this becomes

$$I_n^+(0) = \frac{1}{1} - \frac{1}{2^n} + \frac{1}{3^n} - \frac{1}{4^n} + \dots = \sum_{k=0}^{\infty} \frac{1}{k^n} - 2^{1-n} \sum_{k=0}^{\infty} \frac{1}{k^n} = (1 - 2^{1-n}) \zeta(n). \quad (2.280)$$

In the opposite limit $\alpha \rightarrow -\infty$, the sum yields the same constant as in (2.278):

$$I_n^+(\alpha) \rightarrow e^\alpha \Gamma(n). \quad (2.281)$$

At a fixed particle number N , the chemical potential changes with temperature in a way determined by the vanishing of the derivative of (2.270), which yields the equation

$$T \partial_T \frac{\mu}{k_B T} = -3 \frac{I_{3/2}^\mp(\frac{\mu}{k_B T})}{I_{1/2}^\mp(\frac{\mu}{k_B T})}. \quad (2.282)$$

Here we have used the property

$$\partial_z I_n^\mp(z) = (n-1) I_{n-1}^\mp(z), \quad (2.283)$$

which follows directly from the series expansion (2.273). For large T , we obtain from Eqs. (2.276) and (2.278) the limit

$$T \partial_T \frac{\mu}{k_B T} \xrightarrow{T \rightarrow \infty} -\frac{3}{2}. \quad (2.284)$$

Relation (2.269) can also be obtained from the general thermodynamic calculation:

$$E - \mu N = -Z_G^{-1} \frac{\partial Z_G}{\partial \beta} = \frac{\partial}{\partial \beta} \beta F_G, \quad (2.285)$$

which follows directly from (2.250) by differentiating with respect to $\beta = 1/k_B T$.

The grand-canonical free energy is from (2.267), using (2.260), (2.264), (2.271), and (2.272):

$$\begin{aligned} F_G(T, \mu, V) = -pV &= -g \frac{V}{\lambda^3(T)} k_B T \frac{2}{3} \frac{1}{\Gamma(3/2)} I_{5/2}^{\mp} \left(\frac{\mu}{k_B T} \right) \\ &= -N(T, \mu) k_B T \frac{2}{3} \frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \end{aligned} \quad (2.286)$$

For large T where $\alpha \rightarrow -\infty$, the limiting formula (2.278) shows that F_G has the correct Dulong-Petit-like behavior $-Nk_B T$, implying the *ideal-gas law*

$$pV = Nk_B T. \quad (2.287)$$

Due to the relation (2.268), the energy is

$$E = N(T, \mu) k_B T \frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \quad (2.288)$$

For large temperatures, this has the correct Dulong-Petit limit of free particles $3Nk_B T/2$.

We may check the first line in Eq. (2.286) by differentiating it with respect to μ and using the relation (2.283) to reobtain the thermodynamic relation $N = -\partial F_G / \partial \mu$.

According to Eq. (1.520), the entropy S is obtained from the negative derivative of (2.286) with respect to T . This yields

$$S = k_B g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_S^{\mp} \left(\frac{\mu}{k_B T} \right) = g k_B N(T, \mu) \frac{2}{3} \frac{I_S^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}, \quad (2.289)$$

where

$$I_S^{\mp}(\alpha) \equiv \frac{5}{2} I_{5/2}^{\mp}(\alpha) - \alpha I_{5/2}^{\mp}{}'(\alpha) = \frac{5}{2} I_{5/2}^{\mp}(\alpha) - \frac{3}{2} \alpha I_{3/2}^{\mp}(\alpha). \quad (2.290)$$

This agrees with the general thermodynamic relation

$$F_G(T, \mu) = E(T, \mu) - \mu N(T, \mu) - TS(T, \mu). \quad (2.291)$$

Adiabatic processes are defined by the condition $S/N = \text{const.}$ which implies by Eq. (2.290) that the ratio $\mu/k_B T$ is also a constant. Inserting this into (2.270) with (2.271) we find that, at a constant particle number, an adiabatic process satisfies

$$VT^{3/2}|_{\text{adiab}} = \text{const.} \quad (2.292)$$

Combining this with (2.287) leads to

$$pV^{5/3}|_{\text{adiab}} = \text{const.} \quad (2.293)$$

The specific heat at a constant volume and particle number is found from the entropy by forming the derivative $C_V = T\partial_T S$ of Eq. (2.289). Using (2.282), this leads to

$$C_V = gk_B N \frac{1}{2} \left[5 \frac{I_{5/2}^\mp(\alpha)}{I_{3/2}^\mp(\alpha)} - 9 \frac{I_{3/2}^\mp(\alpha)}{I_{1/2}^\mp(\alpha)} \right], \quad \alpha = \frac{\mu}{k_B T}. \quad (2.294)$$

For large T , we use (2.278) again to show that this becomes a constant

$$C_V \xrightarrow{T \rightarrow \infty} C_V^{\text{DP}} = g \frac{3}{2} N k_B, \quad (2.295)$$

which complies with the classical rule of Dulong and Petit ($k_B/2$ per degree of freedom).

2.15.2 Degenerate Fermi Gas Near $T = 0$

Consider the Fermi gas close to zero temperature which is called the *degenerate limit*. Then the occupation number (2.264) reduces to

$$f_\varepsilon = \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \quad \text{for} \quad \begin{Bmatrix} \varepsilon < \mu \\ \varepsilon > \mu \end{Bmatrix} = \Theta(\varepsilon - \mu). \quad (2.296)$$

All states with energy lower than μ are filled, all higher states are empty. The chemical potential μ at zero temperature is called Fermi energy ε_F :

$$\mu|_{T=0} \equiv \varepsilon_F. \quad (2.297)$$

The Fermi energy for a given particle number N is found from (2.260), (2.263), and (2.296):

$$N = gV \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon = gV \int_0^{\varepsilon_F} d\varepsilon g_\varepsilon = gV \frac{\sqrt{2} M^{3/2} \varepsilon_F^{3/2}}{3\pi^2 \hbar^3} = gV \frac{p_F^3}{6\pi^2 \hbar^3}, \quad (2.298)$$

where

$$p_F = \sqrt{2M\varepsilon_F} \equiv \hbar k_F \quad (2.299)$$

is the Fermi momentum associated with the Fermi energy. Equation (2.298) is solved for ε_F by

$$\varepsilon_F = \left(\frac{6\pi^2}{g} \right)^{2/3} \left(\frac{N}{V} \right)^{2/3} \frac{\hbar^2}{2M}, \quad (2.300)$$

and for the Fermi momentum by

$$p_F \equiv k_F \hbar = \left(\frac{6\pi^2}{g} \right)^{1/3} \left(\frac{N}{V} \right)^{1/3} \hbar. \quad (2.301)$$

In two dimensions, we find

$$\varepsilon_F = \frac{2\pi}{g} \frac{\rho}{M}. \quad (2.302)$$

Note that in terms of the particle number N , the density of states per unit energy interval and volume (2.260) can be written as

$$gg_\varepsilon \equiv \frac{3}{2} \frac{N}{V} \frac{1}{\varepsilon_F} \sqrt{\frac{\varepsilon}{\varepsilon_F}}. \quad (2.303)$$

As the gas is heated slightly, there is a softening of the degeneracy in the particle distribution (2.296). In order to study this quantitatively it is useful to define a characteristic temperature associated with the Fermi energy ε_F , the so-called *Fermi temperature*

$$T_F \equiv \frac{\varepsilon_F}{k_B} = \frac{1}{k_B} \frac{p_F^2}{2M} = \frac{\hbar^2}{k_B} \frac{k_F^2}{2M}. \quad (2.304)$$

For electrons in a metal, k_F is of the order of $1/\text{\AA}$. Inserting $M = m_e = 9.109558 \times 10^{-28}$ g, $k_B = 1.380622 \times 10^{-16}$ erg/K, and $\hbar = 6.0545919 \times 10^{-27}$ erg sec, we see that the order of magnitude of T_F is

$$T_F \approx 44\,000 \text{ K}. \quad (2.305)$$

Hence the relation

$$T/T_F \ll 1 \quad (2.306)$$

is quite well fulfilled even far above room temperature, and T/T_F can be used as an expansion parameter in evaluating the thermodynamic properties of the electron gas at nonzero temperature.

Let us do this to calculate the corrections to the above equations at small T . Eliminating the particle number in (2.270) in favor of the Fermi temperature with the help of Eqs. (2.298) and (2.304), we find the temperature dependence of the chemical potential from the equation

$$1 = \left(\frac{T}{T_F} \right)^{3/2} \frac{3}{2} I_{3/2}^+ \left(\frac{\mu}{k_B T} \right). \quad (2.307)$$

For $T \rightarrow 0$, the chemical potential μ approaches the Fermi energy ε_F , so that small T corresponds to a large reduced chemical potential $\bar{\mu} = \mu/k_B T$. Let us derive an expansion for $I_{3/2}^+(\bar{\mu})$ in powers of $1/\bar{\mu}$ in this regime. For this we set

$$z - \bar{\mu} \equiv x, \quad (2.308)$$

and write $I_n^+(\bar{\mu})$ as

$$I_n^+(\bar{\mu}) = \int_{-\bar{\mu}}^{\infty} dx \frac{(\bar{\mu} + x)^{n-1}}{e^x + 1} = \int_0^{\bar{\mu}} dx \frac{(\bar{\mu} - x)^{n-1}}{e^{-x} + 1} + \int_0^{\infty} dx \frac{(\bar{\mu} + x)^{n-1}}{e^x + 1}. \quad (2.309)$$

In the first integral on the right-hand side we substitute

$$\frac{1}{e^{-x} + 1} = 1 - \frac{1}{e^x + 1} \quad (2.310)$$

and obtain

$$I_n^+(\bar{\mu}) = \int_0^{\bar{\mu}} dx x^{n-1} + \int_0^{\infty} dx \frac{(\bar{\mu} + x)^{n-1} - (\bar{\mu} - x)^{n-1}}{e^x + 1} + \int_{\bar{\mu}}^{\infty} dx \frac{(\bar{\mu} - x)^{n-1}}{e^x + 1}. \quad (2.311)$$

In the limit $\bar{\mu} \rightarrow \infty$, only the first term survives, whereas the last term

$$L(\bar{\mu}) \equiv \int_{\bar{\mu}}^{\infty} dx \frac{(\bar{\mu} - x)^{n-1}}{e^x + 1} = -(-1)^n \int_0^{\infty} dx \frac{x^{n-1}}{e^{x+\bar{\mu}} + 1} = (-1)^n \Gamma(n) \zeta_n(-e^{-\bar{\mu}}) \quad (2.312)$$

is exponentially small, so that it can be ignored in an expansion in powers of $1/\bar{\mu}$. The second term is expanded as

$$2 \sum_{k=\text{odd}}^{\infty} \binom{n-1}{k} \bar{\mu}^{n-1-k} \int_0^{\infty} dx \frac{x^k}{e^x + 1} = 2 \sum_{k=\text{odd}} \frac{(n-1)!}{(n-1-k)!} \bar{\mu}^{n-1-k} (1 - 2^{-k}) \zeta(k+1). \quad (2.313)$$

At even positive and odd negative integer arguments, the zeta function is related to the Bernoulli numbers by⁴

$$\zeta(1-2n) = -\frac{B_{2n}}{2n}, \quad \zeta(2n) = \frac{(2\pi)^{2n}}{2(2n)!} |B_{2n}|. \quad (2.314)$$

The two equations go over into each other via the identity

$$\zeta(x) = 2^x \pi^{x-1} \sin(\pi x/2) \Gamma(1-x) \zeta(1-x), \quad (2.315)$$

which can also be written as

$$\zeta(x) = 2^{x-1} \pi^x \zeta(1-x) / \Gamma(x) \cos \frac{x\pi}{2}. \quad (2.316)$$

The lowest values of $\zeta(k+1)$ occurring in the expansions (2.313) are⁵

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad (2.317)$$

⁴These and the subsequent formulas are found in I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formulas 9.542 and 9.535.

⁵Other often-needed values are $\zeta(0) = -1/2$, $\zeta'(0) = -\log(2\pi)/2$, $\zeta(-2n) = 0$, $\zeta(3) \approx 1.202057$, $\zeta(5) \approx 1.036928$, ...

so that $I_n^+(\bar{\mu})$ starts out for large $\bar{\mu}$ like

$$I_n^+(\bar{\mu}) = \frac{1}{n}\bar{\mu}^n + 2(n-1)\frac{1}{2}\zeta(2)\bar{\mu}^{n-2} + 2(n-1)(n-2)(n-3)\frac{7}{8}\zeta(4)\bar{\mu}^{n-4} + \dots \quad (2.318)$$

Inserting this with $n = 3/2$ into Eq. (2.307), we find

$$1 = \left(\frac{T}{T_F}\right)^{3/2} \frac{3}{2} \left[\frac{2}{3} \left(\frac{\mu}{k_B T}\right)^{3/2} + \frac{\pi^2}{12} \left(\frac{\mu}{k_B T}\right)^{-1/2} + \frac{7\pi^4}{3 \cdot 320} + \left(\frac{\mu}{k_B T}\right)^{-5/2} \dots \right]. \quad (2.319)$$

From this we derive, by inversion, a small- T/T_F expansion of $\mu/k_B T$. Rewriting the latter ratio as a product $\mu/\varepsilon_F \times T_F/T$, we obtain for μ the series

$$\mu = \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_F}\right)^2 + \frac{7\pi^4}{720} \left(\frac{T}{T_F}\right)^4 + \dots \right]. \quad (2.320)$$

Only exponentially small terms in $e^{-T_F/T}$ coming from the integral $L(\bar{\mu})$ of (2.312) are ignored. Inserting the chemical potential (2.320) into the grand-canonical free energy F_G , we obtain by reexpanding the first line in (2.286):

$$F_G(T, \mu, V) = F_G(0, \mu, V) \left[1 + \frac{5\pi^2}{8} \left(\frac{T}{T_F}\right)^2 - \frac{7\pi^4}{384} \left(\frac{T}{T_F}\right)^4 + \dots \right], \quad (2.321)$$

where

$$F_G(0, \mu, V) \equiv -\frac{2}{5}gV \frac{\sqrt{2}M^{3/2}}{3\pi^2\hbar^3} \mu^{5/2} = -\frac{2}{5}gV \frac{k_\mu^3}{6\pi^2} \mu. \quad (2.322)$$

Here k_μ is the analog of k_F , to which it reduces for $T = 0$ [compare (2.299)]:

$$k_\mu \equiv \frac{1}{\hbar} \sqrt{2M\mu}. \quad (2.323)$$

At $T = 0$ where ε_F , we see from (2.299) that

$$F_G(0, \varepsilon_F, V) = -\frac{2}{5}N\varepsilon_F. \quad (2.324)$$

This can also be obtained from (2.286) using the limiting behavior (2.281).

By differentiating F_G with respect to the temperature at fixed μ , we obtain the low-temperature behavior of the entropy

$$S = k_B \frac{\pi^2}{2} \frac{T}{T_F} \frac{N}{V} + \dots, \quad (2.325)$$

and from this the specific heat

$$C_V = T \frac{\partial S}{\partial T} \Big|_{V,N} = k_B \frac{\pi^2}{2} N \frac{T}{T_F}. \quad (2.326)$$

This is a linear behavior with a slope C_V^{DP} of Eq. (2.295) associated with the high-temperature Dulong-Petit law:

$$C_V = C_V^{\text{DP}} \times \frac{\pi^2}{3g} \frac{T}{T_F}. \quad (2.327)$$

The linear growth is a characteristic feature of the electronic specific heat at low temperature sketched for all temperatures in Fig. 2.3. It is due to the progressive softening of the Fermi distribution with temperature, and this makes a linearly increasing number of electrons thermally excitable. This is directly observable experimentally in metals at low temperature. There the contribution of lattice vibrations are frozen out since they behave like $(T/T_D)^3$. The temperature T_D is the Debye temperature which characterizes the elastic stiffness of a crystal. It ranges typically from $T_D \approx 90$ K in soft metals like lead, over $T_D \approx 389$ K for aluminum, to $T_D \approx 1890$ K for diamonds. The measured experimental slope is usually larger than that for a free electron gas in (2.326). This can be explained mainly by the effect of the lattice which leads to an increased effective mass $M_{\text{eff}} > M$ of the electrons.

Note that the quantity $F_G(0, \mu, V)$ is temperature-dependent via the chemical potential μ . Inserting (2.320) into (2.321), we find the complete T -dependence

$$F_G(T, \mu, V) = F_G(0, \varepsilon_F, V) \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{k_B T}{\varepsilon_F} \right)^4 + \dots \right] \quad (2.328)$$

with $F_G(0, \varepsilon_F, V)$ given by Eq. (2.324) at $\mu = \varepsilon_F$.

Recalling the relation (2.268), the above equation supplies us also with the low-temperature behavior of the internal energy:

$$E = \frac{3}{5} N \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_F} \right)^4 + \dots \right]. \quad (2.329)$$

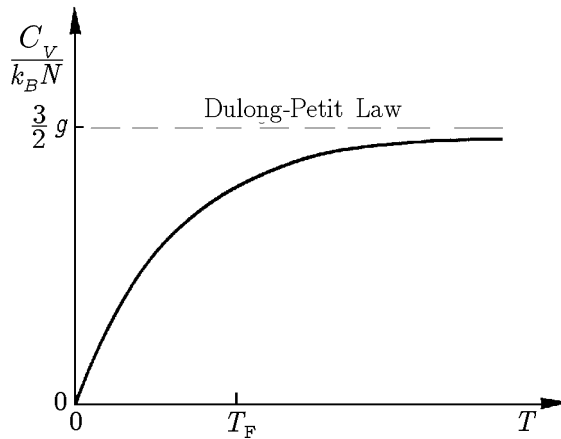


FIGURE 2.3 Temperature behavior of the specific heat of a free Fermi gas.

The first term is the energy of the zero-temperature Fermi sphere. Using the relation $C_V = \partial E / \partial T$, the second term yields once more the leading $T \rightarrow 0$ behavior (2.326) of the specific heat.

This behavior of the specific heat can be observed in metals where the conduction electrons behave like a free electron gas. Due to *Bloch's theorem*, a single electron in a perfect lattice behaves just like a free particle. For many electrons, this is still approximately true, if the mass of the electrons is replaced by an effective mass.

Another important macroscopic system, where the behavior (2.326) can be observed, is a liquid consisting of the fermionic isotope ^3He . There are two electron spins and an odd number of nucleon spins which make this atom a fermion. The atoms interact strongly in the liquid, but it turns out that these interactions produce a screening effect after which the system may be considered approximately as an almost-free gas of quasiparticles which behave like free fermions whose mass is about 8 times that of the strongly interacting atoms [10].

2.15.3 Degenerate Bose Gas Near $T = 0$

For bosons, the low-temperature discussion is quite different. As we can see from Eq. (2.263), the particle density remains positive for all $\varepsilon \in (0, \infty)$ only if the chemical potential μ is negative. A positive μ would also cause a divergence in the integrals (2.270), (2.272). At high temperatures, the chemical potential has a large negative value, which moves closer to zero as the temperature decreases (see Fig. 2.4, compare also with Fig. 2.1).

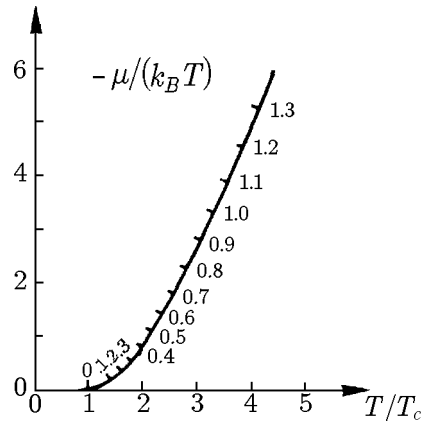


FIGURE 2.4 Temperature behavior of the chemical potential of a free Bose gas.

The chemical potential vanishes at a critical temperature T_c . From Eqs. (2.263), (2.270), and (2.276), this is determined by the equation

$$\begin{aligned} \frac{N}{V} &= g \int d^3p \frac{1}{e^{(\frac{p^2}{2M} - \mu)/k_B T} - 1} = g \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon \\ &= g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_{3/2}^- \left(\frac{\mu}{k_B T} \right), \end{aligned} \quad (2.330)$$

at $\mu = 0$, where it yields, via Eq. (2.276), the particle density

$$\frac{N}{V} = g \frac{V}{\lambda^3(T)} \zeta(3/2). \quad (2.331)$$

Thus the critical temperature T_c satisfies the equation

$$T_c = [g\zeta(3/2)]^{-2/3} \left(\frac{N}{V}\right)^{2/3} \frac{2\pi\hbar^2}{k_B M}, \quad (2.332)$$

with $\zeta(3/2) = 2.61238 \dots$.

It is interesting to rewrite this equation in natural variables. We may introduce an average distance a between the bosons by the relation $N/V \equiv 1/a^3$. There is an energy associated with it,

$$\varepsilon_a \equiv \frac{\hbar^2}{2Ma^2}, \quad (2.333)$$

and a temperature $T_a \equiv \varepsilon_a/k_B$. In these natural units, the critical temperature (2.332) of the free Bose gas is simply

$$T_c = [g\zeta(3/2)]^{-2/3} 4\pi T_a. \quad (2.334)$$

We may rewrite Eq. (2.330) in the form

$$1 = \left(\frac{T}{T_c}\right)^{3/2} \frac{I_{3/2}(\bar{\mu})}{I_{3/2}(0)}, \quad \bar{\mu} = \frac{\mu}{k_B T}. \quad (2.335)$$

For $\bar{\mu}$ between 0 and 1, this equation yields $T/T_c > 1$, while Eq. (2.294) gives us the associated specific heat. The result is displayed in Fig. 2.5. To understand the figure we must realize what happens in the regime of low temperatures $T < T_c$ where (2.270) has no solution.

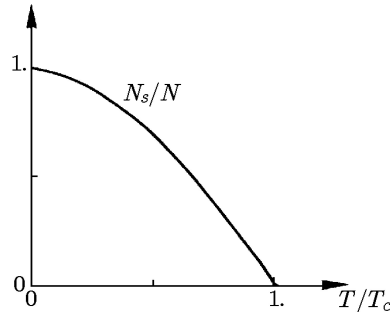


FIGURE 2.5 Temperature behavior of the fraction of zero-momentum bosons in a free Bose gas.

A glance at Eq. (2.331) shows that a phase transition takes place when the average distance a between atoms becomes smaller than the De Broglie wavelength of thermal motion (2.271). In natural units, this may be expressed as

$$\lambda(T) = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{T_a}{T}}. \quad (2.336)$$

For helium, this length scale has roughly the value $5.64 \text{ \AA}$.⁶

For $T < T_c$, Eq. (2.330) has no solution even though the physical system can be cooled further. The apparent contradiction has its origin in a failure of the integral approximation (2.257) to replace the sum over momenta for $T < T_c$. The reason is that the state with $\mathbf{p} = 0$ is not properly included in the energy integral over all states in Eq. (2.270). To avoid this we have to write more properly:

$$N = N_{\mathbf{p}=0} + N_{\mathbf{p} \neq 0} \equiv N_s + gV \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon|_{\mu=0}, \quad (2.337)$$

where $N_s \equiv N_{\mathbf{p}=0}$ is the number of Bose particles at zero momentum and energy. Below T_c , a finite fraction of all particles N_s/N accumulates in this single degenerate state. It can be calculated from the modified Eq. (2.330):

$$\begin{aligned} N - N_s &= Vg \int_0^\infty d\varepsilon g_\varepsilon f_\varepsilon|_{\mu=0} \\ &= g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_{3/2}^-(0) = N \left(\frac{T}{T_c} \right)^{3/2}. \end{aligned} \quad (2.338)$$

Thus we find that the number of degenerate bosons has the temperature behavior

$$N_s = N \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right], \quad (2.339)$$

which is plotted in Fig. 2.5.

The phenomenon of a macroscopic accumulation of particles in a single state is called *Bose condensation* and plays a central role in the understanding of the phenomenon of *superfluidity* in liquid helium consisting of the bosonic atoms of ^4He . In fact, the temperature T_c calculated from Eq. (2.332) is $T_c \sim 3.1 \text{ K}$, which is roughly of the same order as the experimental value⁷

$$T_c^{\text{exp}} \equiv 2.18 \text{ K}. \quad (2.340)$$

The discrepancy is due to the strong interactions between the ^4He atoms in the liquid state, which have all been neglected in deriving Eq. (2.340).

There exists a phenomenological two-fluid description of superfluidity in which the condensate of the $\mathbf{p} = \mathbf{0}$ -bosons is identified with the *superfluid component* of

⁶See p. 256 in the textbook Ref. [11].

⁷The mass density is $\rho \approx 0.145 \text{ g/cm}^3$. With the mass of the helium atoms being $M_{^4\text{He}} \approx 4m_p \approx 4 \times 1.6762 \times 10^{-24} \text{ g}$, this implies a volume per atom of $V/N \approx 46.2 \text{ \AA}^3$.

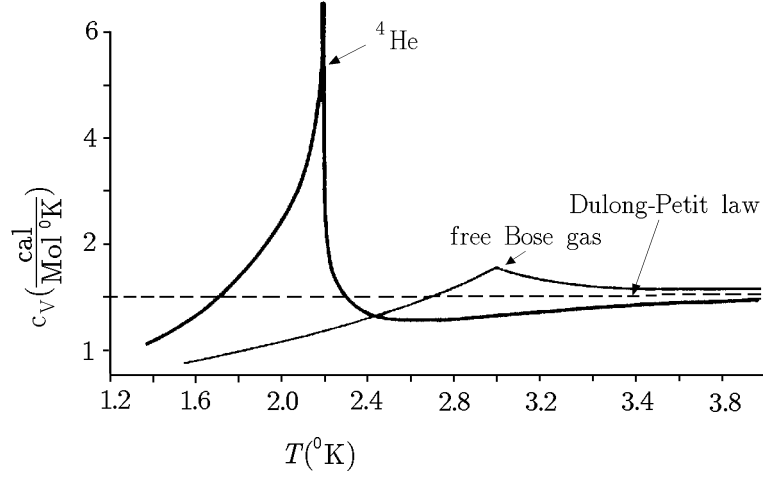


FIGURE 2.6 Temperature behavior of the specific heat of a free Bose gas. For comparison we show the specific heat of the strongly interacting Bose liquid ${}^4\text{He}$, scaled down by a factor of 2 to match the Dulong-Petit limit of the free Bose gas.

the liquid. This is the reason why we have used the subscript s in (2.338). The complementary piece

$$N_n = N - N_s \quad (2.341)$$

is usually referred to as the *normal component* of the superfluid.

For $T < T_c$, the energy of the normal liquid is equal to the total energy. Using Eq. (2.288) with $\mu = 0$ we obtain

$$\begin{aligned} E &= E_n = g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} k_B T I_{5/2}^-(0) = g \frac{I_{5/2}^-(0)}{I_{3/2}^-(0)} N k_B T \left(\frac{T}{T_c} \right)^{3/2} \\ &\approx g 0.7703 N k_B T \left(\frac{T}{T_c} \right)^{3/2} \equiv E_c \left(\frac{T}{T_c} \right)^{3/2}, \end{aligned} \quad (2.342)$$

where we have expressed $I_n^-(0)$ via Eq. (2.276). From this energy we derive the specific heat below T_c :

$$\begin{aligned} C_V &= T \left. \frac{\partial S}{\partial T} \right|_{V,N} = \left. \frac{\partial E}{\partial T} \right|_{V,N} \\ &= \frac{5}{2} \frac{E}{T} \propto T^{3/2}. \end{aligned} \quad (2.343)$$

Integrating this with respect to the temperature gives the entropy

$$S = \frac{5}{3} \frac{E}{T}, \quad (2.344)$$

and the free energy $F = E - TS$ takes the simple form

$$F = -\frac{2}{3} E. \quad (2.345)$$

This is consistent with the general relation (2.268), since for $\mu = 0$ the grand canonical free energy F_G coincides with the free energy F [recall the Euler relation (1.529)].

The special role of the Bose condensate lies in the fact that it provides the system with a particle reservoir, with the relation (2.270) being replaced by Eq. (2.330) and Eq. (2.338).

Inserting (2.342) into (2.343), the low-temperature behavior of the specific heat becomes explicitly

$$C_V = \frac{\partial E}{\partial T} = gk_B N \frac{5}{2} \frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)} \left(\frac{T}{T_c}\right)^{3/2} \approx gk_B N 1.92567 \left(\frac{T}{T_c}\right)^{3/2}. \quad (2.346)$$

Comparing (2.346) with (2.294) and using the fact that $I_{1/2}(0) = \infty$, we see that at T_c the peak in (2.346) has the same maximal value as in the $T > T_c$ -solution (since $I_{1/2}(0) = \infty$).

As T passes T_c , the chemical potential becomes negative. To calculate the behavior of $-\mu$ in this regime, we use Eq. (2.335), and replace $I_{3/2}^-(\bar{\mu})$ by $I_{3/2}^-(0) + \Delta I_{3/2}^-(\bar{\mu})$ with

$$\Delta I_{3/2}^-(\bar{\mu}) = \int_0^\infty dz z^{1/2} \left(\frac{1}{e^{z-\bar{\mu}} - 1} - \frac{1}{e^z - 1} \right). \quad (2.347)$$

This function receives its main contribution from $z \approx 0$, where it can be approximated by⁸

$$\Delta I_{3/2}^-(\bar{\mu}) \approx \bar{\mu} \int_0^\infty dz \frac{1}{z^{1/2}(z - \bar{\mu})} = -\pi\sqrt{-\bar{\mu}}. \quad (2.348)$$

Hence we obtain from (2.335) the relation

$$1 = \left(\frac{T}{T_c}\right)^{3/2} \left[1 + \frac{\Delta I_{3/2}^-(\frac{\mu}{k_B T})}{I_{3/2}^-(0)} \right]. \quad (2.349)$$

Inserting here the small- $\bar{\mu}$ behavior (2.348), we see that, for T slightly above T_c , the negative chemical potential $-\mu$ becomes nonzero behaving like

$$-\mu \approx \frac{1}{\pi^2} k_B T_c [I_{3/2}^-(0)]^2 \left[\left(\frac{T}{T_c}\right)^{3/2} - 1 \right]^2, \quad (2.350)$$

where $I_{3/2}^-(0)$ is given by Eq. (2.276).

Let us use this result to find the internal energy slightly above the critical temperature T_c . With the help of relation (2.268) we calculate the derivative of the energy with respect to the chemical potential as

$$\left. \frac{\partial E}{\partial \mu} \right|_{T,V} = -\frac{3}{2} \left. \frac{\partial F_G}{\partial \mu} \right|_{T,V} = \frac{3}{2} gN. \quad (2.351)$$

⁸In general, the small- $\bar{\mu}$ expansion of $I_\nu^-(\bar{\mu}) = \Gamma(\nu)\zeta_\nu(e^{\bar{\mu}})$ follows from the so-called *Robinson expansion*: $\zeta_\nu(e^{\bar{\mu}}) = \Gamma(1-\nu)\bar{\mu}^{\nu-1} + \zeta(\nu) + \sum_{k=1}^\infty (-\bar{\mu})^k \zeta(\nu-k)/k!$, derived in Subsec. 2.15.6 of the textbook in Ref. [1].

This allows us to find the internal energy slightly above the critical temperature T_c , where $-\mu$ is small, as

$$\begin{aligned} E &\approx E_c + \frac{3}{2}gN\mu \\ &= E_c - \frac{3}{2\pi^2}gNk_BT_c [I_{3/2}^-(0)]^2 \left[\left(\frac{T}{T_c} \right)^{3/2} - 1 \right]^2. \end{aligned} \quad (2.352)$$

Here E_c is the internal energy at the critical point defined in Eq. (2.342). Forming the derivative with respect to the temperature as in (2.343) we see that at T_c the specific heat has a kink. Its slope jumps by

$$\Delta \left(\frac{\partial C_V}{\partial T} \right) \approx \frac{27}{4\pi^2} [I_{3/2}^-(0)]^2 gN \frac{k_B}{T_c} \equiv 3.6658 gN \frac{k_B}{T_c}, \quad (2.353)$$

the slopes being below T_c from (2.342):

$$\left(\frac{\partial C_V}{\partial T} \right) = \frac{5}{2} \frac{3}{2} \frac{I_{5/2}(0)}{I_{3/2}(0)} \frac{gNk_B}{T_c} \approx \frac{5}{2} \frac{3}{2} 0.7703 \frac{gNk_B}{T_c} \approx 2.8885 \frac{gNk_B}{T_c}, \quad T \leq T_c, \quad (2.354)$$

and above T_c from (2.352):

$$\left(\frac{\partial C_V}{\partial T} \right) = \left\{ \frac{5}{2} \frac{3}{2} \frac{I_{5/2}(0)}{I_{3/2}(0)} - \frac{27}{4\pi^2} [I_{3/2}^-(0)]^2 \right\} \frac{gNk_B}{T_c} \approx -0.7715 \frac{gNk_B}{T_c}, \quad T > T_c. \quad (2.355)$$

Let us compare the behavior of the specific heat of the free Bose gas with the experimental results for the Bose liquid ^4He (see Fig. 2.6). The latter also rises like T^3 for small T , but it has a sharp singularity at $T = T_c$. Considering the crudeness of the free-gas approximation, the similarity of the curves is quite surprising, indicating the physical relevance of the above idealized quantum-statistical description.

2.15.4 High Temperatures

At high temperatures, the particles are distributed over a large volume in phase space, so that the occupation numbers of each energy level are very small. As a consequence, the difference between bosons and fermions disappears, and the distribution functions (2.264) become

$$f_\varepsilon \equiv -\frac{\partial}{\partial \mu} F_\varepsilon(T, \mu) \approx e^{(\mu - \varepsilon)/k_B T}, \quad (2.356)$$

for either statistics. The high-temperature limit of the thermodynamic quantities can therefore all be calculated from the fermion expressions. The corresponding limit in the functions $I_n^\mp(\bar{\mu})$ in Eq. (2.272) is $\bar{\mu} \rightarrow -\infty$, for which we obtain

$$I_n^\mp(\bar{\mu}) \xrightarrow{\bar{\mu} \rightarrow -\infty} \int_0^\infty z^n e^{\bar{\mu} - z} = n! e^{\bar{\mu}}. \quad (2.357)$$

Inserting this into (2.307) for $n = 1/2$, we find that at a fixed particle number N , the chemical potential has the large- T behavior

$$\frac{\mu}{k_B T} \approx \frac{3}{2} \log \left[\frac{T}{T_F} \left(\frac{3\sqrt{\pi}}{4} \right)^{2/3} \right]. \quad (2.358)$$

In the same limit, the grand-canonical free energy (2.286) behaves like

$$F_G(T, \mu, V) \approx -gN(T, \mu) k_B T. \quad (2.359)$$

With the definition of the pressure (1.527), this is the equation of state for the *ideal gas*. Using the relation (2.268), we obtain from this the internal energy at a fixed particle number

$$E \approx \frac{3}{2} gN k_B T. \quad (2.360)$$

This equation is a manifestation of the *Dulong-Petit law*: Each of the $3N$ degrees of freedom of the system carries an internal energy $k_B T/2$.

The corresponding specific heat per constant unit volume is

$$C_V^{\text{DP}} = \frac{3}{2} gN k_B \quad (2.361)$$

[compare with the fermion formula (2.295)]. The low-temperature behavior (2.346) is related to this by the factor [compare with (2.327)]:

$$C_V \underset{\text{small } T}{\approx} C_V^{\text{DP}} \times 5 \frac{\zeta(5/2)}{\zeta(3/2)} \left(\frac{T}{T_c} \right)^{3/2} \approx C_V^{\text{DP}} \times 1.2838 \left(\frac{T}{T_c} \right)^{3/2}. \quad (2.362)$$

2.16 Noninteracting Bose Gas in a Trap

In 1995, Bose-Einstein condensation was observed in a dilute gas in a way that fits the above simple theoretical description [9]. When ^{87}Rb atoms were cooled down in a magnetic trap to temperatures less than 170 nK, about 50 000 atoms were observed to form a condensate, a kind of “superatom”. Such condensates have been set into rotation and shown to become perforated by vortex lines [12, 13, 14] just as in rotating superfluid helium II.

2.16.1 Bose Gas in a Finite Box

Consider first the condensation process in a finite number N of bosons enclosed in a large cubic box of size L . Then the momentum sum in Eq. (2.263) has to be carried out over the discrete momentum vectors $\mathbf{p}_n = \hbar\pi(n_1, n_2, \dots, n_D)/L$ with $n_i = 1, 2, 3, \dots$:

$$N = \frac{V_D}{l_e^D(\hbar\beta)} \zeta_{D/2}^{\text{box}}(z) \equiv \sum_{\mathbf{p}_n} \frac{1}{e^{\beta \mathbf{p}_n^2/2M - \beta\mu} - 1}, \quad (2.363)$$

where $z \equiv e^{\mu\beta}$ is the so-called *fugacity*. This can be expressed in terms of the one-dimensional auxiliary partition function of a particle in a one-dimensional “box”:

$$Z_1(b) \equiv \sum_{n=1}^{\infty} e^{-bn^2/2}, \quad b \equiv \beta\hbar^2\pi^2/ML^2 = \pi l_e^2(\hbar\beta)/2L^2. \quad (2.364)$$

Using this, we can rewrite (2.363) in the form of a so-called *fugacity expansion*

$$N = \frac{V_D}{l_e^D(\hbar\beta)} \zeta_{D/2}^{\text{box}}(z) \equiv \sum_w Z_1^D(wb) z^w, \quad (2.365)$$

where the function $Z_1(b)$ is related to the *elliptic theta function*

$$\vartheta_3(u, z) \equiv 1 + 2 \sum_{n=1}^{\infty} z^{n^2} \cos 2nu \quad (2.366)$$

by $Z_1(b) = [\vartheta_3(0, e^{-b/2}) - 1]/2$. The small- b behavior of this function is easily calculated as follows. We rewrite the sum as a sum over integrals

$$\begin{aligned} \vartheta_3(0, e^{-b/2}) &= \sum_{k=-\infty}^{\infty} e^{-k^2 b/2} = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dk e^{-k^2 b/2 + 2\pi i k m} \\ &= \sqrt{\frac{2\pi}{b}} \left(1 + 2 \sum_{m=1}^{\infty} e^{-2\pi^2 m^2/b} \right). \end{aligned} \quad (2.367)$$

Thus, up to exponentially small corrections, we may replace $\vartheta_3(0, e^{-b/2})$ by $\sqrt{2\pi/b}$, so that for small b (i.e., large $L/\sqrt{\beta}$):

$$Z_1(b) = \sqrt{\frac{\pi}{2b}} - \frac{1}{2} + \mathcal{O}(e^{-2\pi^2/b}). \quad (2.368)$$

For large b , $Z_1(b)$ falls exponentially fast to zero.

In the sum (2.363), the lowest energy level with $\mathbf{p}_{1,\dots,1} = \hbar\pi(1, \dots, 1)/L$ plays a special role. Its contribution to the total particle number is the number of particles in the condensate:

$$N_{\text{cond}}(T) = \frac{1}{e^{Db/2 - \beta\mu} - 1} = \frac{z_D}{1 - z_D}, \quad z_D \equiv e^{\beta\mu - Db/2}. \quad (2.369)$$

This number diverges for $z_D \rightarrow 1$, where the box function $\zeta_{D/2}^{\text{box}}(z)$ has a pole $1/(Db/2 - \beta\mu)$. This pole prevents $\beta\mu$ from becoming exactly equal to $Db/2$ when solving the equation (2.363) for the particle number in the box.

For a large but finite system near $T = 0$, almost all particles will go into the condensate, so that $Db/2 - \beta\mu$ will be very small, of the order $1/N$, but not zero. The thermodynamic limit can be performed smoothly by defining a regularized function $\bar{\zeta}_{D/2}^{\text{box}}(z)$ in which the lowest (singular) term in the sum (2.363) is omitted. Let us define the number of *normal* particles which have not condensed into the state of

zero momentum as $N_n(T) = N - N_{\text{cond}}(T)$. Then we can rewrite Eq. (2.363) as an equation for the number of normal particles:

$$N_n(T) = \frac{V_D}{l_e^D(\hbar\beta)} \bar{\zeta}_{D/2}^{\text{box}}(z(\beta)), \quad (2.370)$$

which reads more explicitly

$$N_n(T) = S_D(z_D) \equiv \sum_{w=1}^{\infty} [Z_1^D(wb) e^{wDb/2} - 1] z_D^w. \quad (2.371)$$

A would-be critical point may now be determined by setting here $z_D = 1$ and equating the resulting N_n with the total particle number N . If N is sufficiently large, we need only the small- b limit of $S_D(1)$ which is calculated in Appendix 2B [see Eq. (2B.14)], so that the associated temperature $T_c^{(1)}$ is determined from the equation

$$N = \sqrt{\frac{\pi}{2b_c}}^3 \zeta(3/2) + \frac{3\pi}{4b_c^{(1)}} \log C_3 b_c + \dots, \quad (2.372)$$

where $C_3 \approx 0.0186$. In the thermodynamic limit, the critical temperature $T_c^{(0)}$ is obtained by ignoring the second term, yielding

$$N = \sqrt{\frac{\pi}{2b_c^{(0)}}}^3 \zeta(3/2), \quad (2.373)$$

in agreement with Eq. (2.331) for T_c , if we recall b from (2.364). Using this we rewrite (2.372) as

$$1 \equiv \left(\frac{T_c^{(1)}}{T_c^{(0)}} \right)^{3/2} + \frac{3}{2N} \frac{\pi}{2b_c^{(0)}} \log C_3 b_c^{(0)}. \quad (2.374)$$

Expressing $b_c^{(0)}$ in terms of N from (2.373), this implies

$$\frac{\delta T_c^{(1)}}{T_c^{(0)}} \approx \frac{1}{\zeta^{2/3}(3/2) N^{1/3}} \log \frac{2}{\pi C_3} \frac{N^{2/3}}{\zeta^{2/3}(3/2)}. \quad (2.375)$$

Experimentally, the temperature $T_c^{(1)}$ is not immediately accessible. What is easy to find is the place where the condensate density has the largest curvature, i.e., where $d^3 N_{\text{cond}}/dT^3 = 0$. The associated temperature T_c^{exp} is larger than $T_c^{(1)}$ by a factor $1 + \mathcal{O}(1/N)$, so that it does not modify the leading finite-size correction which is of the order $1/N^{1/3}$.

Alternatively we may use the phase space formula

$$\begin{aligned} N_n &= \int d^D x \frac{d^D p}{(2\pi\hbar)^D} \frac{1}{e^{\beta[p^2/2M + V(\mathbf{x})]} - 1} = \sum_{n=1}^{\infty} \int d^D x \frac{d^D p}{(2\pi\hbar)^D} e^{-n\beta[p^2/2M + V(\mathbf{x})]} \\ &= \sum_{n=1}^{\infty} \frac{1}{\sqrt{2\pi\hbar^2 n\beta/M}^D} \int d^D x e^{-n\beta V(\mathbf{x})}, \end{aligned} \quad (2.376)$$

where the spatial integration produces a factor $\sqrt{2\pi/M\omega^2 n\beta}$ so that the right-hand side becomes again $(T/T_c^{(0)})^D N$.

2.16.2 Harmonic and General Power Trap

For a D -dimensional harmonic trap $V = M\omega^2 \mathbf{x}^2/2$, the critical temperature is reached if N_n is equal to the total particle number N where

$$k_B T_c^{(0)} = \hbar\omega \left[\frac{N}{\zeta(D)} \right]^{1/D}. \quad (2.377)$$

This formula has a solution only for $D > 1$.

The equation (2.376) for the particle number can be easily calculated for a more general trap where the potential has the anisotropic power behavior

$$V(\mathbf{x}) = \frac{M}{2} \tilde{\omega}^2 \tilde{a}^2 \sum_{i=1}^D \left(\frac{|x_i|}{a_i} \right)^{p_i}. \quad (2.378)$$

The parameter $\tilde{\omega}$ denotes some frequency parameter, and $\tilde{a}$ the geometric average $\tilde{a} \equiv [\prod_{i=1}^D a_i]^{1/D}$. Inserting (2.378) into (2.376) we encounter a product of integrals:

$$\prod_{i=1}^D \int_{-\infty}^{\infty} dx e^{-n\beta M \tilde{\omega}^2 \tilde{a}^2 (|x_i|/a_i)^{p_i}/2} = \prod_{i=1}^D \frac{a_i}{(\beta M \tilde{\omega}^2 \tilde{a}^2/2)^{1/p_i}} \Gamma(1 + 1/p_i), \quad (2.379)$$

so that the right-hand side of (2.376) becomes $(T/T_c^{(0)})^{\tilde{D}} N$, with the critical temperature

$$k_B T_c^{(0)} = \frac{M \tilde{a}^2 \tilde{\omega}^2}{2} \left(\frac{\hbar \tilde{\omega}}{M \tilde{a}^2 \tilde{\omega}^2} \right)^{D/\tilde{D}} \left[\frac{N \pi^{D/2}}{\zeta(\tilde{D}) \prod_{i=1}^D \Gamma(1 + 1/p_i)} \right]^{1/\tilde{D}}. \quad (2.380)$$

Here $\tilde{D}$ is the dimensionless parameter

$$\tilde{D} \equiv \frac{D}{2} + \sum_{i=1}^D \frac{1}{p_i} \quad (2.381)$$

that takes over the role of D in the harmonic formula (2.377). A harmonic trap, that has different oscillator frequencies $\omega_1, \dots, \omega_D$ along the D Cartesian axes, is a special case of (2.378) with $p_i \equiv 2$, $\omega_i^2 = \tilde{\omega}^2 \tilde{a}^2/a_i^2$, and $\tilde{D} = D$, and formula (2.380) reduces to (2.377), with ω replaced by the geometric average $\tilde{\omega} \equiv (\omega_1 \cdots \omega_D)^{1/D}$ of the frequencies. The parameter $\tilde{a}$ disappears from the formula. A free Bose gas in a box of size $V_D = \prod_{i=1}^D (2a_i) = 2^D \tilde{a}^D$ is described by (2.378) in the limit $p_i \rightarrow \infty$, where $\tilde{D} = D/2$. Then Eq. (2.380) reduces to

$$k_B T_c^{(0)} = \frac{\pi \hbar^2}{2M \tilde{a}^2} \left[\frac{N}{\zeta(D/2)} \right]^{2/D} = \frac{2\pi \hbar^2}{M} \left[\frac{N}{V_D \zeta(D/2)} \right]^{2/D}, \quad (2.382)$$

in agreement with Eq. (2.331).

Another interesting limiting case is that of a box of length $L = 2a_1$ in the x -direction with $p_1 = \infty$, and two different oscillators of frequency ω_2 and ω_3 in the

other two directions. To find $T_c^{(0)}$ for such a Bose gas we identify $\tilde{\omega}^2 \tilde{a}^2 / a_{2,3}^2 = \omega_{2,3}^2$ in the potential (2.378), so that $\tilde{\omega}^4 / \tilde{a}^2 = \omega_2^2 \omega_3^2 / a_1^2$, and we obtain

$$k_B T_c^{(0)} = \hbar \tilde{\omega} \left(\frac{\pi \hbar}{2M \tilde{\omega}} \right)^{1/5} \left[\frac{N}{a_1 \zeta(5/2)} \right]^{2/5} = \hbar \tilde{\omega} \left(\frac{2\pi \lambda_{\omega_1} \lambda_{\omega_2}}{L^2} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \quad (2.383)$$

2.16.3 Anharmonic Trap in Rotating Bose-Einstein Gas

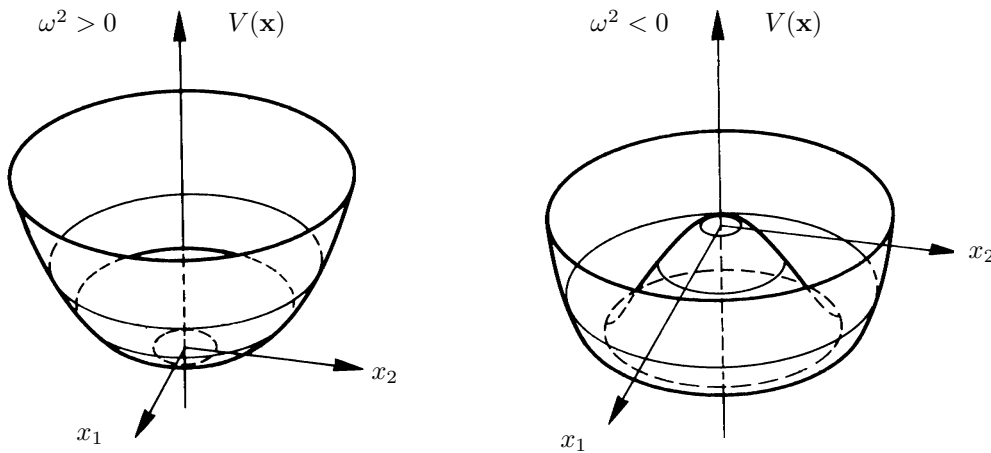
Another interesting potential can be prepared in the laboratory by rotating a Bose condensate [13] with an angular velocity Ω around the z -axis. The vertical trapping frequency is $\omega_z \approx 2\pi \times 11.0 \text{ Hz} \approx 0.58 \times \text{nK}$, while the horizontal one is $\omega_{\perp} \approx 6 \times \omega_z$. The centrifugal forces create an additional repulsive harmonic potential, bringing the rotating potential to the form

$$V(\mathbf{x}) = \frac{M\omega_z^2}{2} \left(z^2 + 36\eta r_{\perp}^2 + \frac{\kappa}{2} \frac{r_{\perp}^4}{\lambda_{\omega_z}^2} \right) = \frac{\hbar\omega_z}{2} \left(\frac{z^2}{\lambda_{\omega_z}^2} + 36\eta \frac{r_{\perp}^2}{\lambda_{\omega_z}^2} + \frac{\kappa}{2} \frac{r_{\perp}^4}{\lambda_{\omega_z}^4} \right), \quad (2.384)$$

where $r_{\perp}^2 = x^2 + y^2$, $\eta \equiv 1 - \Omega^2 / \omega_{\perp}^2$, $\kappa \approx 0.4$, and $\lambda_{\omega_z} \equiv 3.245 \mu\text{m} \approx 1.42 \times 10^{-3} \text{ K}$. For $\Omega > \omega_{\perp}$, η turns negative and the potential takes the form of a Mexican hat as shown in Fig. 2.7, with a circular minimum at $r_m^2 = -36\eta \lambda_{\omega_z}^2 / \kappa$. For a large rotation speed Ω , the potential may be approximated by a circular harmonic well, so that we may apply formula (2.383) with $a_1 = 2\pi r_m$, to obtain the η -independent critical temperature

$$k_B T_c^{(0)} \approx \hbar \omega_z \left(\frac{\kappa}{\pi} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \quad (2.385)$$

FIGURE 2.7 Rotating trap potential for $\omega^2 > 0$ and $\omega^2 < 0$, pictured for the case of two components x_1, x_2 . The right-hand figure looks like a Mexican hat or the bottom of a champagne bottle.



For $\kappa = 0.4$ and $N = 300\,000$, this yields $T_c \approx 53\text{nK}$.

At the critical rotation speed $\Omega = \omega_\perp$, the potential is purely quartic $r_\perp = \sqrt{(x^2 + y^2)}$. To estimate $T_c^{(0)}$ we approximate it for a moment by the slightly different potential (2.378) with the powers $p_1 = 2, p_2 = 4, p_3 = 4$, $a_1 = \lambda_{\omega_z}, a_2 = a_3 = \lambda_{\omega_z}(\kappa/2)^{1/4}$, so that formula (2.380) becomes

$$k_B T_c^{(0)} = \hbar \omega_z \left[\frac{\pi^2 \kappa}{16 \Gamma^4(5/4)} \right]^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \quad (2.386)$$

It is easy to change this result so that it holds for the potential $\propto r^4 = (x + y)^4$ rather than $x^4 + y^4$. We use the semiclassical formula for the number of normal particles in the form

$$N_n = \int_{E_{\min}}^{\infty} dE \frac{\rho_{\text{cl}}(E)}{e^{E/k_B T} - 1}, \quad (2.387)$$

where $E_{\min}$ is the classical ground state energy, and

$$\rho_{\text{cl}}(E) = \left(\frac{M}{2\pi\hbar^2} \right)^{D/2} \frac{1}{\Gamma(D/2)} \int d^D x [E - V(\mathbf{x})]^{D/2-1} \quad (2.388)$$

is the semiclassical density of states. For a harmonic trap, the spatial integral can be done, after which the energy integral on the right-hand side of (2.387) yields $[k_B T / \hbar \omega]^D \zeta(D) = (T/T_c^{(0)})^D N$, thus leading back to (2.377). Hence the critical temperature for the potential $\propto r^4 = (x + y)^4$ rather than $x^4 + y^4$ is obtained by multiplying the right-hand side of Eq. (2.387) for N by a factor

$$\frac{2\pi \int r dr dx dy e^{-r^4}}{\int dx dy e^{-x^4 - y^4}} = \frac{\pi^{3/2}}{\Gamma[5/4]^2}. \quad (2.389)$$

This factor arrives inversely in front of N in Eq. (2.390), so that we obtain the critical temperature of the critically rotating Bose gas:

$$k_B T_c^{(0)} = \hbar \omega_z \left(\frac{4\kappa}{\pi} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \quad (2.390)$$

The critical temperature at $\Omega = \omega_\perp$ is therefore by a factor $4^{1/5} \approx 1.32$ larger than at infinite Ω . Actually, this limit is somewhat academic in a semiclassical approximation since it ignores the quantum nature of the oscillator.

For more details see Chapter 7 in the textbook [1].

2.17 Temperature Green Functions of Free Particles

As argued in Section 1.7, all properties of a system in thermodynamic equilibrium are calculable by continuing the quantum theory to imaginary times $t = -i\tau$, with real τ . We shall see later that the calculation of small interaction effects to the

free-particle results, presented in the last section, can be done perturbatively. It involves the analytically continued analog of the free-particle propagator (2.249).

In a grand-canonical ensemble, the relevant quantity is the so called *finite-temperature Green function* or *finite-temperature propagator* of the free particles:

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}' \tau') &= \frac{\text{Tr} \left[e^{-\hat{H}_G/k_B T} \hat{T}_\tau \left(\hat{\psi}(\mathbf{x}, \tau) \hat{\psi}^\dagger(\mathbf{x}', \tau') \right) \right]}{\text{Tr} (e^{-\hat{H}_G/k_B T})} \\ &= e^{F_G/k_B T} \text{Tr} \left[e^{-\hat{H}_G/k_B T} \hat{T}_\tau \left(\hat{\psi}(\mathbf{x}, \tau) \hat{\psi}^\dagger(\mathbf{x}', \tau') \right) \right]. \end{aligned} \quad (2.391)$$

Here $\hat{T}_\tau$ is the τ -ordering operator defined in complete analogy to the time-ordering operator $\hat{T}$ in (2.231). The fields $\hat{\psi}(\mathbf{x}, \tau)$, $\hat{\psi}^\dagger(\mathbf{x}, \tau)$ are defined in analogy to (2.133) and (2.134) via an analytically continued time evolution operator as follows:

$$\hat{\psi}(\mathbf{x}, \tau) = e^{\hat{H}_G \tau / \hbar} a_{\mathbf{x}} e^{-\hat{H}_G \tau / \hbar}, \quad (2.392)$$

$$\hat{\psi}^\dagger(\mathbf{x}, \tau) = e^{-\hat{H}_G \tau / \hbar} a_{\mathbf{x}}^\dagger e^{\hat{H}_G \tau / \hbar}. \quad (2.393)$$

At equal imaginary time, these satisfy canonical commutation relations analogous to (2.205):

$$\begin{aligned} [\hat{\psi}(\mathbf{x}, \tau), \hat{\psi}(\mathbf{x}', \tau)]_\mp &= 0, \\ [\hat{\psi}^\dagger(\mathbf{x}, \tau), \hat{\psi}^\dagger(\mathbf{x}', \tau)]_\mp &= 0, \\ [\hat{\psi}(\mathbf{x}, \tau), \hat{\psi}^\dagger(\mathbf{x}', \tau)]_\mp &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (2.394)$$

The time evolution of these field operators is governed by the grand-canonical Hamiltonian

$$\hat{H}_G = \hat{H} - \mu \hat{N}. \quad (2.395)$$

Note that while $\psi_{\mathbf{p}}^\dagger$ in (2.393) at $\tau = 0$ is the Hermitian conjugate of $\psi_{\mathbf{p}}$ in (2.392), this is no longer true for $\tau \neq 0$. The advantages of using these non-Hermitian fields will become apparent later when we discuss perturbation theory.

When it comes to calculating physical phenomena in thermal equilibrium, all Green functions will be needed whose imaginary time τ lies in the interval

$$\tau \in (0, \hbar/k_B T). \quad (2.396)$$

Differentiating (2.392) and (2.393) with respect to τ , we obtain the Heisenberg equations

$$\hat{\partial}_\tau \hat{\psi}(\mathbf{x}, \tau) = [\hat{H}_G, \hat{\psi}(\mathbf{x}, \tau)], \quad (2.397)$$

$$\hat{\partial}_\tau \hat{\psi}^\dagger(\mathbf{x}, \tau) = -[\hat{H}_G, \hat{\psi}^\dagger(\mathbf{x}, \tau)]. \quad (2.398)$$

Using the canonical field commutation relations (2.394), the fields $\hat{\psi}(\mathbf{x}, \tau)$ and $\hat{\psi}^\dagger(\mathbf{x}, \tau)$ are seen to satisfy the analytically continued Schrödinger equations

$$\left(-\hbar \partial_\tau + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + \mu \right) \hat{\psi}(\mathbf{x}, \tau) = 0, \quad (2.399)$$

$$\hat{\psi}^\dagger(\mathbf{x}, \tau) \left(\hbar \overleftarrow{\partial}_\tau + \frac{\hbar^2}{2M} \overleftarrow{\partial}_{\mathbf{x}}^2 + \mu \right) = 0. \quad (2.400)$$

If we apply these differential operators to the Green function (2.391), we obtain the equation

$$\begin{aligned} \left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu \right) G(\mathbf{x}, \tau; \mathbf{x}', \tau') \\ = e^{F_G/k_B T} \text{Tr} \left\{ e^{-\hat{H}_G/k_B T} \delta(\tau - \tau') \left[\hat{\psi}(\mathbf{x}, \tau), \hat{\psi}^\dagger(\mathbf{x}', \tau') \right] \right\}. \end{aligned} \quad (2.401)$$

Using the commutation rule (2.395), this becomes

$$\left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu \right) G(\mathbf{x}, \tau; \mathbf{x}', \tau') = \delta(\tau - \tau') \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (2.402)$$

which is the general defining equation of a Green function [recall (1.315)].

The plane-wave solutions of Eqs. (2.399) and (2.400) are the analytically-continued versions of the plane-wave solutions (2.206),

$$\begin{aligned} \hat{\psi}_{\mathbf{p}}(\mathbf{x}, \tau) &= \hat{a}_{\mathbf{p}} e^{i\mathbf{p}\mathbf{x} - \xi(\mathbf{p})\tau/\hbar}, \\ \hat{\psi}_{\mathbf{p}}^\dagger(\mathbf{x}, \tau) &= \hat{a}_{\mathbf{p}}^\dagger e^{-i\mathbf{p}\mathbf{x} + \xi(\mathbf{p})\tau/\hbar}, \end{aligned} \quad (2.403)$$

where

$$\xi(\mathbf{p}) \equiv \frac{\mathbf{p}^2}{2M} - \mu \quad (2.404)$$

with particle energies counted from the chemical potential μ rather than from zero. The canonical field operators solving (2.399) and (2.400) have momentum-space expansions of the type (2.215), namely

$$\begin{aligned} \hat{\psi}(\mathbf{x}, \tau) &= \int \tilde{d}^3 p e^{i\mathbf{p}\mathbf{x}/\hbar - \xi(\mathbf{p})\tau/\hbar} \hat{a}_{\mathbf{p}}, \\ \hat{\psi}^\dagger(\mathbf{x}, \tau) &= \int \tilde{d}^3 p e^{-i\mathbf{p}\mathbf{x}/\hbar + \xi(\mathbf{p})\tau/\hbar} \hat{a}_{\mathbf{p}}^\dagger. \end{aligned} \quad (2.405)$$

Inserting these into (2.391), we now calculate the Green function for $\tau > \tau'$:

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= G(\mathbf{x} - \mathbf{x}', \tau - \tau') \\ &= e^{F_G/k_B T} \text{Tr} \left[e^{-\hat{H}_G/k_B T} \hat{\psi}(\mathbf{x}, \tau) \hat{\psi}^\dagger(\mathbf{x}', \tau') \right] \\ &= e^{F_G/k_B T} \int \tilde{d}^3 p \int \tilde{d}^3 p' \text{Tr} \left(e^{-\hat{H}_G/k_B T} \hat{a}_{\mathbf{p}} \hat{a}_{\mathbf{p}'}^\dagger \right) e^{i[\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}']/\hbar - i[\xi(\mathbf{p})\tau - \xi(\mathbf{p}')\tau']/\hbar}. \end{aligned} \quad (2.406)$$

Here we observe that the expression

$$e^{F_G/k_B T} \text{Tr} \left(e^{-\hat{H}_G/k_B T} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}'} \right) = \frac{\text{Tr} \left(e^{-\hat{H}_G/k_B T} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}'} \right)}{\text{Tr} \left(e^{-\hat{H}_G/k_B T} \right)} \quad (2.407)$$

is simply the average particle number of Eq. (2.264) for the energy $\xi(\mathbf{p})$:

$$f_{\xi(\mathbf{p})} = \frac{1}{e^{\xi(\mathbf{p})/k_B T} \mp 1}, \quad (2.408)$$

apart from a Dirac δ -function in the momenta $\delta^{(3)}(\mathbf{p} - \mathbf{p}')$. Hence we find for $\tau > 0$:

$$G(\mathbf{x}, \tau) \equiv \int d^3p e^{i\mathbf{p}\mathbf{x}/\hbar - \xi(\mathbf{p})\tau/\hbar} (1 \pm f_{\xi(\mathbf{p})}). \quad (2.409)$$

For $\tau < 0$, the operator order is reversed, and we obtain directly

$$G(\mathbf{x}, \tau) \equiv \pm \int d^3p e^{i\mathbf{p}\mathbf{x}/\hbar - \xi(\mathbf{p})\tau/\hbar} f_{\xi(\mathbf{p})}. \quad (2.410)$$

From these expressions we can derive an important property of the temperature Green function. Using the identity

$$e^{\xi/k_B T} f_{\xi} = 1 \pm f_{\xi}, \quad (2.411)$$

we see that $G(\mathbf{x}, \tau)$ is periodic or antiperiodic under the replacement

$$\tau \rightarrow \tau + \frac{\hbar}{k_B T}, \quad (2.412)$$

depending on whether the particles are bosons or fermions, respectively. Explicitly, the Green function satisfies the relation

$$G(\mathbf{x}, \tau) = \pm G(\mathbf{x}, \tau + \hbar/k_B T), \quad \tau \in (-\hbar/k_B T, \hbar/k_B T]. \quad (2.413)$$

At zero imaginary time this reduces to $G(\mathbf{x}, 0) = \pm G(\mathbf{x}, \hbar/k_B T)$, implying that $G(\mathbf{x}, \tau)$ has a Fourier transform

$$G(\mathbf{x}, \tau) = \frac{k_B T}{\hbar} \sum_{\omega_m} e^{-i\omega_m \tau} G(\mathbf{x}, \omega_m) \quad (2.414)$$

with the frequencies

$$\omega_m \equiv \omega_m = \frac{2\pi}{\hbar\beta} \begin{cases} m & \text{for bosons,} \\ m + \frac{1}{2} & \text{for fermions,} \end{cases} \quad (2.415)$$

where m runs through all integer values $m = 0, \pm 1, \pm 2, \dots$. These are known as *Matsubara frequencies*.

The Fourier components are given by the integrals

$$G(\mathbf{x}, \omega_m) = \int_0^{\hbar/k_B T} d\tau e^{i\omega_m \tau} G(\mathbf{x}, \tau). \quad (2.416)$$

The full Fourier representation in space and imaginary time reads

$$G(\mathbf{x}, \tau) = \frac{k_B T}{\hbar} \sum_{\omega_m} \int d^3p e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} G(\mathbf{p}, \omega_m), \quad (2.417)$$

with the components

$$\begin{aligned} G(\mathbf{p}, \omega_m) &= \int d^3x \int_0^{\hbar/k_B T} d\tau e^{i\omega_m \tau - i\mathbf{p}\mathbf{x}/\hbar} G(\mathbf{x}, \tau) \\ &= \frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})} (1 \pm f_{\xi(\mathbf{p})}) \left\{ e^{[i\hbar\omega_m - \xi(\mathbf{p})]/k_B T} - 1 \right\}. \end{aligned} \quad (2.418)$$

Inserting (2.408) and the explicit form of the Matsubara frequencies (2.415), we obtain

$$G(\mathbf{p}, \omega_m) = -\frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})}. \quad (2.419)$$

Due to a marvelous cancellation, this has become very simple. In fact, the result can be obtained from the Fourier transform (2.248) of the quantum field theoretic Green function $G(\mathbf{p}, E)$ in two steps: First, we continue (2.248) analytically in the energy E to the imaginary off-shell values $E = i\hbar\omega_m$, and second, we shift the single-particle energy from $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2M$ to $\xi(\mathbf{p}) = \varepsilon(\mathbf{p}) - \mu$, this being a trivial consequence of the use of $\hat{H}_G = \hat{H} - \mu\hat{N}$ instead of $\hat{H}$.

As a cross check, let us calculate $G(\mathbf{x}, \tau)$ for a very small negative $\tau = -\eta$ from the Fourier representation (2.417) with the components (2.419) for bosons:

$$G(\mathbf{x}, -\eta) = - \int d^3p e^{i\mathbf{p}\mathbf{x}/\hbar} \frac{k_B T}{\hbar} \sum_{\omega_m} e^{i\omega_m \eta} \frac{\hbar}{-i\omega_m + \xi(\mathbf{p})}. \quad (2.420)$$

The phase factor $e^{i\omega_m \eta}$ is necessary to ensure convergence of the otherwise logarithmically-divergent sums. The sum can be performed by rephrasing it as the contour integral

$$-k_B T \sum_{\omega_m} e^{i\omega_m \eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \mp \frac{k_B T}{2\pi i} \int_C dz \frac{e^{\eta z}}{e^{z/k_B T} \mp 1} \frac{1}{z - \xi}. \quad (2.421)$$

The contour of integration C encircles the imaginary z -axis in the positive sense, thereby enclosing all integer or half-integer valued poles at $z = i\omega_m$. The upper signs on the right-hand side of (14.196) holds for bosons, the lower for fermions.

The closed contour C may be viewed as the result of two straight contours, which lie next to each other: one runs upwards to the right of the imaginary axis and the other that runs downwards to the left of it. The two parts may be closed by infinite semicircles Γ_l and Γ_r at infinity (see Fig. 2.8). These contribute nothing since the right-semicircle is suppressed by an exponential factor $e^{-z/k_B T}$, and the left-hand by a factor $e^{\eta z}$. The two resulting closed contours may now be distorted and shrunk to zero. There is a pole only on the right-hand side, at $z = \xi$, which contributes by Cauchy's residue theorem:

$$\mp k_B T \sum_{\omega_m} e^{i\omega_m \eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \pm \frac{1}{e^{\xi(\mathbf{p})/k_B T} \mp 1} = \pm f_{\xi(\mathbf{p})}. \quad (2.422)$$

Via Eq. (2.420) these lead to the Bose and Fermi distribution functions represented by Eq. (2.410) for small negative τ .

In the opposite limit $\tau = +\eta$, the phase factor in the sum would be $e^{-i\omega_n \eta}$. In this case, the sum is converted into the contour integral

$$-k_B T \sum_{\omega_n} e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi(\mathbf{p})} = \pm \frac{k_B T}{2\pi i} \int_C dz \frac{e^{-\eta z}}{e^{-z/k_B T} \mp 1} \frac{1}{z - \xi}, \quad (2.423)$$

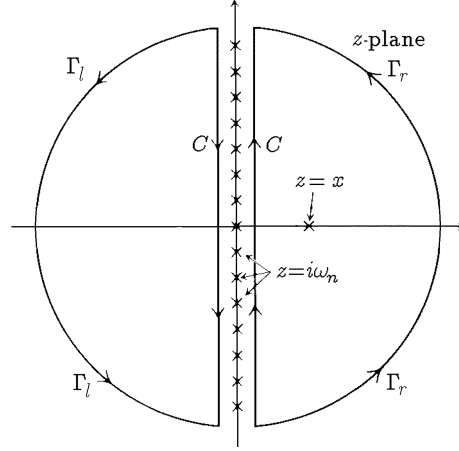


FIGURE 2.8 Contour C in the complex z -plane for evaluating the Matsubara sum (2.422). The semicircles at infinity Γ_l and Γ_r do not contribute. After shrinking the contours, only the pole on the right-hand side contributes via Cauchy's residue theorem.

from which we would find $1 \pm f_{\xi(\mathbf{p})}$, corresponding to Eq. (2.409) for small positive τ .

While the phase factors $e^{\pm i\omega_m \eta}$ are needed to make the logarithmically-divergent sums converge, they become superfluous if the two sums are combined. Indeed, adding the two sums yields

$$\begin{aligned}
 -k_B T \sum_{\omega_n} \left[e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi} + e^{-i\omega_n \eta} \frac{1}{i\omega_n - \xi} \right] &= -k_B T \sum_{\omega_n} e^{i\omega_n \eta} \left[\frac{1}{i\omega_n - \xi} + \frac{1}{-i\omega_n - \xi} \right] \\
 &= \frac{k_B T}{\hbar} \sum_{\omega_m} \frac{2\xi}{\omega_m^2 + \xi^2} = 1 \pm 2 f_{\xi} \\
 &= \left\{ \begin{array}{l} \coth(\hbar\xi/k_B T) \\ \tanh(\hbar\xi/k_B T) \end{array} \right\} \text{ for } \left\{ \begin{array}{l} \text{bosons} \\ \text{fermions} \end{array} \right\}.
 \end{aligned} \tag{2.424}$$

The right-hand side is the thermal expectation value of $\hat{a}_{\mathbf{p}}\hat{a}_{\mathbf{p}}^{\dagger} + \hat{a}_{\mathbf{p}}^{\dagger}\hat{a}_{\mathbf{p}}$.

2.18 Calculating the Matsubara Sum via Poisson Formula

There exists another way of calculating the Matsubara sum in the finite-temperature propagator (2.417). At very low temperatures, the Matsubara frequencies $\omega_m = 2m\pi k_B T/\hbar$ or $\omega_m = (2m+1)\pi k_B T/\hbar$ move infinitely close to each other, so that the sum over ω_m becomes an integral

$$\frac{k_B T}{\hbar} \sum_{n=-\infty}^{\infty} \rightarrow \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \tag{2.425}$$

for Bose and Fermi fields. The propagator (2.417) becomes therefore, with (2.419),

$$\begin{aligned} G(\mathbf{x}, \tau) &= \frac{k_B T}{\hbar} \sum_{m=-\infty}^{\infty} \int d^3 p e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} \\ &\rightarrow \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \int d^3 p e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar}. \end{aligned} \quad (2.426)$$

The integral over ω_m can be performed trivially with the help of the residue theorem, as in Eq. (2.243), yielding

$$G(\mathbf{p}, \tau) = \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} e^{-i\omega_m \tau} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} = \Theta(\tau) e^{-\xi(\mathbf{p})\tau/\hbar}. \quad (2.427)$$

For finite temperatures we make use of Poisson's summation formula (1.213) to write

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i \mu n} f(\mu), \quad (2.428)$$

from which we derive

$$\sum_{m=-\infty}^{\infty} f(m + 1/2) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} (-1)^n e^{2\pi i \mu n} f(\mu). \quad (2.429)$$

A direct application of this formula shows that

$$\frac{k_B T}{\hbar} \sum_{m=-\infty}^{\infty} e^{-i\omega_m \tau} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} = \sum_{n=-\infty}^{\infty} \left\{ \frac{1}{(-1)^n} \right\} \Theta(\tau + n\hbar\beta) e^{-\xi(\mathbf{p})(\tau + n\hbar\beta)/\hbar}. \quad (2.430)$$

Thus the finite-temperature Green function is obtained from the zero-temperature function by making it periodic or antiperiodic by forming a simple sum over all periods, with equal or alternating signs. This guarantees the property (2.413). The sum over n on the right-hand side of (2.430) is a geometric series in powers of $e^{-\xi(\mathbf{p})n\hbar\beta}$, which can be performed trivially. For $\tau \in (0, \hbar\beta)$, the Heaviside function forces the sum to run only over positive n , so that we find

$$G(\mathbf{p}, \tau) = \sum_{n=0}^{\infty} \left\{ \frac{1}{(-1)^n} \right\} \Theta(\tau + n\hbar\beta) e^{-\xi(\mathbf{p})\tau/\hbar} e^{-n\xi(\mathbf{p})\beta} = \frac{e^{-\xi(\mathbf{p})\tau/\hbar}}{1 \mp e^{-\xi(\mathbf{p})\beta}}. \quad (2.431)$$

This can also be rewritten in terms of the Bose and Fermi distribution functions (2.408) as

$$G(\mathbf{p}, \tau) = e^{-\xi(\mathbf{p})\tau/\hbar} (1 \pm f_{\xi(\mathbf{p})}). \quad (2.432)$$

For free particles with zero chemical potential where $\xi(\mathbf{p}) = \mathbf{p}^2/2M$, the momentum integral can be done at zero temperature as in Eq. (2.239), and we obtain the imaginary-time version of the Schrödinger propagator (2.241):

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= \Theta(\tau - \tau') \frac{1}{\sqrt{2\pi\hbar^2(\tau - \tau')/M}} e^{-M(\mathbf{x} - \mathbf{x}')^2/2\hbar^2(\tau - \tau')} \\ &= G(\mathbf{x} - \mathbf{x}', \tau - \tau'). \end{aligned} \quad (2.433)$$

This Gaussian function coincides with the end-to-end distribution of random walk of length proportional to $\hbar(\tau - \tau')$. Thus the quantum-mechanical propagator is a complex version of a particle performing a random walk. The random walk is caused by *quantum fluctuations*. This fluctuation picture of the Schrödinger theory is exhibited best in the path-integral formulation of quantum mechanics.⁹ In the imaginary-time formulation of quantum field theory, we describe ensembles of particles. They correspond therefore to ensembles of random walks of fixed length. For this reason, nonrelativistic quantum field theories can be used efficiently to formulate theories of fluctuating polymers. In this context, they are called *disorder field theories*.¹⁰

2.19 Nonequilibrium Quantum Statistics

The physical systems which can be described by the above imaginary-time Green functions are quite limited. They must be in thermodynamic equilibrium, with a constant temperature enforced by a thermal reservoir. Only then can a partition function and a particle distribution be calculated from an analytic continuation of quantum-mechanical time evolution amplitudes to an imaginary time $t_b - t_a = -i\hbar/k_B T$. In this section we want to go beyond such equilibrium physics and extend the path-integral formalism to nonequilibrium time-dependent phenomena.

2.19.1 Linear Response and Time-Dependent Green Functions for $T \neq 0$

If the deviations of a quantum system from thermal equilibrium are small, the easiest description of nonequilibrium phenomena proceeds via the *theory of linear response*. In operator quantum mechanics, this theory is introduced as follows. First, the system is assumed to have a time-independent Hamiltonian operator $\hat{H}$. The ground state is determined by the Schrödinger equation, evolving as a function of time according to the equation

$$|\Psi_S(t)\rangle = e^{-i\hat{H}t}|\Psi_S(0)\rangle \quad (2.434)$$

(in natural units with $\hbar = 1$, $k_B = 1$). The subscript S denotes the Schrödinger picture.

Next, the system is slightly disturbed by adding to $\hat{H}$ a time-dependent external interaction,

$$\hat{H} \rightarrow \hat{H} + \hat{H}^{\text{ext}}(t), \quad (2.435)$$

where $\hat{H}^{\text{ext}}(t)$ is assumed to set in at some time t_0 , i.e., $\hat{H}^{\text{ext}}(t)$ vanishes identically for $t < t_0$. The disturbed Schrödinger ground state has the time dependence

$$|\Psi_S^{\text{dist}}(t)\rangle = e^{-i\hat{H}t}\hat{U}_H(t)|\Psi_S(0)\rangle, \quad (2.436)$$

⁹See the textbook Ref. [1].

¹⁰See the textbooks Refs. [1] and [11].

where $\hat{U}_H(t)$ is the time translation operator in the Heisenberg picture. It satisfies the equation of motion

$$i\dot{\hat{U}}_H(t) = \hat{H}_H^{\text{ext}}(t)\hat{U}_H(t), \quad (2.437)$$

with¹¹

$$\hat{H}_H^{\text{ext}}(t) \equiv e^{i\hat{H}t} \hat{H}^{\text{ext}}(t) e^{-i\hat{H}t}. \quad (2.438)$$

To lowest-order perturbation theory, the operator $\hat{U}_H(t)$ is given by

$$\hat{U}_H(t) = 1 - i \int_{t_0}^t dt' \hat{H}_H^{\text{ext}}(t') + \dots \quad (2.439)$$

In the sequel, we shall assume the onset of the disturbance to lie at $t_0 = -\infty$. Consider an arbitrary time-independent Schrödinger observable $\hat{O}$ whose Heisenberg representation has the time dependence

$$\hat{O}_H(t) = e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t}. \quad (2.440)$$

Its time-dependent expectation value in the disturbed state $|\Psi_S^{\text{dist}}(t)\rangle$ is given by

$$\begin{aligned} \langle \Psi_S^{\text{dist}}(t) | \hat{O} | \Psi_S^{\text{dist}}(t) \rangle &= \langle \Psi_S(0) | \hat{U}_H^\dagger(t) e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} \hat{U}_H(t) | \Psi_S(0) \rangle \\ &\approx \langle \Psi_S(0) | \left(1 + i \int_{-\infty}^t dt' \hat{H}_H^{\text{ext}}(t') + \dots \right) \hat{O}_H(t) \\ &\quad \times \left(1 - i \int_{-\infty}^t dt' \hat{H}_H^{\text{ext}}(t') + \dots \right) | \Psi_S(0) \rangle \\ &= \langle \Psi_H | \hat{O}_H(t) | \Psi_H \rangle - i \langle \Psi_H | \int_{-\infty}^t dt' [\hat{O}_H(t), \hat{H}_H^{\text{ext}}(t')] | \Psi_H \rangle + \dots \quad (2.441) \end{aligned}$$

We have identified the time-independent Heisenberg state with the time-dependent Schrödinger state at zero time in the usual manner, i.e., $|\Psi_H\rangle \equiv |\Psi_S(0)\rangle$. Thus the expectation value of $\hat{O}$ deviates from equilibrium by

$$\begin{aligned} \delta \langle \Psi_S(t) | \hat{O} | \Psi_S(t) \rangle &\equiv \langle \Psi_S^{\text{dist}}(t) | \hat{O}(t) | \Psi_S^{\text{dist}}(t) \rangle - \langle \Psi_S(t) | \hat{O}(t) | \Psi_S(t) \rangle \\ &= -i \int_{-\infty}^t dt' \langle \Psi_H | [\hat{O}_H(t), \hat{H}_H^{\text{ext}}(t')] | \Psi_H \rangle. \quad (2.442) \end{aligned}$$

If the left-hand side is transformed into the Heisenberg picture, it becomes

$$\delta \langle \Psi_S(t) | \hat{O} | \Psi_S(t) \rangle = \delta \langle \Psi_H | \hat{O}_H(t) | \Psi_H \rangle = \langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle,$$

¹¹Note that after the replacements $H \rightarrow H_0$, $H_H^{\text{ext}} \rightarrow H_I^{\text{int}}$, Eq. (2.437) coincides with the equation for the time evolution operator in the interaction picture to appear in Section 9.1.3. In contrast to that section, however, the present interaction is a nonpermanent artifact to be set equal to zero at the end, and H is the complicated total Hamiltonian, not a simple free one. This is why we do not speak here of an interaction picture.

so that Eq. (2.442) takes the form

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = -i \int_{-\infty}^t dt' \langle \Psi_H | [\hat{O}_H(t), \hat{H}_H^{\text{ext}}(t')] | \Psi_H \rangle. \quad (2.443)$$

It is useful to use the retarded Green function of the operators $\hat{O}_H(t)$ and $\hat{H}_H(t')$ in the state $|\Psi_H\rangle$

$$G_{OH}^R(t, t') \equiv \Theta(t - t') \langle \Psi_H | [\hat{O}_H(t), \hat{H}_H(t')] | \Psi_H \rangle. \quad (2.444)$$

Then the deviation from equilibrium is given by the integral

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = -i \int_{-\infty}^{\infty} dt' G_{OH}^R(t, t'). \quad (2.445)$$

Suppose now that the observable $\hat{O}_H(t)$ is capable of undergoing oscillations. Then an external disturbance coupled to $\hat{O}_H(t)$ will in general excite these oscillations. The simplest coupling is a linear one, with an interaction energy

$$\hat{H}^{\text{ext}}(t) = -\hat{O}_H(t) \delta j(t), \quad (2.446)$$

where $j(t)$ is some external source. Inserting (2.446) into (2.445) yields the linear-response formula

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = i \int_{-\infty}^{\infty} dt' G_{OO}^R(t, t') \delta j(t'), \quad (2.447)$$

where G_{OO}^R is the retarded Green function of two operators $\hat{O}$:

$$G_{OO}^R(t, t') = \Theta(t - t') \langle \Psi_H | [\hat{O}_H(t), \hat{O}_H(t')] | \Psi_H \rangle. \quad (2.448)$$

At frequencies where the Fourier transform of $G_{OO}(t, t')$ is singular, the slightest disturbance causes a large response. This is the well-known resonance phenomenon found in any oscillating system. Whenever the external frequency ω hits an eigenfrequency, the Fourier transform of the Green function diverges. Usually, the eigenfrequencies of a complicated N -body system are determined by calculating (2.448) and by finding the singularities in ω .

It is easy to generalize this description to a thermal ensemble at a nonzero temperature. The principal modification consists in the replacement of the ground state expectation by the thermal average

$$\langle \hat{O} \rangle_T \equiv \frac{\text{Tr}(e^{-\hat{H}/T} \hat{O})}{\text{Tr}(e^{-\hat{H}/T})}.$$

Using the free energy

$$F = -T \log \text{Tr}(e^{-\hat{H}/T}),$$

this can also be written as

$$\langle \hat{O} \rangle_T = e^{F/T} \text{Tr}(e^{-\hat{H}/T} \hat{O}). \quad (2.449)$$

In a grand-canonical ensemble, $\hat{H}$ must be replaced by $\hat{H} - \mu\hat{N}$ and F by its grand-canonical version F_G (see Section 1.16). At finite temperatures, the linear-response formula (2.447) becomes

$$\delta \langle \hat{O}(t) \rangle_T = i \int_{-\infty}^{\infty} dt' G_{OO}^R(t, t') \delta j(t'), \quad (2.450)$$

where $G_{OO}^R(t, t')$ is the *retarded Green function at nonzero temperature* defined by [recall (1.313)]

$$G_{OO}^R(t, t') \equiv G_{OO}^R(t - t') \equiv \Theta(t - t') e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H(t), \hat{O}_H(t')] \right\}. \quad (2.451)$$

In a realistic physical system, there are usually many observables, say $\hat{O}_H^i(t)$ for $i = 1, 2, \dots, l$, which perform coupled oscillations. Then the relevant retarded Green function is some $l \times l$ matrix

$$G_{ij}^R(t, t') \equiv G_{ij}^R(t - t') \equiv \Theta(t - t') e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^i(t), \hat{O}_H^j(t')] \right\}. \quad (2.452)$$

After a Fourier transformation and diagonalization, the singularities of this matrix render the important physical information on the resonance properties of the system.

The retarded Green function at $T \neq 0$ occupies an intermediate place between the real-time Green function of field theories at $T = 0$, and the imaginary-time Green function used before to describe thermal equilibria at $T \neq 0$. The Green function (2.452) depends both on the real time and on the temperature via an imaginary time.

2.19.2 Spectral Representations of Green Functions for $T \neq 0$

The retarded Green functions are related to the imaginary-time Green functions of equilibrium physics by an analytic continuation. For two arbitrary operators $\hat{O}_H^1$, $\hat{O}_H^2$, the latter is defined by the thermal average

$$G_{12}(\tau, 0) \equiv G_{12}(\tau) \equiv e^{F/T} \text{Tr} \left[e^{-\hat{H}/T} \hat{T}_\tau \hat{O}_H^1(\tau) \hat{O}_H^2(0) \right], \quad (2.453)$$

where $\hat{O}_H(\tau)$ is the *imaginary-time Heisenberg operator*

$$\hat{O}_H(\tau) \equiv e^{\hat{H}\tau} \hat{O} e^{-\hat{H}\tau}. \quad (2.454)$$

To see the relation between $G_{12}(\tau)$ and the retarded Green function $G_{12}^R(t)$, we take a complete set of states $|n\rangle$, insert them between the operators $\hat{O}^1$, $\hat{O}^2$, and expand $G_{12}(\tau)$ for $\tau \geq 0$ into the spectral representation

$$G_{12}(\tau) = e^{F/T} \sum_{n, n'} e^{-E_n/T} e^{(E_n - E_{n'})\tau} \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle. \quad (2.455)$$

Since $G_{12}(\tau)$ is periodic under $\tau \rightarrow \tau + 1/T$, its Fourier representation contains only the discrete Matsubara frequencies $\omega_m = 2\pi mT$:

$$\begin{aligned} G_{12}(\omega_m) &= \int_0^{1/T} d\tau e^{i\omega_m \tau} G_{12}(\tau) \\ &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left(1 - e^{(E_n - E_{n'})/T}\right) \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \\ &\quad \times \frac{-1}{i\omega_m - E_{n'} + E_n}. \end{aligned} \quad (2.456)$$

The retarded Green function satisfies no periodic (or antiperiodic) boundary condition. It possesses Fourier components with *all* real frequencies ω :

$$\begin{aligned} G_{12}^R(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} \Theta(t) e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^1(t), \hat{O}_H^2(0)]_{\mp} \right\} \\ &= e^{F/T} \int_0^{\infty} dt e^{i\omega t} \sum_{n,n'} \left[e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \right. \\ &\quad \left. \mp e^{-E_{n'}/T} e^{-i(E_n - E_{n'})t} \langle n | \hat{O}^2 | n' \rangle \langle n' | \hat{O}^1 | n \rangle \right]. \end{aligned} \quad (2.457)$$

In the second sum we exchange n and n' and perform the integral, after having attached to ω an infinitesimal positive-imaginary part $i\eta$ to ensure convergence. The result is

$$\begin{aligned} G_{12}^R(\omega) &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 - e^{(E_n - E_{n'})/T}\right] \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \\ &\quad \times \frac{i}{\omega - E_{n'} + E_n + i\eta}. \end{aligned} \quad (2.458)$$

By comparing this with (2.456), we see that the thermal Green functions are obtained from the retarded ones by the replacement (for a discussion see [15])

$$\frac{i}{\omega - E_{n'} + E_n + i\eta} \rightarrow \frac{-1}{i\omega_m - E_{n'} + E_n}. \quad (2.459)$$

A similar procedure holds for fermion operators $\hat{O}^i$ (which are not observable). There are only two changes with respect to the boson case. First, in the Fourier expansion of the imaginary-time Green functions, the bosonic Matsubara frequencies ω_m in (2.456) become fermionic. Second, in the definition of the retarded Green functions (2.452), the commutator is replaced by an anticommutator, i.e., the retarded Green function of fermion operators $\hat{O}_H^i$ is defined by

$$G_{ij}^R(t, t') \equiv G_{ij}^R(t - t') \equiv \Theta(t - t') e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^i(t), \hat{O}_H^j(t')]_{+} \right\}. \quad (2.460)$$

These changes produce an opposite sign in front of the $e^{(E_n - E_{n'})/T}$ -term in both of the formulas (2.456) and (2.458). Apart from that, the relation between the two Green functions is again given by the replacement rule (2.459).

At this point it is customary to introduce the *spectral function*

$$\begin{aligned} \rho_{12}(\omega') &= (1 \mp e^{-\omega'/T}) e^{F/T} \\ &\times \sum_{n,n'} e^{-E_n/T} 2\pi \delta(\omega - E_{n'} + E_n) \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle, \end{aligned} \quad (2.461)$$

where the upper and the lower sign hold for bosons and fermions, respectively. Under an interchange of the two operators it behaves like

$$\rho_{12}(\omega') = \mp \rho_{12}(-\omega'). \quad (2.462)$$

Using this spectral function, we may rewrite the Fourier-transformed retarded and thermal Green functions as the following spectral integrals:

$$G_{12}^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \frac{i}{\omega - \omega' + i\eta}, \quad (2.463)$$

$$G_{12}(\omega_m) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \frac{-1}{i\omega_m - \omega'}. \quad (2.464)$$

These equations show how the imaginary-time Green functions arise from the retarded Green functions by a simple analytic continuation in the complex frequency plane to the discrete Matsubara frequencies, $\omega \rightarrow i\omega_m$. The inverse problem is not solvable. It is impossible to reconstruct the retarded Green functions in the entire upper half-plane of ω from the imaginary-time Green functions defined only at the Matsubara frequencies ω_m . The problem is solvable only approximately if other information is available [16]. For instance, the sum rules for canonical fields, which will be derived later in Eq. (2.499) with the ensuing asymptotic condition (2.500), are sufficient to make the continuation unique [17].

Going back to the time variables t and τ , the Green functions are

$$G_{12}^R(t) = \Theta(t) \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') e^{-i\omega' t}, \quad (2.465)$$

$$G_{12}(\tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') T \sum_{\omega_m} e^{-i\omega_m \tau} \frac{-1}{i\omega_m - \omega'}. \quad (2.466)$$

The sum over even or odd Matsubara frequencies on the right-hand side of $G_{12}(\tau)$ was evaluated before as [recall (2.422)]

$$\begin{aligned} T \sum_n e^{-i\omega_n \tau} \frac{-1}{i\omega_n - \omega} &= G_{\omega,e}^p(\tau) = e^{-\omega(\tau-1/2T)} \frac{1}{2 \sin(\omega/2T)} \\ &= e^{-\omega\tau} (1 + f_\omega), \end{aligned} \quad (2.467)$$

and

$$\begin{aligned} T \sum_n e^{-i\omega_n \tau} \frac{-1}{i\omega_n - \omega} &= G_{\omega,e}^a(\tau) = e^{-\omega(\tau-1/2T)} \frac{1}{2 \cos(\omega/2T)} \\ &= e^{-\omega\tau} (1 - f_\omega), \end{aligned} \quad (2.468)$$

with the Bose and Fermi distribution functions (2.422)

$$f_\omega = \frac{1}{e^{\omega/T} \mp 1}, \quad (2.469)$$

respectively.

2.20 Other Important Green Functions

In studying the dynamics of systems at finite temperature, several other Green functions are useful. Let us derive their spectral functions and general properties.

By complete analogy with the retarded Green functions for bosonic and fermionic operators, we may introduce their counterparts, the so-called *advanced Green functions* (compare page 39):

$$G_{12}^A(t, t') \equiv G_{12}^A(t - t') = -\Theta(t' - t) e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^1(t), \hat{O}_H^2(t')]_{\mp} \right\}. \quad (2.470)$$

Their Fourier transforms have the spectral representation

$$G_{12}^A(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \frac{i}{\omega - \omega' - i\eta}, \quad (2.471)$$

differing from the retarded case (2.463) only by the sign of the $i\eta$ -term. This makes the Fourier transforms vanish for $t > 0$, so that the time-dependent Green function has the spectral representation [compare (2.465)]

$$G_{12}^A(t) = -\Theta(-t) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_{12}(\omega) e^{-i\omega t}. \quad (2.472)$$

By subtracting retarded and advanced Green functions, we obtain the thermal expectation value of commutator or anticommutator:

$$C_{12}(t, t') = e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^1(t), \hat{O}_H^2(t')]_{\mp} \right\} = G_{12}^R(t, t') - G_{12}^A(t, t'). \quad (2.473)$$

Note the simple relations:

$$G_{12}^R(t, t') = \Theta(t - t') C_{12}(t, t'), \quad (2.474)$$

$$G_{12}^A(t, t') = -\Theta(t' - t) C_{12}(t, t'). \quad (2.475)$$

When inserting into (2.473) the spectral representations (2.463) and (2.472) of $G_{12}^R(t)$ and $G_{12}^A(t)$ and using the identity (1.337),

$$\frac{i}{\omega - \omega' + i\eta} - \frac{i}{\omega - \omega' - i\eta} = 2 \frac{\eta}{(\omega - \omega')^2 + \eta^2} = 2\pi\delta(\omega - \omega'), \quad (2.476)$$

we obtain the spectral integral representation for the commutator function:¹²

$$C_{12}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_{12}(\omega) e^{-i\omega t}. \quad (2.477)$$

Thus a knowledge of the commutator function $C_{12}(t)$ determines directly the spectral function $\rho_{12}(\omega)$ by its Fourier components

$$C_{12}(\omega) = \rho_{12}(\omega). \quad (2.478)$$

An important role in studying the dynamics of a system in a thermal environment is played by the time-ordered Green functions. They are defined by

$$G_{12}(t, t') \equiv G_{12}(t - t') = e^{F/T} \text{Tr} \left[e^{-\hat{H}/T} \hat{T} \hat{O}_H^1(t) \hat{O}_H^2(t') \right]. \quad (2.479)$$

Inserting intermediate states as in (2.456) we find the spectral representation

$$\begin{aligned} G_{12}(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} \Theta(t) e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} \hat{O}_H^1(t) \hat{O}_H^2(0) \right\} \\ &+ \int_{-\infty}^{\infty} dt e^{i\omega t} \Theta(-t) e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} \hat{O}_H^2(t) \hat{O}_H^1(0) \right\} \\ &= e^{F/T} \int_0^{\infty} dt e^{i\omega t} \sum_{n, n'} e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \\ &\pm e^{F/T} \int_{-\infty}^0 dt e^{i\omega t} \sum_{n, n'} e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n | \hat{O}^2 | n' \rangle \langle n' | \hat{O}^1 | n \rangle. \end{aligned} \quad (2.480)$$

Interchanging again n and n' , this can be written in terms of the spectral function (2.461) as

$$G_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{1}{1 \mp e^{-\omega'/T}} \frac{i}{\omega - \omega' + i\eta} + \frac{1}{1 \mp e^{\omega'/T}} \frac{i}{\omega - \omega' - i\eta} \right]. \quad (2.481)$$

Let us also write down the spectral decomposition of a further operator expression complementary to $C_{12}(t)$ of (2.473), in which boson or fermion fields appear with the “wrong” commutator:

$$A_{12}(t - t') \equiv e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^1(t), \hat{O}_H^2(t')]_{\pm} \right\}. \quad (2.482)$$

This function characterizes the size of fluctuations of the operators O_H^1 and O_H^2 . Inserting intermediate states, we find

$$\begin{aligned} A_{12}(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{O}_H^1(t), \hat{O}_H^2(0)]_{\pm} \right\} \\ &= e^{F/T} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{n, n'} \left[e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \right. \\ &\quad \left. \pm e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n | \hat{O}^2 | n' \rangle \langle n' | \hat{O}^1 | n \rangle \right]. \end{aligned} \quad (2.483)$$

¹²Due to the relation (2.474), the same representation is found by dropping the factor $\Theta(t)$ in (2.465).

In the second sum we exchange n and n' and perform the integral, which now runs over the entire time interval and therefore gives a δ -function:

$$A_{12}(\omega) = e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 \pm e^{(E_n - E_{n'})/T} \right] \langle n | \hat{O}^1 | n' \rangle \langle n' | \hat{O}^2 | n \rangle \times 2\pi \delta(\omega - E_{n'} + E_n). \quad (2.484)$$

In terms of the spectral function (2.461), this has the simple form

$$A_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \tanh^{\mp 1} \frac{\omega'}{2T} \rho_{12}(\omega') 2\pi \delta(\omega - \omega') = \tanh^{\mp 1} \frac{\omega}{2T} \rho_{12}(\omega). \quad (2.485)$$

Thus the expectation value (2.482) of the “wrong” commutator has the time dependence

$$A_{12}(t, t') \equiv A_{12}(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_{12}(\omega) \tanh^{\mp 1} \frac{\omega}{2T} e^{-i\omega(t-t')}. \quad (2.486)$$

There exists another way of writing the spectral representation of the various Green functions. For retarded and advanced Green functions G_{12}^R , G_{12}^A , we decompose in the spectral representations (2.463) and (2.471) according to the rule (1.338):

$$\frac{i}{\omega - \omega' \pm i\eta} = i \left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi \delta(\omega - \omega') \right], \quad (2.487)$$

where $\mathcal{P}$ indicates principal value integration across the singularity, leading to

$$G_{12}^{R,A}(\omega) = i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi \delta(\omega - \omega') \right]. \quad (2.488)$$

Inserting (2.487) into (2.481) we find the alternative representation of the time-ordered Green function

$$G_{12}(\omega) = i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} - i\pi \tanh^{\mp 1} \frac{\omega}{2T} \delta(\omega - \omega') \right]. \quad (2.489)$$

The term proportional to $\delta(\omega - \omega')$ in the spectral representation is commonly referred to as the *absorptive* or *dissipative part* of the Green function. The first term proportional to the principal value is called the *dispersive* or *fluctuation part*.

The relevance of the spectral function $\rho_{12}(\omega')$ in determining both the *fluctuation part* as well as the *dissipative part* of the time-ordered Green function is the content of the important *fluctuation-dissipation theorem*. In more detail, this may be restated as follows: The common spectral function $\rho_{12}(\omega')$ which appears in the commutator function in (2.477), in the retarded Green function in (2.463), and in the *fluctuation part* of the time-ordered Green function in (2.489) determines, after multiplication by a factor $\tanh^{\mp 1}(\omega'/2T)$, the *dissipative part* of the time-ordered Green function in Eq. (2.489).

The three Green functions $-iG_{12}(\omega)$, $-iG_{12}^R(\omega)$, and $-iG_{12}^A(\omega)$ have the same real parts. By comparing Eqs. (2.463) and (2.464), we see that retarded and advanced

Green functions are simply related to the imaginary-time Green function via an analytic continuation. The spectral decomposition (2.489) shows that this is not true for the time-ordered Green function, due to the extra factor $\tanh^{\mp 1}(\omega/2T)$ in the absorptive term.

Another representation of the time-ordered Green function is useful. It is obtained by expressing $\tanh^{\mp 1}$ in terms of the Bose and Fermi distribution functions (2.469) as $\tanh^{\mp 1} = 1 \pm 2f_{\omega}$. Then we can decompose

$$G_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{i}{\omega - \omega' + i\eta} \pm 2\pi f_{\omega} \delta(\omega - \omega') \right]. \quad (2.490)$$

2.21 Hermitian Adjoint Operators

If the two operators $\hat{O}_H^1(t)$, $\hat{O}_H^2(t)$ are Hermitian adjoint to each other,

$$\hat{O}_H^2(t) = [\hat{O}_H^1(t)]^{\dagger}, \quad (2.491)$$

the spectral function (2.461) can be rewritten as

$$\begin{aligned} \rho_{12}(\omega') &= (1 \mp e^{-\omega'/T}) e^{F/T} \\ &\times \sum_{n,n'} e^{-E_n/T} 2\pi \delta(\omega' - E_{n'} + E_n) |\langle n | \hat{O}_H^1(t) | n' \rangle|^2. \end{aligned} \quad (2.492)$$

This shows that

$$\begin{aligned} \rho_{12}(\omega') \omega' &\geq 0 && \text{for bosons,} \\ \rho_{12}(\omega') &\geq 0 && \text{for fermions.} \end{aligned} \quad (2.493)$$

This property makes it possible to derive several useful inequalities between various diagonal Green functions.

Under the condition (2.491), the expectation values of anticommutators and commutators satisfy the time-reversal relations

$$G_{12}^A(t, t') = \mp G_{21}^R(t', t)^*, \quad (2.494)$$

$$A_{12}(t, t') = \pm A_{21}(t', t)^*, \quad (2.495)$$

$$C_{12}(t, t') = \mp C_{21}(t', t)^*, \quad (2.496)$$

$$G_{12}(t, t') = \pm G_{21}(t', t)^*. \quad (2.497)$$

Examples are the corresponding functions for creation and annihilation operators which will be treated in detail below. More generally, these properties hold for any interacting nonrelativistic particle fields $\hat{O}_H^1(t) = \hat{\psi}_{\mathbf{p}}(t)$, $\hat{O}_H^2(t) = \hat{\psi}_{\mathbf{p}}^{\dagger}(t)$ of a specific momentum $\mathbf{p}$.

Such operators satisfy, in addition, the canonical equal-time commutation rules at each momentum:

$$[\hat{\psi}_{\mathbf{p}}(t), \hat{\psi}_{\mathbf{p}}^{\dagger}(t)] = 1. \quad (2.498)$$

Using (2.473) and (2.477), we derive from this the *spectral function sum rule*:

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') = 1. \quad (2.499)$$

For a canonical free field with $\rho_{12}(\omega') = 2\pi\delta(\omega' - \omega)$, this sum rule is of course trivially fulfilled. In general, the sum rule ensures the large- ω behavior of imaginary-time Green functions of canonically conjugate field operators, the retarded expressions depending on real time, and the advanced expressions to be the same as for a free particle, i.e.,

$$G_{12}(\omega_m) \xrightarrow{\omega_m \rightarrow \infty} \frac{i}{\omega_m}, \quad G_{12}^{R,A}(\omega) \xrightarrow{\omega \rightarrow \infty} \frac{1}{\omega}. \quad (2.500)$$

2.22 Harmonic Oscillator Green Functions for $T \neq 0$

As an example, consider a single harmonic oscillator of frequency Ω or, equivalently, a free particle at a point in the second-quantized field formalism. We shall start with the second representation.

2.22.1 Creation Annihilation Operators

The operators $\hat{O}_H^1(t)$ and $\hat{O}_H^2(t)$ are the creation and annihilation operators in the Heisenberg picture

$$\hat{a}_H^\dagger(t) = \hat{a}^\dagger e^{i\Omega t}, \quad \hat{a}_H(t) = \hat{a} e^{-i\Omega t}. \quad (2.501)$$

The eigenstates of the Hamilton operator

$$\hat{H} = \frac{1}{2} (\hat{p}^2 + \Omega^2 \hat{x}^2) = \frac{\omega}{2} (\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger) = \omega \left(\hat{a}^\dagger \hat{a} \pm \frac{1}{2} \right) \quad (2.502)$$

are

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle, \quad (2.503)$$

with the eigenvalues $E_n = (n \pm 1/2)\Omega$ for $n = 0, 1, 2, 3, \dots$ or $n = 0, 1$, if $\hat{a}^\dagger$ and $\hat{a}$ commute or anticommute, respectively. In the second-quantized field interpretation the energies are $E_n = n\Omega$ and the final Green functions are the same. The spectral function $\rho_{12}(\omega')$ is trivial to calculate. The Schrödinger operator $\hat{O}^2 = \hat{a}^\dagger$ can connect the state $|n\rangle$ only to $\langle n+1|$, with the matrix element $\sqrt{n+1}$. The operator $\hat{O}^1 = \hat{a}$ does the opposite. Hence we have

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega)(1 \mp e^{-\Omega/T})e^{F/T} \sum_{n=0}^{\infty,0} e^{-(n \pm 1/2)\Omega/T} (n+1). \quad (2.504)$$

Now we make use of the explicit partition functions of the oscillator whose paths satisfy periodic and antiperiodic boundary conditions:

$$Z_\Omega \equiv e^{-F/T} = \sum_{n=0}^{\infty,1} e^{-(n \pm 1/2)\Omega/T} = \left\{ \begin{array}{cc} [2 \sinh(\Omega/2T)]^{-1} & \text{for bosons} \\ 2 \cosh(\Omega/2T) & \text{for fermions} \end{array} \right\}. \quad (2.505)$$

These allow us to calculate the sums in (2.504) as follows

$$\begin{aligned} \sum_{n=0}^{\infty} e^{-(n+1/2)\Omega/T} (n+1) &= \left(-T \frac{\partial}{\partial \Omega} + \frac{1}{2} \right) e^{-F/T} = (1 \mp e^{-\Omega/T})^{-1} e^{-F/T}, \\ \sum_{n=0}^0 e^{-(n-1/2)\Omega/T} (n+1) &= e^{\Omega/2T} = (1 + e^{-\Omega/T})^{-1} e^{-F/T}. \end{aligned} \quad (2.506)$$

The spectral function $\rho_{12}(\omega')$ of the single oscillator quantum of frequency Ω is therefore given by

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega). \quad (2.507)$$

With it, the retarded and imaginary-time Green functions become

$$G_\Omega^R(t, t') = \Theta(t - t') e^{-\Omega(t-t')}, \quad (2.508)$$

$$G_\Omega(\tau, \tau') = -T \sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')} \frac{1}{i\Omega_m - \Omega} \quad (2.509)$$

$$= e^{-\Omega(\tau-\tau')} \left\{ \begin{array}{cc} 1 \pm n_\Omega & \text{for } \tau \geq \tau' \\ \pm n_\Omega & \text{for } \tau < \tau' \end{array} \right\}, \quad (2.510)$$

with the average particle number f_Ω of (2.469). The commutation function, for instance, is by (2.477) and (2.507):

$$C_{12}(t, t') = e^{-i\Omega(t-t')}, \quad (2.511)$$

and the correlation function of the “wrong commutator” is from (2.486) and (2.507):

$$A_\Omega(t, t') = \tanh^{\mp 1} \frac{\Omega}{2T} e^{-i\Omega(t-t')}. \quad (2.512)$$

Of course, these harmonic-oscillator expressions could have been obtained directly by starting from the defining operator equations. For example, the commutator function

$$C_\Omega(t, t') = e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} [\hat{a}_H(t), \hat{a}_H^\dagger(t')]_{\mp} \right\} \quad (2.513)$$

turns into (2.511) by using the commutation rule at different times:

$$[\hat{a}_H(t), \hat{a}_H^\dagger(t')] = e^{-i\Omega(t-t')}, \quad (2.514)$$

which follows from (2.501). Since the right-hand side is a c -number, the thermodynamic average is trivial:

$$e^{F/T} \text{Tr}(e^{-\hat{H}/T}) = 1. \quad (2.515)$$

After this, the relations (2.474) and (2.475) determine the retarded and advanced Green functions

$$G_{\Omega}^R(t - t') = \Theta(t - t') e^{-i\Omega(t-t')}, \quad G_{\Omega}^A(t - t') = -\Theta(t' - t) e^{-i\Omega(t-t')}. \quad (2.516)$$

For the Green function at imaginary times

$$G_{\Omega}(\tau, \tau') \equiv e^{F/T} \text{Tr} \left[e^{-\hat{H}/T} \hat{T}_{\tau} \hat{a}_H(\tau) \hat{a}_H^{\dagger}(\tau') \right], \quad (2.517)$$

the expression (2.510) is found using [see (2.518)]

$$\begin{aligned} \hat{a}_H^{\dagger}(\tau) &\equiv e^{\hat{H}\tau} \hat{a}^{\dagger} e^{-\hat{H}\tau} = \hat{a}^{\dagger} e^{\Omega\tau}, \\ \hat{a}_H(\tau) &\equiv e^{\hat{H}\tau} \hat{a} e^{-\hat{H}\tau} = \hat{a} e^{-\Omega\tau}, \end{aligned} \quad (2.518)$$

and the summation formula (2.506).

The “wrong” commutator function (2.512) can, of course, be immediately derived from the definition

$$A_{12}(t - t') \equiv e^{F/T} \text{Tr} \left\{ e^{-\hat{H}/T} \left[\hat{a}_H(t), \hat{a}_H^{\dagger}(t') \right]_{\pm} \right\} \quad (2.519)$$

using (2.501) and inserting intermediate states.

For the temporal behavior of the time-ordered Green function we find from (2.481):

$$G_{\Omega}(\omega) = \left(1 \mp e^{-\Omega/T}\right)^{-1} G_{\Omega}^R(\omega) + \left(1 \mp e^{\Omega/T}\right)^{-1} G_{\Omega}^A(\omega), \quad (2.520)$$

and from this by a Fourier transformation:

$$\begin{aligned} G_{\Omega}(t, t') &= \left(1 \mp e^{-\Omega/T}\right)^{-1} \Theta(t - t') e^{-i\Omega(t-t')} - \left(1 \mp e^{\Omega/T}\right)^{-1} \Theta(t' - t) e^{-i\Omega(t-t')} \\ &= \left[\Theta(t - t') \pm (e^{\Omega/T} \mp 1)^{-1} \right] e^{-i\Omega(t-t')} = [\Theta(t - t') \pm f_{\Omega}] e^{-i\Omega(t-t')}. \end{aligned} \quad (2.521)$$

The same result is easily obtained by directly evaluating the defining equation using (2.501) and inserting intermediate states:

$$\begin{aligned} G_{\Omega}(t, t') &\equiv G_{\Omega}(t - t') = e^{F/T} \text{Tr} \left[e^{-\hat{H}/T} \hat{T} \hat{a}_H(t) \hat{a}_H^{\dagger}(t') \right] \\ &= \Theta(t - t') \langle \hat{a} \hat{a}^{\dagger} \rangle e^{-i\Omega(t-t')} \pm \Theta(t' - t) \langle \hat{a}^{\dagger} \hat{a} \rangle e^{-i\Omega(t-t')} \\ &= \Theta(t - t') (1 \pm f_{\Omega}) e^{-i\Omega(t-t')} \pm \Theta(t' - t) f_{\Omega} e^{-i\Omega(t-t')}, \end{aligned} \quad (2.522)$$

which is the same as (2.521). For the correlation function with a and $a^{\dagger}$ interchanged,

$$\bar{G}_{\Omega}(t, t') \equiv G_{\Omega}(t - t') = e^{F/T} \text{Tr} \left[e^{-\hat{H}/T} \hat{T} \hat{a}_H^{\dagger}(t) \hat{a}_H(t') \right], \quad (2.523)$$

we find in this way

$$\begin{aligned} \bar{G}_{\Omega}(t, t') &= \Theta(t - t') \langle \hat{a}^{\dagger} \hat{a} \rangle e^{-i\Omega(t-t')} \pm \Theta(t' - t) \langle \hat{a} \hat{a}^{\dagger} \rangle e^{-i\Omega(t-t')} \\ &= \Theta(t - t') f_{\Omega} e^{-i\Omega(t-t')} \pm \Theta(t' - t) (1 \pm f_{\Omega}) e^{-i\Omega(t-t')} \end{aligned} \quad (2.524)$$

in agreement with (2.497).

2.22.2 Real Field Operators

From the above expressions it is easy to construct the corresponding Green functions for the position operators of the harmonic oscillator $\hat{x}(t)$. It will be useful to keep the discussion more general by admitting oscillators which are not necessarily mass points in space but can be field variables. Thus we shall use, instead of $\hat{x}(t)$, the symbol $\varphi(t)$, and call this a field variable. We decompose the field as

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2M\Omega}} (\hat{a}e^{-i\Omega t} + \hat{a}^\dagger e^{i\Omega t}), \quad (2.525)$$

using in this section physical units. The commutator function (2.473) is directly

$$C(t, t') \equiv \langle [\hat{\varphi}(t), \hat{\varphi}(t')]_{\mp} \rangle_{\rho} = -\frac{\hbar}{2M\Omega} 2i \sin \Omega(t - t'), \quad (2.526)$$

implying a spectral function [recall (2.477)]

$$\rho(\omega') = \frac{1}{2M\Omega} 2\pi [\delta(\omega' - \Omega) - \delta(\Omega' + \Omega)]. \quad (2.527)$$

The real operator $\hat{\varphi}(t)$ behaves like the difference of a particle of frequency Ω and $-\Omega$, with an overall factor $1/2M\Omega$. It is then easy to find the retarded and advanced Green functions of the operators $\hat{\varphi}(t)$ and $\hat{\varphi}(t')$:

$$G^R(t, t') = \frac{\hbar}{2M\Omega} [G_{\Omega}^R(t, t') - G_{-\Omega}^R(t, t')] = -\frac{\hbar}{2M\Omega} \Theta(t - t') 2i \sin \Omega(t - t'), \quad (2.528)$$

$$G^A(t, t') = \frac{\hbar}{2M\Omega} [G_{\Omega}^A(t, t') - G_{-\Omega}^A(t, t')] = \frac{\hbar}{2M\Omega} \Theta(t - t') 2i \sin \Omega(t' - t). \quad (2.529)$$

From the spectral representation (2.486), we obtain for the “wrong commutator”

$$A(t, t') = \langle [\hat{\varphi}(t), \hat{\varphi}(t')]_{\mp} \rangle = \frac{\hbar}{2M\Omega} \coth^{\pm 1} \frac{\Omega}{2k_B T} 2 \cos \Omega(t - t'). \quad (2.530)$$

The relation with (2.526) is again a manifestation of the fluctuation-dissipation theorem (2.486).

The average of these two functions yields the time-dependent correlation function at finite temperature, containing only the product of the operators:

$$G^P(t, t') \equiv \langle \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} [(1 \pm 2f_{\Omega}) \cos \Omega(t - t') - i \sin \Omega(t - t')], \quad (2.531)$$

with the average particle number f_{Ω} of (2.469). In the limit of zero temperature where $f_{\Omega} \equiv 0$, this reduces to

$$G^P(t, t') = \langle \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} e^{-i\Omega(t-t')}. \quad (2.532)$$

The time-ordered Green function is obtained from this by the obvious relation

$$G(t, t') = \Theta(t - t')G^P(t, t') \pm \Theta(t' - t)G^P(t', t) = \frac{1}{2} [A(t, t') + \epsilon(t - t')C(t, t')], \quad (2.533)$$

where $\epsilon(t - t')$ is the step function of Eq. (1.323). Explicitly, the time-ordered Green function is

$$G(t, t') \equiv \langle \hat{T} \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} [(1 \pm 2f_\Omega) \cos \Omega|t - t'| - i \sin \Omega|t - t'|], \quad (2.534)$$

which reduces for $T \rightarrow 0$ to

$$G(t, t') = \langle \hat{T} \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} e^{-i\Omega|t-t'|}. \quad (2.535)$$

Thus, as a mnemonic rule, a finite temperature is introduced into a zero-temperature Green function by simply multiplying the real part of the exponential function by a factor $1 \pm 2f_\Omega$. This is another way of stating the *fluctuation-dissipation theorem*.

There is another way of writing the time-ordered Green function (2.534) in the bosonic case:

$$G(t, t') \equiv \langle \hat{T} \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} \frac{\cosh \left[\frac{\Omega}{2} (\hbar\beta - i|t - t'|) \right]}{\sinh \frac{\hbar\Omega\beta}{2}}. \quad (2.536)$$

For $t - t' > 0$, this coincides precisely with the periodic Green function $G_e^p(\tau, \tau') = G_e^p(\tau - \tau')$ at imaginary-times $\tau > \tau'$ [see (2.431)], if τ and τ' are continued analytically to it and it' , respectively. Decomposing (2.534) into real and imaginary parts, we see by comparison with (2.533) that anticommutator and commutator functions are the doubled real and imaginary parts of the time-ordered Green function:

$$A(t, t') = 2 \operatorname{Re} G(t, t'), \quad C(t, t') = 2i \operatorname{Im} G(t, t'). \quad (2.537)$$

In the fermionic case, the hyperbolic functions $\cosh$ and $\sinh$ in numerator and denominator are simply interchanged, and the result coincides with the analytically continued antiperiodic imaginary-time Green function [see again (2.431)].

For real fields $\hat{\varphi}(t)$, the time-reversal properties (2.494)–(2.497) of the Green functions become

$$G^A(t, t') = \mp G^R(t', t), \quad (2.538)$$

$$A(t, t') = \pm A(t', t), \quad (2.539)$$

$$C(t, t') = \mp C(t', t), \quad (2.540)$$

$$G(t, t') = \pm G(t', t). \quad (2.541)$$

Appendix 2A Permutation Group and Representations on n -Particle Wave Functions

A permutation of n particles is given by

$$P = \begin{pmatrix} 1 & 2 & \dots & n \\ p(1) & p(2) & \dots & p(n) \end{pmatrix}, \quad (2A.1)$$

where $p(i)$ are all possible one-to-one mappings of the integers $1, 2, 3, \dots, n$ onto themselves. In the notation (2A.1) the order of the columns is irrelevant, i.e., the same permutation can be written in any other form in which the columns are interchanged with each other, for example:

$$P = \begin{pmatrix} 2 & 1 & \dots & n \\ p(2) & p(1) & \dots & p(n) \end{pmatrix}. \quad (2A.2)$$

Given n particles at positions $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, the permutation P may be taken to change the position $\mathbf{x}_1$ to $\mathbf{x}_{p(1)}$, $\mathbf{x}_2$ to $\mathbf{x}_{p(2)}$, etc., i.e., we define P to act directly on the indices:

$$P\mathbf{x}_i \equiv \mathbf{x}_{p(i)}. \quad (2A.3)$$

Given an n -particle wave function $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t)$, it behaves under P as follows:

$$\begin{aligned} P\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t) &= \psi(P\mathbf{x}_1, P\mathbf{x}_2, \dots, P\mathbf{x}_n; t) \\ &= \psi(\mathbf{x}_{p(1)}, \mathbf{x}_{p(2)}, \dots, \mathbf{x}_{p(n)}; t). \end{aligned} \quad (2A.4)$$

There exists a different but equivalent definition of permutations, to be denoted by P' , in which the variables $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ of the wave functions are taken from their places $1, 2, \dots, n$ in the list of arguments of $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t)$ and moved to the positions $p(1), p(2), \dots, p(n)$ in this list, i.e.,

$$P'\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t) \equiv \psi(\dots, \mathbf{x}_1, \dots, \mathbf{x}_2, \dots; t), \quad (2A.5)$$

where $\mathbf{x}_1$ is now at position $p(1)$, $\mathbf{x}_2$ at position $p(2)$, etc. The difference between the two definitions is seen in the simple example:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1; t), \quad (2A.6)$$

to be compared with

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}' \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2; t). \quad (2A.7)$$

In the following we shall use only the first definition, but all statements to be derived would hold as well if we use the second one throughout the remainder of this appendix.

For n elements there are $n!$ different permutations P . Given any two permutations

$$P = \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix}$$

and

$$Q = \begin{pmatrix} 1 & \dots & n \\ q(1) & \dots & q(n) \end{pmatrix},$$

a product is defined by rewriting Q as

$$Q = \begin{pmatrix} p(1) & \dots & p(n) \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix}$$

and setting

$$\begin{aligned} QP &\equiv \begin{pmatrix} p(1) & \dots & p(n) \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix} \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix} \\ &\equiv \begin{pmatrix} 1 & \dots & n \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix}. \end{aligned} \quad (2A.8)$$

Every element has an inverse. Indeed, if we apply first P and multiply it by

$$P^{-1} \equiv \begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix}, \quad (2A.9)$$

the operation $P^{-1}P$ returns all elements to their original places:

$$P^{-1}P = \begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix} \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix} = \begin{pmatrix} 1 & \dots & n \\ 1 & \dots & n \end{pmatrix} \equiv I. \quad (2A.10)$$

The right-hand side is defined as the *identity permutation* I .

It can easily be checked that for three permutations PQR , the product is associative:

$$P(QR) = (PQ)R. \quad (2A.11)$$

Thus the $n!$ permutations of n elements form a group, also called the *symmetric group* S_n .

If P is such that only two elements $p(i)$ are different from i , it can be written as

$$T_{ij} = \begin{Bmatrix} 1 & 2 & \dots & i & \dots & j & \dots & n \\ 1 & 2 & \dots & p(i) & \dots & p(j) & \dots & n \end{Bmatrix}. \quad (2A.12)$$

It is called a *transposition*, also denoted in short by (i, j) . Only the elements i and j are interchanged. Every permutation can be decomposed into a product of transpositions. There are many ways of doing this. However, each permutation decomposes either into an even or an odd number of transpositions. Therefore each permutation can be characterized by this property. As mentioned on p. 86, it is called the *parity of the permutation*. It is useful to introduce the function

$$\epsilon_P = \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \text{ for } \begin{Bmatrix} P=\text{even} \\ P=\text{odd} \end{Bmatrix}, \quad (2A.13)$$

which indicates the parity. This function satisfies the identity

$$\epsilon_{PQ} \equiv \epsilon_P \epsilon_Q. \quad (2A.14)$$

Indeed, if P and Q are decomposed into transpositions,

$$\begin{aligned} P &= \prod_{(ij)} T_{(ij)}, & n \text{ factors,} \\ Q &= \prod_{(i'j')} T_{(i'j')}, & m \text{ factors,} \end{aligned} \quad (2A.15)$$

then the product

$$PQ = \prod_{(ij)} \prod_{(i'j')} T_{(ij)} T_{(i'j')} \quad (2A.16)$$

contains $n \times m$ transpositions. This number is even if n and m are both even or odd, and odd, if one of them is odd and the other even. Since the identity is trivially even, the inverse P^{-1} of a permutation has the same parity as P itself, i.e.,

$$\epsilon_{P^{-1}} = \epsilon_P. \quad (2A.17)$$

Let us find the irreducible representations of the permutation group on the Hilbert space of n -particle wave functions. The permutation on this space is defined by (2A.4). The irreducible representations can be classified with the help of so-called *Young tableaux*. These are arrays of n boxes of the form

$$\begin{array}{cccccccccc}
 \boxed{1} & \boxed{2} & \boxed{3} & \boxed{4} & \boxed{5} & \boxed{6} & \boxed{7} & \boxed{8} & \boxed{9} & \boxed{\cdot} & \boxed{\cdot} \\
 \boxed{\cdot} & \boxed{\cdot} & \boxed{\cdot} & & & & & & & & \\
 \boxed{\cdot} & \boxed{\cdot} & \boxed{\cdot} & & & & & & & & \\
 \boxed{\cdot} & \boxed{\cdot} & & & & & & & & & \\
 \boxed{\cdot} & & & & & & & & & & \\
 \boxed{n} & & & & & & & & & &
 \end{array} \quad (2A.18)$$

The boxes are filled successively with the numbers 1 to n . The numbers of boxes in the rows $m_1, m_2, m_3, \dots$ are ordered as

$$m_1 \geq m_2 \geq m_3 \geq \dots \quad \sum_{k=1}^n m_k = n.$$

Each tableau defines a symmetry type of a set of wave functions on which the group of permutations is represented irreducibly. The symmetry types are constructed as follows. Let p_i be all permutations of the numbers i in the row (including the identity), and let q_j be the corresponding operations in the column j . Then we define the operations P and Q as

$$\begin{aligned}
 P &= \prod_i (\sum p_i), \\
 Q &= \prod_j (\sum \epsilon_{q_j} q_j).
 \end{aligned}$$

The product is taken over all rows i or all columns j , and ϵ_q is the parity function (2A.13). Now apply the operation QP to the *indices* of the wave function $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$.

As an example, take the Hilbert space of three-particle wave functions. There are three different Young tableaux corresponding to the following irreducible representations of S_3 :

$$\begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline \end{array} \quad P = \sum p \text{ (sum over all 6 elements of } S_3), \quad Q = 1 \quad (2A.19)$$

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array} \quad P = 1 + (1, 2), \quad Q = 1 - (1, 3) \quad (2A.20)$$

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} \quad P = 1, \quad Q = \sum \epsilon_q q \text{ (sum over all 6 elements of } S_3). \quad (2A.21)$$

The wave functions associated with these have the form

$$\begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline \end{array} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \begin{aligned} &\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1) \\ &+ \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) + \psi(\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) \\ &+ \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) + \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1), \end{aligned} \quad (2A.22)$$

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \begin{aligned} &\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) \\ &- \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1), \end{aligned} \quad (2A.23)$$

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \begin{aligned} &\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1) \\ &+ \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) - \psi(\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) \\ &- \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1). \end{aligned} \quad (2A.24)$$

These wave functions are easily normalized by dividing them by the square root of the number of terms in each expression, i.e., $\sqrt{6}$, 2 , $\sqrt{6}$, in the three cases. The horizontal array leads to the completely symmetrized wave function, the vertical array to the completely antisymmetrized one. The second tableau results in a mixed symmetry.

Four-particle wave functions are classified with the following tableaux:

$$\begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline \end{array} + \begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline 4 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} + \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} + \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline \end{array}. \quad (2A.25)$$

Consider, for instance, the third of these

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array}.$$

This stands for the permutation operator QP with

$$P = (1 + (3, 4))(1 + (1, 2)), \quad Q = (1 - (2, 4))(1 - (1, 3)), \quad (2A.26)$$

so that

$$\begin{aligned} P\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) &= \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4) \\ &\quad + \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3), \\ QP\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) &= \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4) \\ &\quad - \psi(\mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_2) + \psi(\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_2) \\ &\quad + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_4) \\ &\quad - \psi(\mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) + \psi(\mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) \\ &\quad + \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_1) \\ &\quad - \psi(\mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_2, \mathbf{x}_1) \\ &\quad + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_1) \\ &\quad - \psi(\mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1). \end{aligned} \quad (2A.27)$$

There exists an alternative but mathematically equivalent prescription of forming the wave functions of different symmetry types based on the permutations P' introduced in (2A.5). Instead of performing the permutations on the indices, one exchanges the positions of the arguments in the wave functions to produce $\psi(\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_n)$. As an example, take the tableaux

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array},$$

whose associated wave function was written down in (2A.23). The alternative wave function would be

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array}' \quad \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1) - \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2), \quad (2A.29)$$

with the last two terms differing from those in (2A.23).

The following formula specifies the dimensionality with which the group elements of the permutation group are represented for these symmetry classes:

$$d = \frac{n!}{\prod_{i,j} h_{ij}}, \quad (2A.30)$$

where h_{ij} is the number of boxes to the right of the position ij , plus the number of boxes below the position ij in the tableau, plus 1 for the box on the position ij itself.

As a useful check for the calculated dimensions we may use the *dimensionality theorem*, by which the squares of the dimensions d of all inequivalent, irreducible, unitary representations add up to the order of the group, here $n!$:

$$\sum d^2 = n! . \quad (2A.31)$$

This is a direct consequence of the *great orthogonality theorem* of such representations for any finite group.

For the permutation group at hand, one has the additional property that the defining representation contains each irreducible representation with a multiplicity equal to its dimension.

For three particles, the symmetric and antisymmetric representations

$$\boxed{1}\boxed{2}\boxed{3}$$

and

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array}$$

are $3!/3 \times 2 \times 1 = 1$ -dimensional. The mixed representation

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array}$$

is $3!/3 \times 1 \times 1 = 2$ -dimensional. These dimensions fulfill the dimensionality formula (2A.31):

$$1^2 + 1^1 + 2^2 = 3! . \quad (2A.32)$$

Similarly, one has for four particles the dimensionalities

$$\begin{array}{ll} \boxed{1}\boxed{2}\boxed{3}\boxed{4} & d = \frac{4!}{4 \times 3 \times 2 \times 1} = 1, \\ \begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline 4 & & \\ \hline \end{array} & d = \frac{4!}{4 \times 2 \times 1 \times 1} = 3, \\ \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} & d = \frac{4!}{3 \times 2 \times 2 \times 1} = 2, \\ \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline 4 & \\ \hline \end{array} & d = \frac{4!}{4 \times 1 \times 2 \times 1} = 3, \\ \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline \end{array} & d = \frac{4!}{4 \times 3 \times 2 \times 1} = 1. \end{array} \quad (2A.33)$$

Again we check that these dimensions fulfill the dimensionality formula (2A.31):

$$1^2 + 3^2 + 2^2 + 3^2 + 1^2 = 4! . \quad (2A.34)$$

Appendix 2B Treatment of Singularities in Zeta-Function

Here we show how to evaluate the sums which determine the would-be critical temperatures of a Bose gas in a box and in a harmonic trap.

2B.1 Finite Box

According to Eqs. (2.364), (2.369), and (2.371), the relation between temperature $T = \hbar^2 \pi^2 / b M L^2 k_B$ and the fugacity z_D at a fixed particle number N in a finite D -dimensional box is determined by the equation

$$N = N_n(T) + N_{\text{cond}}(T) = S_D(z_D) + \frac{z_D}{1 - z_D}. \quad (2B.1)$$

Here $S_D(z_D)$ is the subtracted infinite sum

$$S_D(z_D) \equiv \sum_{w=1}^{\infty} [Z_1^D(wb) e^{wDb/2} - 1] z_D^w, \quad (2B.2)$$

containing the D th power of a one-particle partition function in the box $Z_1(b) = \sum_{k=1}^{\infty} e^{-bk^2/2}$. The would-be critical temperature is found by equating this sum at $z_D = 1$ with the total particle number N . We shall rewrite $Z_1(b)$ as

$$Z_1(b) = e^{-b/2} \left[1 + e^{-3b/2} \sigma_1(b) \right], \quad (2B.3)$$

where $\sigma_1(b)$ is related to the elliptic theta function (2.366) by

$$\sigma_1(b) \equiv \sum_{k=2}^{\infty} e^{-(k^2-4)b/2} = \frac{e^{2b}}{2} \left[\vartheta_3(0, e^{-b/2}) - 1 - 2e^{-b/2} \right]. \quad (2B.4)$$

According to Eq. (2.368), this has the small- b behavior

$$\sigma_1(b) = \sqrt{\frac{\pi}{2b}} e^{2b} - e^{3b/2} - \frac{1}{2} e^{2b} + \dots \quad (2B.5)$$

The omitted terms are exponentially small as long as $b < 1$ [see the sum over m in Eq. (2.367)]. For large b , these terms become important to ensure an exponentially fast falloff like $e^{-3b/2}$. Inserting (2B.3) into (2B.2), we find

$$S_D(1) \equiv D \sum_{w=1}^{\infty} \left[\sigma_1(wb) e^{-3wb/2} + \frac{D-1}{2} \sigma_1^2(wb) e^{-6wb/2} + \frac{(D-1)(D-2)}{6} \sigma_1^3(wb) e^{-9wb/2} \right]. \quad (2B.6)$$

Inserting here the small- b expression (2B.5), we obtain

$$S_2(1) \equiv \sum_{w=1}^{\infty} \left(\frac{\pi}{2wb} e^{wb} - \sqrt{\frac{\pi}{2wb}} e^{wb} + \frac{1}{4} e^{wb} - 1 \right) + \dots, \quad (2B.7)$$

$$S_3(1) \equiv \sum_{w=1}^{\infty} \left(\sqrt{\frac{\pi}{2wb}}^3 e^{3wb/2} - \frac{3}{2} \frac{\pi}{2wb} e^{3wb/2} + \frac{3}{4} \sqrt{\frac{\pi}{2wb}} e^{3wb/2} - \frac{1}{8} e^{3wb/2} - 1 \right) + \dots, \quad (2B.8)$$

the dots indicating again exponentially small terms. The sums are convergent only for negative b , this being a consequence of the approximate nature of these expressions. If we evaluate them in this regime, the sums produce polylogarithmic functions

$$\zeta \nu(z) \equiv \sum_{w=1}^{\infty} \frac{z^w}{w^\nu}, \quad (2B.9)$$

and we find, using the property at the origin,¹³

$$\zeta(0) = -1/2, \quad \zeta'(0) = -\frac{1}{2} \log 2\pi, \quad (2B.10)$$

¹³I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 9.541.4.

which imply $\sum_{w=1}^{\infty} 1 = \zeta(0) = -1/2$, $-\sum_{w=1}^{\infty} \log w = \zeta'(0) = -\frac{1}{2} \log 2\pi$, such that

$$S_2(1) = \zeta_1(e^b) - \sqrt{\frac{\pi}{2b}} \zeta_{1/2}(e^b) + \frac{1}{4} \zeta_0(e^b) - \zeta(0) + \dots \quad (2B.11)$$

$$S_3(1) = \sqrt{\frac{\pi^3}{2b}} \zeta_{3/2}(e^{3b/2}) - \frac{3}{2} \frac{\pi}{2b} \zeta_1(e^{3b/2}) + \frac{3}{4} \sqrt{\frac{\pi}{2b}} \zeta_1(e^{3b/2}) - \frac{1}{8} \zeta_0(e^{3b/2}) - \zeta(0) + \dots \quad (2B.12)$$

These expressions can now be expanded in powers of b with the help of the Robinson expansion given in the footnote on p. 8. Afterwards, b is continued analytically to positive values and we obtain

$$S_2(1) = -\frac{\pi}{2b} \log(C_2 b) - \sqrt{\frac{\pi}{2b}} \zeta(1/2) + \frac{1}{8} (3 - 2\pi) + \mathcal{O}(b^{1/2}), \quad (2B.13)$$

$$S_3(1) = \sqrt{\frac{\pi^3}{2b}} \zeta(3/2) + \frac{3\pi}{4b} \log(C_3 b) + \frac{3}{4} \sqrt{\frac{\pi}{2b}} \zeta(1/2) (1 + \pi) + \frac{9}{16} (1 + \pi) + \mathcal{O}(b^{1/2}). \quad (2B.14)$$

The constants $C_{2,3}, C'_{2,3}$ inside the logarithms turn out to be complex, implying that the limiting expressions (2B.7) and (2B.8) cannot be used reliably. A proper way to proceed goes as follows: We subtract from $S_D(1)$ terms which remove the small- b singularities by means of modifications of (2B.7) and (2B.8) which have the same small- b expansion up to b^0 :

$$\tilde{S}_2(1) \equiv \sum_{w=1}^{\infty} \left(\frac{\pi}{2wb} - \sqrt{\frac{\pi}{2wb}} + \frac{4\pi - 3}{4} \right) e^{-wb} + \dots, \quad (2B.15)$$

$$\tilde{S}_3(1) \equiv \sum_{w=1}^{\infty} \left[\sqrt{\frac{\pi^3}{2wb}} - \frac{3}{2} \frac{\pi}{2wb} + \frac{3}{4} (1 + 2\pi) \sqrt{\frac{\pi}{2wb}} - \frac{9}{8} (1 + 2\pi) \right] e^{-3wb/2} + \dots \quad (2B.16)$$

In these expressions, the sums over w can be performed for positive b , yielding

$$\tilde{S}_2(1) \equiv \frac{\pi}{2b} \zeta_1(e^{-b}) - \sqrt{\frac{\pi}{2b}} \zeta_{1/2}(e^{-b}) + \frac{4\pi - 3}{4} \zeta_0(e^{-b}) + \dots, \quad (2B.17)$$

$$\begin{aligned} \tilde{S}_3(1) \equiv & \sqrt{\frac{\pi^3}{2b}} \zeta_{3/2}(e^{-3b/2}) - \frac{3}{2} \frac{\pi}{2b} \zeta_1(e^{-3b/2}) + \frac{3}{4} (1 + 2\pi) \sqrt{\frac{\pi}{2b}} \zeta_{1/2}(e^{-3b/2}) \\ & - \frac{9}{8} (1 + 2\pi) \zeta_0(e^{-3b/2}) + \dots \end{aligned} \quad (2B.18)$$

Inserting again the Robinson expansion in the footnote on p. 8, we obtain once more the above expansions (2B.13) and (2B.14), but now with the well-determined real constants

$$\tilde{C}_2 = e^{3/2\pi - 2 + \sqrt{2}} \approx 0.8973, \quad \tilde{C}_3 = \frac{3}{2} e^{-2 + 1/\sqrt{3} - 1/\pi} \approx 0.2630. \quad (2B.19)$$

The subtracted expressions $S_D(1) - \tilde{S}_D(1)$ are smooth near the origin, so that the leading small- b behavior of the sums over these can simply be obtained from a numeric integral over w :

$$\int_0^{\infty} dw [S_2(1) - \tilde{S}_2(1)] = -\frac{1.1050938}{b}, \quad \int_0^{\infty} dw [S_3(1) - \tilde{S}_3(1)] = 3.0441. \quad (2B.20)$$

These modify the constants $\tilde{C}_{2,3}$ to

$$C_2 = 1.8134, \quad C_3 = 0.9574. \quad (2B.21)$$

The corrections to the sums over $S_D(1) - \tilde{S}_D(1)$ are of order b^0 and higher. They were already included in the expansions (2B.13) and (2B.14), which only were unreliable as far as $C_{2,3}$ is concerned.

Let us calculate from (2B.14) the finite-size correction to the critical temperature by equating $S_3(1)$ with N . Expressing this in terms of $b_c^{(0)}$ via (2.373), and introducing the ratio $\hat{b}_c \equiv b_c/b_c^{(0)}$ which is close to unity, we obtain the expansion in powers of the small quantity $2b_c^{(0)}/\pi = [\zeta(3/2)/N]^{2/3}$:

$$\hat{b}_c^{3/2} = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{3\sqrt{\hat{b}_c}}{2\zeta(3/2)} \log(C_3 b_c^{(0)} \hat{b}_c) + \frac{2b_c^{(0)}}{\pi} \frac{3}{4\zeta(3/2)} \zeta(1/2)(1+\pi)\hat{b}_c + \dots \quad (2B.22)$$

To lowest order, the solution is simply

$$\hat{b}_c = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{1}{\zeta(3/2)} \log(C_3 b_c^{(0)}) + \dots, \quad (2B.23)$$

yielding the would-be critical temperature to first order in $1/N^{1/3}$ as stated in (2.375). To next order we insert, into the last term, the zero-order solution $\hat{b}_c \approx 1$, and into the second term, the first-order solution (2B.23). This leads to

$$\begin{aligned} \hat{b}_c^{3/2} = & 1 + \frac{3}{2} \sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{1}{\zeta(3/2)} \log(C_3 b_c^{(0)}) \\ & + \frac{2b_c^{(0)}}{\pi} \frac{3}{4\zeta(3/2)} \left\{ \zeta(1/2)(1+\pi) + \frac{1}{\zeta(3/2)} \left[2\log(C_3 b_c^{(0)}) + \log^2(C_3 b_c^{(0)}) \right] \right\} + \dots \end{aligned} \quad (2B.24)$$

Replacing $b_c^{(0)}$ by $(2/\pi) [\zeta(3/2)/N]^{2/3}$, we obtain the ratio $(T_c^{(0)}/T_c)^{3/2}$ between finite- and infinite-size critical temperatures T_c and $T_c^{(0)}$. The first and second-order corrections are plotted in Fig. 2.9, together with precise results from a numeric solution of the equation $N = S_3(1)$.

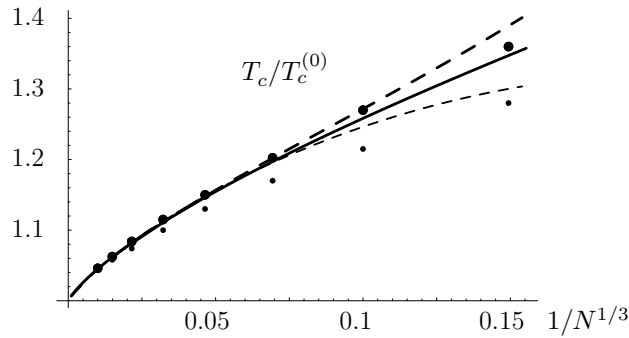


FIGURE 2.9 Finite-size corrections to the critical temperature for $N > 300$, calculated once from the formula $N = S_3(1)$ (solid curve), and once from the expansion (2B.24) (short-dashed up to the order $[b_c^{(0)}]^{1/2} \propto 1/N^{1/3}$, long-dashed up to the order $b_c^{(0)} \propto 1/N^{2/3}$). The fat dots show the peaks in the second derivative $d^2 N_{\text{cond}}(T)/dT^2$. The small dots show the corresponding values for canonical ensembles, for comparison.

2B.2 Harmonic Trap

The sum relevant for the would-be phase transition in a harmonic trap is

$$S_D(b, z_D) = \sum_{w=1}^{\infty} \left[\frac{1}{(1 - e^{-wb})^D} - 1 \right] z_D^w, \quad (2B.25)$$

which determines the number of normal particles in the harmonic trap via

$$N_n(T) = Z_\omega(\beta) \bar{\zeta}_D(\beta \hbar \omega; z_D) \equiv S_D(\beta \hbar \omega, z_D). \quad (2B.26)$$

We consider only the point $z_D = 1$ which determines the critical temperature by the condition $N_n = N$. Restricting ourselves to the physical cases $D = 1, 2, 3$, we rewrite the sum as

$$S_D(b, 1) = \sum_{w=1}^{\infty} D \left[e^{-wb} - \frac{(D-1)}{2} e^{-2wb} + \frac{(D-1)(D-2)}{6} e^{-3wb} \right] \frac{1}{(1 - e^{-wb})^D}. \quad (2B.27)$$

According to the method developed in the evaluation of the Robinson expansion in the footnote on p. 8, we obtain such a sum in two steps. First we go to small b where the sum reduces to an integral over w . After this we calculate the difference between sum and integral by a naive power series expansion.

As it stands, the sum (2B.27) cannot be converted into an integral due to singularities at $w = 0$. These must first be removed by subtractions. Thus we decompose $S_D(b, 1)$ into a subtracted sum plus a remainder as

$$S_D(b, 1) = \bar{S}_D(b, 1) + \Delta_D S_D(b, 1) + b \frac{D}{2} \Delta_{D-1} S_D(b, 1) + b^2 \frac{D(3D-1)}{24} \Delta_{D-2} S_D(b, 1). \quad (2B.28)$$

Here

$$\begin{aligned} \bar{S}_D(b, 1) &= \sum_{w=1}^{\infty} D \left[e^{-wb} - \frac{D-1}{2} e^{-2wb} + \frac{(D-1)(D-2)}{6} e^{-3wb} \right] \\ &\times \left[\frac{1}{(1 - e^{-wb})^D} - \frac{1}{w^D b^D} - \frac{D}{2w^{D-1} b^{D-1}} - \frac{D(3D-1)}{24w^{D-2} b^{D-2}} \right] \end{aligned} \quad (2B.29)$$

is the subtracted sum and

$$\Delta_{D'} S_D(b, 1) \equiv \frac{D}{b^D} \left[\zeta_{D'}(e^{-b}) - \frac{D-1}{2} \zeta_{D'}(e^{-2b}) + \frac{(D-1)(D-2)}{6} \zeta_{D'}(e^{-3b}) \right] \quad (2B.30)$$

collects the remainders. The subtracted sum can now be done in the limit of small b as an integral over w , using the well-known integral formula for the Beta function:

$$\int_0^\infty dx \frac{e^{-ax}}{(1 - e^{-x})^b} = B(a, 1-b) = \frac{\Gamma(a)\Gamma(1-b)}{\Gamma(1+a-b)}. \quad (2B.31)$$

This yields the small- b contributions to the subtracted sums

$$\begin{aligned} \bar{S}_1(b, 1) &\xrightarrow{b \rightarrow 0} \frac{1}{b} \left(\gamma - \frac{7}{12} \right) \equiv s_1, \\ \bar{S}_2(b, 1) &\xrightarrow{b \rightarrow 0} \frac{1}{b} \left(\gamma + \log 2 - \frac{9}{8} \right) \equiv s_2, \\ \bar{S}_3(b, 1) &\xrightarrow{b \rightarrow 0} \frac{1}{b} \left(\gamma + \log 3 - \frac{19}{24} \right) \equiv s_3, \end{aligned} \quad (2B.32)$$

where $\gamma = 0.5772 \dots$ is the *Euler-Mascheroni number*. The remaining sum-minus-integral is obtained by a series expansion of $1/(1 - e^{-wb})^D$ in powers of b and performing the sums over w using the formula:

$$\left(\sum_{n=1}^{\infty} - \int_0^\infty \right) \frac{e^{n\beta \hbar \omega}}{n^\nu} = \sum_{k=1}^{\infty} \frac{1}{k!} (-\beta \hbar \omega)^k \zeta(\nu - k) \equiv \bar{\zeta}_\nu(e^{\beta \hbar \omega}). \quad (2B.33)$$

However, due to the subtractions, the corrections are all small of order $(1/b^D)\mathcal{O}(b^3)$. They will be ignored here. Thus we obtain

$$S_D(b, 1) = \frac{s_D}{b^D} + \Delta S_D(b, 1) + \frac{1}{b^D}\mathcal{O}(b^3). \quad (2B.34)$$

We now expand $\Delta_{D'}S_D(b, 1)$ using Robinson's formula stated in the footnote on p. 8 up to b^2/b^D and find

$$\Delta_{D'}S_1(b, 1) = \frac{1}{b}\zeta_{D'}(e^{-b}), \quad (2B.35)$$

$$\Delta_{D'}S_2(b, 1) = \frac{1}{b^2} [2\zeta_{D'}(e^{-b}) - \zeta_{D'}(e^{-2b})], \quad (2B.36)$$

$$\Delta_{D'}S_3(b, 1) = \frac{1}{b^3} [3\zeta_{D'}(e^{-b}) - 3\zeta_{D'}(e^{-2b}) + \zeta_{D'}(e^{-3b})], \quad (2B.37)$$

where

$$\begin{aligned} \zeta_1(e^{-b}) &= -\log(1 - e^{-b}) = -\log b + \frac{b}{2} - \frac{b^2}{24} + \dots, \\ \zeta_2(e^{-b}) &= \zeta(2) + b(\log b - 1) - \frac{b^2}{4} + \dots, \end{aligned} \quad (2B.38)$$

$$\zeta_3(e^{-b}) = \zeta(3) - \frac{b}{6}\zeta(2) - \frac{b^2}{2} \left(\log b - \frac{3}{2} \right) + \dots. \quad (2B.39)$$

The results are

$$\begin{aligned} S_1(b, 1) &= \frac{1}{b} \left[(-\log b + \gamma) + \frac{b}{4} - \frac{b^2}{144} + \dots \right], \\ S_2(b, 1) &= \frac{1}{b^2} \left[\zeta(2) - b \left(\log b - \gamma + \frac{1}{2} \right) + \frac{7b^2}{24} + \dots \right], \\ S_3(b, 1) &= \frac{1}{b^3} \left[\zeta(3) + \frac{3b}{2}\zeta(2) - b^2 \left(\log b - \gamma + \frac{19}{24} \right) + \dots \right]. \end{aligned} \quad (2B.40)$$

Note that the calculation cannot be shortened by simply expanding the factor $1/(1 - e^{-wb})^D$ in the unsubtracted sum (2B.27) in powers of w , which would yield the result (2B.28) without the first term $\bar{S}_1(b, 1)$, and thus without the integrals (2B.32).

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*Every existing thing is born without reason,
prolongs itself out of weakness,
and dies by chance.*

JEAN-PAUL SARTRE (1905-1980)

3

Interacting Nonrelativistic Particles

If the particles in a nonrelativistic many-body system are no longer free, quantum field theory turns from a trivial to a very difficult subject. Solvable models exist only in certain limiting situations, in particular in a reduced number of $D = 1 + 1$ spacetime dimensions. Some of them have given useful insights into the behavior of a number of quasi-two-dimensional statistical systems.

In general, the physical properties of an interacting field system can be calculated only on the basis of some simple and crude approximations. Among these, the most common consists of an expansion of the interacting theory in powers of the interaction strength, say g (see Chapter 8). Such a *weak-coupling expansion* has at first many mathematical problems since the underlying function is usually not analytic at $g = 0$, but possesses a branch cut starting at this point. The radius of convergence is therefore zero. Thus the expansion can at best be of an asymptotic nature, in which only first few terms can yield useful approximations to the result. Higher orders improve the result only in the limit of an extremely small interaction strength. For any nonzero value of g , however, the asymptotic power series always diverge.

Fortunately, there exists a simple procedure to reconstruct approximately such functions from their divergent weak-coupling expansion. This procedure is called *Variational Perturbation Theory* (VPT), which turns divergent weak-coupling expansions into convergent strong-coupling expansions [1]. In these, the series is not expanded in powers of g but in powers of $1/g^\omega$. For large g , the convergence of the latter allows their evaluation with any desired accuracy.

Even before such mathematical methods were invented, the perturbative approach has led to remarkable results in quantum electrodynamics (QED), the quantum field theory of electrons and phonons. There, the expansion parameter is the fine-structure constant $\alpha = e^2/\hbar c = 1/137$, and numerical results obtained to third order in α do agree with experiment up to an amazing accuracy of one part in a million. Before developing the general perturbation expansion of quantum field theory, it is useful to treat two important weakly interacting quantum systems in a more conventional way, using only the methods of old-fashioned quantum mechanical perturbation theory. In this way, we shall better appreciate the beautiful systematics which the general quantum field theoretic methods are able to offer for treating such problems.

3.1 Weakly Interacting Bose Gas

If the particles in a Bose gas interact with each other, the full power of quantum field theory is needed to understand its behavior. For weak and short-range interactions, the Bose condensation in the limit of low temperature and low density can be studied by a very simple theoretical procedure due to Bogoliubov [4]. Until 1995, the condensation process was not observed due to the difficulty in reaching the required ultralow temperature in this limit. But in that year, several laboratories found it independently. First, there was a group at the Joint Institute for Laboratory Astrophysics in Boulder, Colorado [5]. Second was an independent measurement at MIT [6], and third a measurement at Rutgers [7]. Three years later, also a gas of atomic helium was found to form a condensate [8].

Atom	m (amu)	T_c (μK)	a (nm)	a/λ_T	N_c
H	1	50	0.06	2.7×10^{-4}	10^9
Li	7	0.3	-1.5	-1.2×10^{-3}	10^3
Na	23	2.0	2.8	1.1×10^{-2}	10^7
Rb	87	0.7	5.4	2.4×10^{-2}	10^6

FIGURE 3.1 Typical values of mass, s -wave scattering length a , and the number of atoms N_c in the condensate of various atomic gases. The dimensionless ratio a_s/λ_T characterizes the interaction strength, where $\lambda_T \equiv \sqrt{2\pi\hbar/Mk_BT}$ is the thermal length scale.

For a while it was hoped that superfluid ^4He poured into a container filled with a very fine glass powder could act like a weakly interacting Bose gas, due to the diluting effect of the powder. The grains of the powder would have to be smaller than the scale over which the wave function of the condensate acts coherently. This is the Compton wave length $\hbar/\langle p \rangle$ associated with the momentum distribution in the degenerate Bose gas. However, this did not work well. Presently, the condensation process observed in such a system is explained by the superfluid transition in an ensemble of very small micrograin fluid elements of ^4He .

The condition of being dilute allows us to include only the s -wave in the scattering process. Accordingly, the interaction can be approximated by a δ -function repulsion which acts only upon the s -wave.

The time-independent second quantized grand-canonical energy has a free-particle term:

$$H_0 = \int d^3x a_{\mathbf{x}}^\dagger \left(\frac{1}{2M} \hat{\mathbf{p}}^2 - \mu \right) a_{\mathbf{x}}. \quad (3.1)$$

The interaction has the form (2.129):

$$H_{\text{int}} = \frac{1}{2} \int d^3x \int d^3x' a_{\mathbf{x}}^\dagger a_{\mathbf{x}'}^\dagger V(\mathbf{x} - \mathbf{x}') a_{\mathbf{x}'} a_{\mathbf{x}}. \quad (3.2)$$

We have seen in the discussion of the degenerate non-interacting Bose gas that the state of momentum $\mathbf{p} = 0$ plays a special role, and we expect the same thing to happen here.

Consider the system in a finite volume V , such that the momentum states are discrete $p_i = (2\pi/L)n_i$. Then we may decompose $a_{\mathbf{x}}$ in momentum space as

$$a_{\mathbf{x}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{p}\mathbf{x}} a_{\mathbf{p}}. \quad (3.3)$$

The free-particle Hamiltonian (3.1) becomes

$$H_0 \equiv \sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger (\varepsilon_{\mathbf{p}} - \mu) a_{\mathbf{p}} = \sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger \xi_{\mathbf{p}} a_{\mathbf{p}}, \quad (3.4)$$

where

$$\varepsilon_{\mathbf{p}} \equiv \frac{\mathbf{p}^2}{2M} \quad (3.5)$$

are the single-particle energies and $\xi_{\mathbf{p}} \equiv \varepsilon_{\mathbf{p}} - \mu$ the relevant energies (2.256) in a grand-canonical ensemble. Now we use the Fourier representation of the potential

$$V(\mathbf{x}) = \int \frac{d^3q}{(2\pi\hbar)^3} e^{i\mathbf{q}\mathbf{x}/\hbar} V(\mathbf{q}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{x}/\hbar} V(\mathbf{q}), \quad (3.6)$$

to rewrite the interaction Hamiltonian as

$$H_{\text{int}} = \frac{g}{2V^3} \int d^3x \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4, \mathbf{q}} e^{i\mathbf{q}\mathbf{x}/\hbar} e^{-i\mathbf{p}_3\mathbf{x}/\hbar} e^{-i\mathbf{p}_4\mathbf{x}/\hbar} e^{i\mathbf{p}_2\mathbf{x}/\hbar} e^{i\mathbf{p}_1\mathbf{x}/\hbar} V(\mathbf{q}) a_{\mathbf{p}_4}^\dagger a_{\mathbf{p}_3}^\dagger a_{\mathbf{p}_2} a_{\mathbf{p}_1}. \quad (3.7)$$

The integral over $\mathbf{x}$ yields a $\delta^{(3)}$ -function for overall momentum conservation $(2\pi)^3 \delta^{(3)}(\mathbf{p}_3 + \mathbf{p}_4 - \mathbf{p}_1 - \mathbf{p}_2)$, which for the discrete momenta is equivalent to $V \delta_{\mathbf{p}_3 + \mathbf{p}_4, \mathbf{p}_1 + \mathbf{p}_2}$. This can easily be verified by recalling relation (1.189) and summing the latter over $\mathbf{p}_1$, say, while integrating the former with the phase-space measure $\int d^3p V / (2\pi)^3$. Hence we obtain

$$H_{\text{int}} = \frac{1}{2V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} V(\mathbf{q}) a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} a_{\mathbf{p}}. \quad (3.8)$$

If we want to include only s -wave scattering, we restrict the potential to the simple repulsive δ -function potential

$$V(\mathbf{x} - \mathbf{x}') = g \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (3.9)$$

Then we can write H_{int} as follows:

$$H_{\text{int}} = \frac{g}{2V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} a_{\mathbf{p}}. \quad (3.10)$$

In scattering experiments at low momentum, one measures the phase shift a_s of s -wave scattering. This shows up in a limiting scattering amplitude:

$$f_{\Omega} = -a. \quad (3.11)$$

Its square is the differential cross section, making the total cross section σ in the limit of small momentum equal to $4\pi a^2$. The phase shift is related to the renormalized version g_R of the coupling constant g by

$$a_s = \frac{M}{4\pi\hbar^2} g_R. \quad (3.12)$$

This will be discussed in detail in Chapter 9. The renormalized coupling constant g_R will be defined in Eq. (3.58).

At very low temperatures, the state with $\mathbf{p} = 0$ will contain a macroscopic number of particles N_0 which is much larger than the number of excited particles $N - N_0$. We separate out the terms containing the zero modes and rewrite the interaction Hamiltonian as

$$H_{\text{int}} = H_{\text{int}}^0 + H'_{\text{int}} + H''_{\text{int}}, \quad (3.13)$$

with

$$H_{\text{int}}^0 = \frac{g}{2V} \left[a_0^{\dagger 2} a_0^2 + \sum_{\mathbf{p} \neq 0} \left(2a_{\mathbf{p}}^{\dagger} a_0^{\dagger} a_{\mathbf{p}} a_0 + 2a_{-\mathbf{p}}^{\dagger} a_0^{\dagger} a_{-\mathbf{p}} a_0 + a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} a_0 a_0 + a_0^{\dagger} a_0^{\dagger} a_{\mathbf{p}} a_{-\mathbf{p}} \right) \right], \quad (3.14)$$

and the interaction Hamiltonians

$$H'_{\text{int}} = \frac{g}{2V} \sum_{\mathbf{p} \neq 0, \mathbf{p}' \neq 0, \mathbf{q} \neq 0} a_{\mathbf{p}+\mathbf{q}}^{\dagger} a_{\mathbf{p}'-\mathbf{q}}^{\dagger} a_{\mathbf{p}'} a_{\mathbf{p}}, \quad (3.15)$$

and

$$H''_{\text{int}} = \frac{g}{V} a_0 \sum_{\mathbf{p}, \mathbf{p}'} \left(a_{\mathbf{p}+\mathbf{p}'}^{\dagger} a_{\mathbf{p}} a_{\mathbf{p}'} + \text{c.c.} \right). \quad (3.16)$$

In the Hamiltonian H_{int}^0 we include the excited particles with $\mathbf{p} \neq 0$ only up to quadratic order and keep the full quartic order only for the operators $a_0^{\dagger}, a_0$. The cubic terms in $a_0^{\dagger}, a_0$, which are linear in $a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}$ with $\mathbf{p} \neq 0$, vanish by momentum conservation. The second interaction Hamiltonian H''_{int} does not conserve the particle number and contributes only in second-order perturbation theory.

Since the particle number N_0 is very large, the harmonic oscillator associated with the term $a_0^{\dagger}, a_0$ in the Hamiltonian operator behaves almost classically, so that we can consider $a_0^{\dagger}, a_0$ approximately as c -numbers and replace them by $A_0 \equiv \sqrt{N_0} e^{\mp i\varphi/2}$ with some unknown phase φ . Then H_{int}^0 becomes approximately

$$H_{\text{int}}^0 = \frac{g}{2V} \left[A_0^{\dagger 2} A_0^2 + 2A_0^{\dagger} A_0 \sum_{\mathbf{p} \neq 0} \left(a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} + a_{-\mathbf{p}}^{\dagger} a_{-\mathbf{p}} \right) + \sum_{\mathbf{p} \neq 0} \left(A_0^2 a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} + \text{h.c.} \right) \right]. \quad (3.17)$$

The total particle number N is given by the operator

$$N = A_0^{\dagger} A_0 + N_{\mathbf{u}} = N_0 + N_{\mathbf{u}}, \quad (3.18)$$

where

$$N_{\mathbf{u}} = \frac{1}{2} \sum_{\mathbf{p} \neq 0} (a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} + a_{-\mathbf{p}}^{\dagger} a_{-\mathbf{p}}) = \sum_{\mathbf{p} \neq 0} a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \quad (3.19)$$

counts the uncondensed particles in the nonzero momentum states. Following Bogoliubov [4], we consider a system with a *fixed total number* of particles and forget about the chemical potential. Thus we work with the free Hamiltonian

$$H_0 = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}, \quad (3.20)$$

and rewrite the interaction Hamiltonian (3.17) as

$$H_{\text{int}}^0 \equiv \frac{g}{2V} \left[N^2 + A_0^{\dagger} A_0 \sum_{\mathbf{p} \neq 0} (a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} + a_{-\mathbf{p}}^{\dagger} a_{-\mathbf{p}}) + \sum_{\mathbf{p} \neq 0} (A_0^2 a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} + \text{h.c.}) \right] + H_{\text{int}}'' \quad (3.21)$$

The last term

$$H_{\text{int}}'' = -\frac{g}{2V} N_{\mathbf{u}}^2 \quad (3.22)$$

is of third order in g , and is neglected in Bogoliubov's weak-coupling theory [4]. Thus we have to deal with the approximate free Hamiltonian

$$H_0' \approx \frac{g}{2V} N^2 + \sum_{\mathbf{p} \neq 0} \left(\varepsilon_{\mathbf{p}} + \frac{g}{V} A_0^{\dagger} A_0 \right) a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left(\frac{g}{V} A_0^2 a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} + \text{h.c.} \right). \quad (3.23)$$

At this point, Bogoliubov introduced particle and condensate *densities* ρ and ρ_0 :

$$\rho \equiv \frac{N}{V}, \quad \rho_0 \equiv \frac{N_s}{V}. \quad (3.24)$$

Then he chose A_0 to have a real phase, so that he may identify

$$A_0 = A_0^{\dagger} = \sqrt{V \rho_0}, \quad (3.25)$$

and bring (3.23) to the form

$$H_0' \approx gV \frac{\rho^2}{2} + \sum_{\mathbf{p} \neq 0} (\varepsilon_{\mathbf{p}} + g\rho_0) a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} + \frac{1}{2} g\rho_0 \sum_{\mathbf{p} \neq 0} (a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} + \text{h.c.}). \quad (3.26)$$

This operator is quadratic in the creation and annihilation operators, and can therefore be diagonalized by means of a canonical transformation. Following Bogoliubov's original treatment, we introduce the new creation and annihilation operators $\alpha_{\mathbf{p}}^{\dagger}$ and $\alpha_{\mathbf{p}}$ [9] as follows:

$$\begin{aligned} a_{\mathbf{p}} &= \cosh \theta_{\mathbf{p}} \alpha_{\mathbf{p}} + \sinh \theta_{\mathbf{p}} \alpha_{-\mathbf{p}}^{\dagger}, \\ a_{\mathbf{p}}^{\dagger} &= \cosh \theta_{\mathbf{p}} \alpha_{\mathbf{p}}^{\dagger} + \sinh \theta_{\mathbf{p}} \alpha_{-\mathbf{p}}. \end{aligned} \quad (3.27)$$

More compactly, we shall write

$$\begin{aligned} a_{\mathbf{p}} &= u_{\mathbf{p}}\alpha_{\mathbf{p}} + v_{\mathbf{p}}\alpha_{-\mathbf{p}}^{\dagger}, \\ a_{\mathbf{p}}^{\dagger} &= u_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\alpha_{-\mathbf{p}}, \quad \text{with} \quad u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2 = 1. \end{aligned} \quad (3.28)$$

For the original particle operators this implies

$$\begin{aligned} a_{\mathbf{p}}^{\dagger}a_{\mathbf{p}} &= (u_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\alpha_{-\mathbf{p}})(u_{\mathbf{p}}\alpha_{\mathbf{p}} + v_{\mathbf{p}}\alpha_{-\mathbf{p}}^{\dagger}) \\ &= v_{\mathbf{p}}^2 + u_{\mathbf{p}}^2\alpha_{\mathbf{p}}^{\dagger}\alpha_{\mathbf{p}} + v_{\mathbf{p}}^2\alpha_{-\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}} + u_{\mathbf{p}}v_{\mathbf{p}}(\alpha_{-\mathbf{p}}\alpha_{\mathbf{p}} + \alpha_{\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}}^{\dagger}) \end{aligned} \quad (3.29)$$

and

$$\begin{aligned} a_{\mathbf{p}}^{\dagger}a_{-\mathbf{p}}^{\dagger} &= (u_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\alpha_{-\mathbf{p}})(u_{\mathbf{p}}\alpha_{-\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\alpha_{\mathbf{p}}) \\ &= u_{\mathbf{p}}v_{\mathbf{p}} + u_{\mathbf{p}}^2\alpha_{\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}}^{\dagger} + v_{\mathbf{p}}^2\alpha_{-\mathbf{p}}\alpha_{\mathbf{p}} + u_{\mathbf{p}}v_{\mathbf{p}}(\alpha_{\mathbf{p}}^{\dagger}\alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}}), \end{aligned} \quad (3.30)$$

which have the vacuum expectation values

$$\langle a_{\mathbf{p}}^{\dagger}a_{\mathbf{p}} \rangle = v_{\mathbf{p}}^2, \quad \langle a_{\mathbf{p}}^{\dagger}a_{-\mathbf{p}}^{\dagger} \rangle = u_{\mathbf{p}}v_{\mathbf{p}}. \quad (3.31)$$

Using these we find from (3.26) the approximate Hamiltonian

$$\begin{aligned} H'_0 &\approx gV\frac{\rho_0^2}{2} + \sum_{\mathbf{p} \neq 0} \left\{ [(\varepsilon_{\mathbf{p}} + g\rho_0)v_{\mathbf{p}}^2 + g\rho_0 u_{\mathbf{p}}v_{\mathbf{p}}] \right. \\ &\quad + \frac{1}{2} [(\varepsilon_{\mathbf{p}} + g\rho_0)(u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) + 2g\rho_0 u_{\mathbf{p}}v_{\mathbf{p}}] (\alpha_{\mathbf{p}}^{\dagger}\alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}}) \\ &\quad \left. + \frac{1}{2} [(\varepsilon_{\mathbf{p}} + g\rho_0)2u_{\mathbf{p}}v_{\mathbf{p}} + g\rho_0(u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2)] (\alpha_{\mathbf{p}}^{\dagger}\alpha_{-\mathbf{p}}^{\dagger} + \alpha_{\mathbf{p}}\alpha_{-\mathbf{p}}) \right\}. \end{aligned} \quad (3.32)$$

We now see that the off-diagonal terms in the last line of (3.32) vanish if we set

$$\frac{2u_{\mathbf{p}}v_{\mathbf{p}}}{u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2} = -\frac{g\rho_0}{\varepsilon_{\mathbf{p}} + g\rho_0}. \quad (3.33)$$

In terms of the angles $\theta_{\mathbf{p}}$ in (3.27), this reads

$$\tanh 2\theta_{\mathbf{p}} = -\frac{g\rho_0}{\varepsilon_{\mathbf{p}} + g\rho_0}. \quad (3.34)$$

Using the trigonometric relation $\cos 2\theta_{\mathbf{p}} = 1/\sqrt{1 - \tanh^2 2\theta_{\mathbf{p}}}$, this implies

$$\cosh 2\theta_{\mathbf{p}} = \frac{\varepsilon_{\mathbf{p}} + g\rho_0}{\mathcal{E}_{\mathbf{p}}}, \quad \sin 2\theta_{\mathbf{p}} = -\frac{g\rho_0}{\mathcal{E}_{\mathbf{p}}}, \quad (3.35)$$

where

$$\mathcal{E}_{\mathbf{p}} \equiv \sqrt{(\varepsilon_{\mathbf{p}} + g\rho_0)^2 - g^2\rho_0^2} \quad (3.36)$$

are the quasiparticle energies. They go to zero for $\mathbf{p} \rightarrow 0$, in accordance with the Nambu-Goldstone theorem. Using further

$$\cosh \theta_{\mathbf{p}} = \sqrt{(\cosh 2\theta_{\mathbf{p}} + 1)/2}, \quad \sinh \theta_{\mathbf{p}} = -\sqrt{(\cosh 2\theta_{\mathbf{p}} - 1)/2}, \quad (3.37)$$

we obtain

$$\cosh^2 \theta_{\mathbf{p}} = u_{\mathbf{p}}^2 = \frac{1}{2} \left(1 + \frac{\varepsilon_{\mathbf{p}} + g\rho_0}{\mathcal{E}_{\mathbf{p}}} \right), \quad \sinh^2 \theta_{\mathbf{p}} = v_{\mathbf{p}}^2 = -\frac{1}{2} \left(1 - \frac{\varepsilon_{\mathbf{p}} + g\rho_0}{\mathcal{E}_{\mathbf{p}}} \right), \quad (3.38)$$

with

$$u_{\mathbf{p}} v_{\mathbf{p}} = -\frac{g\rho_0}{2\mathcal{E}_{\mathbf{p}}}. \quad (3.39)$$

Then

$$H'_0 \approx gV \frac{\rho^2}{2} + \sum_{\mathbf{p} \neq 0} [(\varepsilon_{\mathbf{p}} + g\rho_0) v_{\mathbf{p}}^2 + g\rho_0 u_{\mathbf{p}} v_{\mathbf{p}}] + \sum_{\mathbf{p} \neq 0} \mathcal{E}_{\mathbf{p}} \alpha_{\mathbf{p}}^{\dagger} \alpha_{\mathbf{p}} \quad (3.40)$$

can be rewritten as

$$H'_0 \approx gV \frac{\rho^2}{2} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} [\mathcal{E}_{\mathbf{p}} - (\varepsilon_{\mathbf{p}} + g\rho_0)] + \sum_{\mathbf{p} \neq 0} \mathcal{E}_{\mathbf{p}} \alpha_{\mathbf{p}}^{\dagger} \alpha_{\mathbf{p}}. \quad (3.41)$$

Note that, instead of fixing the Bogoliubov coefficients to be (3.38) by the requirement of vanishing off-diagonal elements in the last line of Eq. (3.32), we could also have obtained the same coefficients by extremizing (3.42) with respect to variations in $v_{\mathbf{p}}$ and $u_{\mathbf{p}}$ with the constraint $u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2 = 1$, so that $\delta u_{\mathbf{p}} = \delta v_{\mathbf{p}} v_{\mathbf{p}}/u_{\mathbf{p}}$. Indeed, this would have lead to

$$2(\varepsilon_{\mathbf{p}} + g\rho_0) v_{\mathbf{p}} \delta v_{\mathbf{p}} + g\rho_0 (u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) \delta v_{\mathbf{p}}/u_{\mathbf{p}} = 0, \quad (3.42)$$

which is solved again by (3.38).

At very low temperatures, the quasiparticles are frozen out, and the ground state energy is given by the first three terms:

$$E'_0 \approx gV \frac{\rho^2}{2} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} [\mathcal{E}_{\mathbf{p}} - (\varepsilon_{\mathbf{p}} + g\rho_0)]. \quad (3.43)$$

The particles with nonzero momentum $\mathbf{p}$ lie outside the condensate and constitute what is called the *uncondensed part of the liquid*. Their number is given by the expectation value in the vacuum state of quasiparticles $|0_{\alpha}\rangle$. This state has the property $\alpha_{\mathbf{p}}|0_{\alpha}\rangle = 0$, $\langle 0| \alpha_{\mathbf{p}} = 0$, so that

$$\langle a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \rangle \equiv \langle 0_{\alpha} | (u_{\mathbf{p}} \alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}} \alpha_{-\mathbf{p}}) (u_{\mathbf{p}} \alpha_{\mathbf{p}} + v_{\mathbf{p}} \alpha_{-\mathbf{p}}^{\dagger}) | 0_{\alpha} \rangle = v_{\mathbf{p}}^2 \quad (3.44)$$

and

$$\langle a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} \rangle \equiv \langle 0_{\alpha} | (u_{\mathbf{p}} \alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}} \alpha_{-\mathbf{p}}) (u_{\mathbf{p}} \alpha_{-\mathbf{p}}^{\dagger} + v_{\mathbf{p}} \alpha_{\mathbf{p}}) | 0_{\alpha} \rangle = u_{\mathbf{p}} v_{\mathbf{p}}. \quad (3.45)$$

The total number of uncondensed particles is found from the sum

$$N_{\mathbf{u}} = \sum_{\mathbf{p} \neq 0} \langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle \equiv V \rho_{\mathbf{u}} \equiv \sum_{\mathbf{p} \neq 0} v_{\mathbf{p}}^2. \quad (3.46)$$

Inserting $v_{\mathbf{p}}^2$ from (3.38) yields

$$\rho_{\mathbf{u}} = \frac{1}{V} \sum_{\mathbf{p}} v_{\mathbf{p}}^2 = \int \frac{d^3 p}{(2\pi\hbar)^3} v_{\mathbf{p}}^2 = \frac{1}{2} \int \frac{d^3 p}{(2\pi\hbar)^3} \left(\frac{\varepsilon_{\mathbf{p}} + g\rho_0}{\mathcal{E}_{\mathbf{p}}} - 1 \right). \quad (3.47)$$

To evaluate this, we replace the sum over $\mathbf{p}$ by an integral,

$$\sum_{\mathbf{p} \neq 0} \rightarrow V \int \frac{d^3 p}{(2\pi\hbar)^2},$$

and measure all momenta in units of

$$k_{g\rho_0} = \frac{\sqrt{2Mg\rho_0}}{\hbar}. \quad (3.48)$$

Expressing the coupling constant g in terms of the experimentally observable s -wave scattering length a_s via (3.12), this is equal to

$$k_{g\rho_0} = 2\sqrt{2\pi a_s \rho_0}. \quad (3.49)$$

This is a characteristic wave number associated with the s -wave scattering length (3.12). Thus we substitute

$$p = \hbar k_{g\rho_0} \kappa, \quad (3.50)$$

and find for the density of uncondensed particles (3.47) the equation

$$\rho_{\mathbf{u}} = \frac{N_{\mathbf{u}}}{V} = k_{g\rho_0}^3 \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2}, \quad (3.51)$$

where $I_{\rho_{\mathbf{u}}}$ is the integral

$$I_{\rho_{\mathbf{u}}} \equiv \int_0^\infty d\kappa \kappa^2 \left(\frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - 1 \right) = \frac{\sqrt{2}}{3}. \quad (3.52)$$

Hence,

$$\rho_{\mathbf{u}} = k_{g\rho_0}^3 \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2} = \frac{8\rho}{3\sqrt{\pi}} \sqrt{a_s^3 \rho_0}. \quad (3.53)$$

The lesson of Eq. (3.51) is that, even at zero temperature, the repulsive interaction scatters a small set of particles out of the condensate, thus causing a depletion to a fraction [13, 14]

$$\frac{\rho_0}{\rho} = 1 - \frac{\rho_{\mathbf{u}}}{\rho} \approx 1 - \frac{8}{3\sqrt{\pi}} \sqrt{a_s^3 \rho_0}. \quad (3.54)$$

In the strongly interacting superfluid ^4He , only about 8% of the particles condenses in the zero-temperature state [15]. Nevertheless, all particles participate in the superfluid motion [16], and the superfluid density is equal to the total density. The condensate and the normal fluid move together.

Let us also calculate the energy of the Bose system. There we encounter a typical divergence of the present local quantum field theory: The momentum sum in the second term of (3.41) does not converge. Indeed, the energy $\mathcal{E}_{\mathbf{p}}$ of (3.38) behaves, at large momenta, like

$$\mathcal{E}_{\mathbf{p}} \approx (\varepsilon_{\mathbf{p}} + g\rho_0) \sqrt{1 - \frac{g^2\rho_0^2}{(\varepsilon_{\mathbf{p}} + g\rho_0)^2}} \approx \varepsilon_{\mathbf{p}} + g\rho_0 - \frac{1}{2} \frac{g^2\rho_0^2}{\varepsilon_{\mathbf{p}}} + \dots \quad (3.55)$$

The integral

$$V \int \frac{d^3p}{(2\pi\hbar)^3} [\mathcal{E}_{\mathbf{p}} - (\varepsilon_{\mathbf{p}} + g\rho_0)] \sim V \int \frac{d^3p}{(2\pi\hbar)^3} \frac{g^2\rho_0^2}{\varepsilon_{\mathbf{p}}} \quad (3.56)$$

diverges linearly. The integral can be made convergent. First we rearrange the terms in (3.43) to

$$E'_0 \approx gV \frac{\rho_0^2}{2} - \frac{1}{4} \sum_{\mathbf{p} \neq 0} \frac{g^2\rho_0^2}{\varepsilon_{\mathbf{p}}} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[\mathcal{E}_{\mathbf{p}} - \varepsilon_{\mathbf{p}} - g\rho_0 + \frac{g^2\rho_0^2}{2\varepsilon_{\mathbf{p}}} \right]. \quad (3.57)$$

The last sum is now convergent, but the sum before it is still divergent. However, the divergence disappears if the energy is expressed in terms of the renormalized coupling constant g_R defined by

$$\frac{1}{g_R} \equiv \frac{1}{g} - \frac{1}{V} \sum_{\mathbf{p} \neq 0} \frac{1}{2\varepsilon_{\mathbf{p}}} = \frac{1}{g} - \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\varepsilon_{\mathbf{p}}}. \quad (3.58)$$

This is precisely the quantity determined by measurements of the s -wave scattering length a_s to which it is related by Eq. (3.12). In terms of this g_R , we find the renormalized energy

$$E'_0 \approx g_R V \frac{\rho^2}{2} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[\mathcal{E}_{\mathbf{p}} - (\varepsilon_{\mathbf{p}} + g_R\rho) + \frac{g_R^2\rho^2}{2\varepsilon_{\mathbf{p}}} \right]. \quad (3.59)$$

The above *renormalization* procedure of going from an unobservable divergent bare coupling g to a finite observable coupling g_R is typical for all quantum field theories. Here is the first place where it appears. This may surprise the reader since we are, after all, dealing with a Schrödinger system which should have no infinities. The puzzle is resolved by the observation, that the three-dimensional Schrödinger equation has no proper solution if the potential is a δ -function. Only in one dimension it does. After the above renormalization, however, the problem of finding the quantum behavior of a particle in a point-like potential becomes

meaningful and solvable. A meaningful limit can, of course, be obtained from a study of a completely finite problem in an extended potential hole and taking at the end the limit of zero range while letting the depth of the potential go to infinity.

With the substitution (3.50) we can rewrite the energy as

$$E'_0 = g_R V \frac{\rho^2}{2} + V g \rho_0 k_{g\rho_0}^3 \frac{I_E}{4\pi^2}, \quad (3.60)$$

where I_E is the integral

$$I_E \equiv \int_0^\infty d\kappa \kappa^2 \left[\sqrt{(\kappa^2 + 1)^2 - 1} - \kappa^2 - 1 + \frac{1}{2\kappa^2} \right] = \frac{8\sqrt{2}}{15}. \quad (3.61)$$

Inserting $g_R = 4\pi\hbar^2 a_s/M$, this can be written as [10]

$$E'_0 = V \frac{2\pi\hbar^2 a_s}{M} \rho^2 \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{a_s^3 \rho_0} \right). \quad (3.62)$$

The operators $\alpha_{\mathbf{p}}$ applied to the vacuum state generate *quasiparticles*. They have the Bogoliubov energies $\mathcal{E}_{\mathbf{p}}$ instead of the original energies $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/2M$. For small momenta, the quasiparticle energy (3.36) starts out like

$$\mathcal{E}_{\mathbf{p}} \approx \sqrt{\frac{g\rho_0}{M}} |\mathbf{p}| + \sqrt{\frac{M}{g\rho_0}} \frac{\mathbf{p}^3}{8M^2} + \dots \quad (3.63)$$

The initial linear behavior defines the velocity of second sound:

$$c \equiv \sqrt{\frac{g\rho_0}{M}}. \quad (3.64)$$

This behavior is a consequence of the famous *Nambu-Goldstone theorem*, according to which a spontaneous breakdown of a continuous symmetry leads to excitation with such an energy-momentum relation. The continuous symmetry of the present Bose system is an invariance of the Hamiltonian under a transformation of all operators by a U(1) phase factor $a_{\mathbf{p}} \rightarrow e^{i\gamma} a_{\mathbf{p}}$. This symmetry is violated by the condensate which is characterized by a ground-state expectation value $A_0 \neq 0$ with a definite phase. That phase was chosen to be real. For more details on this theorem see Section 16.2.1.

For large momenta, the expansion is

$$\mathcal{E}_{\mathbf{p}} \approx \frac{\mathbf{p}^2}{2M} + Mc^2 - \frac{c^4 M^3}{\mathbf{p}^2} + \dots, \quad (3.65)$$

and the particles behave like free particles, but with an apparent rest energy Mc^2 , similar to the low-momentum behavior of relativistic particles. In Fig. 3.2 we have plotted the $\varepsilon_{\mathbf{p}}$ for $M = 1$ and $g\rho_0 = 1$ and compared it with the free-particle curve $\mathbf{p}^2/2$ as well as the experimental determination of the excitation spectrum in bulk superfluid ^4He . We see that the simple approximation (3.36) yields initially a similar

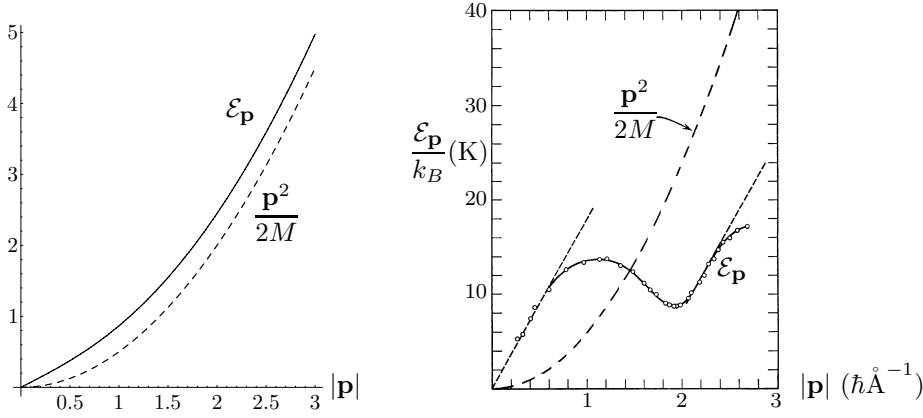


FIGURE 3.2 Plot of the quasiparticle energies as function of momenta in an interacting Bose gas. The dashed curve indicates the free-particle energies. The right-hand part of the figure shows the experimental curve for superfluid helium at 1.12 K measured by neutrons of wavelength 4.04 Å. The slope of the dashed straight lines indicates the sound velocity 2.37×10^4 cm/sec.

behavior as in the superfluid, but it is not quite capable of giving the pronounced minimum in the experimental data. The energy of minimum is referred to as the *roton energy*. An interpretation of these states was first given by Feynman in 1955 [12].

In the neighborhood of the minimum, the experimental energy is roughly

$$\mathcal{E}_{\mathbf{p}} \sim \Delta + \frac{(p - p_0)^2}{\mu}, \quad (3.66)$$

with

$$\Delta \sim 8.96 K k_B, \quad p_0 \approx 1.9 \text{Å}^{-1} \hbar, \quad \mu \approx 0.5 m_e. \quad (3.67)$$

In Eq. (3.64) we deduced the velocity c of second sound from the slope of the quasiparticle spectrum at small momenta. We may also use a classical formula relating the sound velocity to the compressibility of a material. At zero temperature, the compressibility follows from the ground state energy (3.62). Using only the leading first term we may write

$$E'_0 \approx \frac{g N^2}{2V}. \quad (3.68)$$

From this we obtain

$$c \equiv \sqrt{\frac{V^2}{MN} \frac{\partial^2 E}{\partial V^2}} \approx \sqrt{\frac{g_R}{MV}}, \quad (3.69)$$

in agreement with (3.64).

In bulk superfluid ^4He , the sound velocity at atmospheric pressure and zero temperature is

$$c \approx \sqrt{3} \cdot 137 \frac{\text{m}}{\text{sec}} \approx 2.373 \frac{\text{cm}}{\text{sec}} \approx 17.2 \frac{k_B}{\hbar} \text{\AA K}. \quad (3.70)$$

Actually, this number is obtained from measurements of the velocity c_2 of the so-called *second sound*, which can be measured more accurately than c . Second sound arises if the superfluid component oscillates out of phase against the normal component (at a constant total density). The velocity c is larger than c_2 by a factor of $\sqrt{3}$, as shown first by Landau.¹ The result (3.70) agrees very well with the slope in Fig. 3.2.

Note that the interaction between the Bose particles has to be repulsive, otherwise the sound velocity would be imaginary!

3.2 Weakly Interacting Fermi Gas

Two field theoretic models of interacting fermions are of great theoretical and practical importance. One helps to understand the contribution of electrons to the binding energy of metals. The second illustrates the mechanism by which electrons can become superconductive. In particle physics, the second mechanism has inspired all models for explaining the properties of the pion and thus of the most important nuclear forces. It underlies all present attempts to construct a unified theory of strong electromagnetic and weak interactions.

3.2.1 Electrons in a Metal

When electrons run through a metal with crystalline order it is possible to define a momentum of the particles (since there is still a translational symmetry). For small momenta the energy behaves like $p^2/2M$, only that m is no longer the true electronic mass but some effective mass, whose size depends on the interactions with the positive ions.

Since the ions are very heavy, they take little part in the dynamics of the electrons. This is well known for single atoms, where the motion of the electron hardly influences the nucleus. One is therefore justified in approximating the ions simply by a uniform time-independent positive background charge. The Hamiltonian of the electrons is

$$H_{\text{el}} = \sum_{i=1}^N \frac{p_i^2}{2M} + \frac{1}{2} e^2 \sum \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}. \quad (3.71)$$

The Hamiltonian of the uniform positive background is

$$H_{\text{b}} = \frac{e^2}{2} \int d^3x d^3x' \frac{n(\mathbf{x})n(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}, \quad (3.72)$$

¹L.D. Landau, J. Phys, USSR, 5, 71 (1941) (see also L.D. Landau, E.M. Lifshitz, *Fluid Mechanics*, Addison Wesley, Reading, Mass. 1959, Ch. XIV, and *Statistical Physics*, ibid, Ch. VI, pp. 66-67).

with $n(x) \equiv N/V$. Finally, the interaction of the electron with the background reads

$$H_{\text{int}} = -e^2 \sum_i \int d^3x \frac{n(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_i|}. \quad (3.73)$$

In order to keep control over divergencies at long distances it is useful to insert an exponential screening factor $e^{-\mu(x-x')}$ into the Coulomb potential $1/|\mathbf{x} - \mathbf{x}'|$. Otherwise each of the terms diverges in the limit $N \rightarrow \infty, V \rightarrow \infty$, at $\rho \equiv N/V \equiv \text{const}$ (the so-called *thermodynamic limit*).

In the Hamiltonian

$$H = H_{\text{el}} + H_{\text{b}} + H_{\text{eb}}, \quad (3.74)$$

the limit $\mu \rightarrow 0$ can be taken at the end, together with the limit $V \rightarrow \infty$. One has to let the screening length μ^{-1} grow to infinity in the same way as the size $L = \sqrt[3]{V}$ of the system. In order to be able to make use of translational invariance we shall assume the finite system to be a cube of periodically repeated volume $V = L^3$ in all directions, i.e., we assume periodic boundary conditions in all wave functions. Then all Fourier components have the discrete momenta

$$k_i = \frac{2\pi}{L} n_i. \quad (3.75)$$

Let us first integrate the energy of the positive background:

$$\begin{aligned} H_{\text{b}} &= \frac{1}{2} e^2 \left(\frac{N}{V} \right)^2 \int d^3x d^3x' \frac{e^{-\mu|\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} = \frac{1}{2} e^2 \left(\frac{N}{V} \right)^2 \int d^3x \frac{4\pi}{\mu^2} \\ &= \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}. \end{aligned} \quad (3.76)$$

We see the need of using the length μ^{-1} to keep this expression finite.

The electron background interaction energy can be calculated just as easily:

$$H_{\text{e,b}} = -e^2 \sum_{i=1}^N \frac{N}{V} \int d^3x \frac{e^{-\mu|\mathbf{x} - \mathbf{x}_i|}}{|\mathbf{x} - \mathbf{x}_i|} = -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}. \quad (3.77)$$

We may therefore confine our attention purely to the electron's Hamiltonian remembering only to subtract, at the end, the constant energy $-e^2/2N^2V^{-1}4\pi\mu^{-2}$ before taking the limit $\mu \rightarrow 0$.

The kinetic energy of the electron gas is easily written down:

$$E_{\text{el,kin}} = \sum_{\mathbf{p}, \sigma} \varepsilon_{\mathbf{p}} a_{\mathbf{p}, \sigma}^\dagger a_{\mathbf{p}, \sigma}, \quad (3.78)$$

where $\sigma = \pm 1/2$ distinguishes the two spin states. Alternatively, we shall use the spin-up and spin-down symbols $\sigma = \uparrow$ and $\sigma = \downarrow$.

The potential energy is given by

$$H_{\text{el,pot}} = \frac{1}{2} \sum_{\mathbf{x}, \mathbf{x}', \sigma, \sigma'} a_{\mathbf{x}, \sigma}^\dagger a_{\mathbf{x}', \sigma'}^\dagger \frac{e^2}{|\mathbf{x} - \mathbf{x}'|} a_{\mathbf{x}', \sigma'} a_{\mathbf{x}, \sigma}. \quad (3.79)$$

Expanding

$$a_{\mathbf{x}, \sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{p}, \sigma} e^{i\mathbf{p}\mathbf{x}} a_{\mathbf{p}, \sigma} \quad (3.80)$$

and

$$\frac{1}{4\pi} \frac{e^{-\mu|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} = \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\mathbf{q}^2 + \mu^2} e^{i\mathbf{q}\mathbf{x}}, \quad (3.81)$$

we find

$$H_{\text{el,pot}} = \frac{e^2}{2V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}, \sigma, \sigma'} \frac{4\pi}{\mathbf{q}^2 + \mu^2} a_{\mathbf{p}+\mathbf{q}, \sigma}^\dagger a_{\mathbf{p}'-\mathbf{q}, \sigma'}^\dagger a_{\mathbf{p}', \sigma'} a_{\mathbf{p}, \sigma}. \quad (3.82)$$

Consider the terms with $\mathbf{q} = 0$

$$H_{\text{el,pot}}^{\mathbf{q}=0} = \frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\mathbf{p}, \mathbf{p}', \sigma, \sigma'} a_{\mathbf{p}, \sigma}^\dagger a_{\mathbf{p}', \sigma'}^\dagger a_{\mathbf{p}', \sigma'} a_{\mathbf{p}, \sigma}. \quad (3.83)$$

Using the commutator

$$\sum_{\mathbf{p}', \sigma'} \left[a_{\mathbf{p}, \sigma}^\dagger, a_{\mathbf{p}', \sigma'}^\dagger a_{\mathbf{p}', \sigma'} \right] = -a_{\mathbf{p}', \sigma}, \quad (3.84)$$

it can be written as

$$\begin{aligned} H_{\text{el,pot}}^{\mathbf{q}=0} &= \frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\mathbf{p}, \mathbf{p}', \sigma, \sigma'} \left(a_{\mathbf{p}', \sigma}^\dagger a_{\mathbf{p}', \sigma'}^\dagger a_{\mathbf{p}, \sigma}^\dagger a_{\mathbf{p}, \sigma} - \delta_{\mathbf{p}\mathbf{p}'} a_{\mathbf{p}\sigma}^\dagger a_{\mathbf{p}\sigma} \right) \\ &= \frac{e^2}{2V} \frac{4\pi}{\mu^2} (\hat{N}^2 - \hat{N}). \end{aligned} \quad (3.85)$$

For a fixed particle number N , this is equal to

$$E_{\text{el,pot}} = \frac{e^2}{2V} \frac{4\pi}{\mu^2} (N^2 - N). \quad (3.86)$$

The first term cancels with the constant background term. The second term grows linearly with the total particle number. It is of the order

$$\frac{1}{L} \left(\frac{1}{\mu L} \right)^2, \quad (3.87)$$

where $L \approx V^{1/3}$ is the linear size of the system, and disappears for $L \rightarrow \infty$, assuming that μL stays fixed.

The remaining terms in the energy (3.82) have a smooth limit $\mu \rightarrow 0$ so that we can continue the calculation with $\mu = 0$ and study the Hamiltonian operator

$$H = H_{\text{el,kin}} + H'_{\text{el,pot}} = \sum_{\mathbf{p},\sigma} \frac{\mathbf{p}^2}{2M} a_{\mathbf{p},\sigma}^\dagger a_{\mathbf{p},\sigma} + \frac{e^2}{2V} \sum_{\mathbf{p},\mathbf{p}',\mathbf{q} \neq 0,\sigma,\sigma'} \frac{4\pi}{\mathbf{q}^2} a_{\mathbf{p}+\mathbf{q},\sigma}^\dagger a_{\mathbf{p}'-\mathbf{q},\sigma'}^\dagger a_{\mathbf{p}',\sigma'} a_{\mathbf{p},\sigma}. \quad (3.88)$$

We now make the important observation that, even if the potential is not weak and possibly of long range, there exists a physical regime where the interaction can be treated as a small perturbation. This is in the regime of high density. Indeed, the momenta in the first term have the dimension L^{-2} , the second term has the dimension $1/Vq^2 \sim L^{-1}$. The remaining calculations involve only dimensionless sums over integer numbers. Thus, in a very small box, the second term is negligible compared to the first.

Let us calculate the first term. For simplicity, we shall do this in the limit of large L . At zero temperature, the electrons fill all states up to the Fermi momentum. Then

$$\begin{aligned} E^{(0)} &= \frac{1}{2M} \sum_{\mathbf{p},\sigma} p^2 \Theta(p_F - p) \\ &= \frac{V}{2M} \frac{2}{3} \int_0^{p_F} \frac{d^3p}{(2\pi)^3} p^2 \\ &= \frac{V}{2M\hbar^3} \frac{p_F^5}{10\pi^2} = \frac{V}{(2\pi)^3} \frac{4\pi\hbar^2}{5m} k_F^5, \end{aligned} \quad (3.89)$$

and p_F is determined from

$$\frac{N}{V} = \frac{2}{\hbar^3} \int_0^{p_F} \frac{d^3p}{(2\pi)^3} = \frac{2}{\hbar^3} \frac{p_F^3}{6\pi^2}, \quad (3.90)$$

so that

$$\frac{E^{(0)}}{N} = \frac{3}{5} \frac{p_F^2}{2M}. \quad (3.91)$$

Using the Fermi energy

$$\varepsilon_F \equiv \frac{p_F^2}{2M}, \quad (3.92)$$

this can be written as

$$\frac{E^{(0)}}{N} = \frac{3}{5} \varepsilon_F, \quad (3.93)$$

and (3.90) becomes

$$\left(\frac{N}{V} \right) = \frac{2mp_F}{3\pi^2\hbar^3} \varepsilon_F. \quad (3.94)$$

The result is often stated in terms of the length r_s , the spherical volume per particle:

$$\frac{4\pi}{3}r_s^3 = \frac{V}{N}. \quad (3.95)$$

From (3.90) and (3.95) we obtain the relation

$$p_F = \hbar k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{\hbar}{r_s}. \quad (3.96)$$

Remembering the Bohr radius

$$a_H = 4\pi \frac{\hbar^2}{me^2}, \quad (3.97)$$

the energy density at zero temperature can then be written as

$$\begin{aligned} \frac{E^{(0)}}{N} &= \frac{1}{4\pi} \frac{e^2}{2a_H} \frac{3}{5} \left(\frac{9\pi}{4}\right)^{2/3} \left(\frac{a_H}{r_s}\right)^2 \\ &\approx 2.21 \left(\frac{a_H}{r_s}\right)^2 \text{ Ry}, \end{aligned} \quad (3.98)$$

where

$$\text{Ry} \equiv \frac{1}{4\pi} \frac{e^2}{2a_H} \approx 13.5\text{eV} \quad (3.99)$$

is the Rydberg energy, the binding energy of the hydrogen atom. Note that we are using rationalized electrostatic units in which the Coulomb potential is $e^2/4\pi r$.

Consider now the electron-electron interaction. To lowest order, the energy is shifted by

$$\Delta E^{(1)} = \frac{e^2}{2V} \sum_{\mathbf{q} \neq 0} \sum_{\mathbf{p}, \mathbf{p}', \sigma, \sigma'} \frac{4\pi}{q^2} \langle \psi_0 | a_{\mathbf{p}+\mathbf{q}, \sigma}^\dagger a_{\mathbf{p}', \sigma'}^\dagger a_{\mathbf{p}', \sigma'} a_{\mathbf{p}, \sigma} | \psi_0 \rangle, \quad (3.100)$$

where $|\psi_0\rangle$ denotes the ground state of the free electron gas. In order to give a non-zero contribution, the state $|\psi_0\rangle$ must contain an electron in the states $\mathbf{p}', \sigma'$ and $\mathbf{p}, \sigma$ as well as in the states $\mathbf{p} + \mathbf{q}, \sigma$ and $\mathbf{p}' - \mathbf{q}, \sigma'$. Both $\mathbf{p}$ and $\mathbf{p}'$ must therefore lie inside the Fermi sphere $p^2 < p_F^2, p'^2 < p_F^2$. The annihilation operators create two holes. These must subsequently be filled up by $a_{\mathbf{p}+\mathbf{q}, \sigma}^\dagger a_{\mathbf{p}', \sigma'}^\dagger$ so that also $\mathbf{p} + \mathbf{q}, \mathbf{p}' - \mathbf{q}$ are inside the Fermi sphere. Thus one must either have

$$(\mathbf{p} + \mathbf{q}, \sigma) = (\mathbf{p}, \sigma); \quad (\mathbf{p}' - \mathbf{q}, \sigma') = (\mathbf{p}', \sigma'), \quad (3.101)$$

or

$$(\mathbf{p} + \mathbf{q}, \sigma) = (\mathbf{p}', \sigma'), \quad (\mathbf{p}' - \mathbf{q}, \sigma') = (\mathbf{p}, \sigma). \quad (3.102)$$

The first pairing would imply $\mathbf{q} = 0$, but this momentum is not included in the sum. So we are only left with the second case which contributes an expectation value

$$\begin{aligned}\Delta E^{(1)} &= \frac{e^2}{2V} \sum_{\mathbf{q} \neq 0, \sigma} \sum_{\mathbf{p}, \mathbf{p}'} \frac{\hbar^2}{q^2} \delta_{\mathbf{p}', \mathbf{p}+\mathbf{q}} \langle \psi_0 | a_{\mathbf{p}', \sigma}^\dagger a_{\mathbf{p}, \sigma}^\dagger a_{\mathbf{p}', \sigma} a_{\mathbf{p}, \sigma} | \psi_0 \rangle \\ &= -\frac{e^2}{2V} 2 \sum_{\mathbf{q} \neq 0} \frac{\hbar^2}{q^2} \sum_{\mathbf{p}} \Theta(p_F - |\mathbf{p}|) \Theta(p_F - |\mathbf{p} + \mathbf{q}|).\end{aligned}\quad (3.103)$$

The factor 2 in the last expression comes from the sum over σ . Substituting $\mathbf{p} \rightarrow \mathbf{p} - \mathbf{q}/2$, $\mathbf{p} + \mathbf{q} \rightarrow \mathbf{p} + \mathbf{q}/2$, and approximating the sum over $\mathbf{p}$ by an integral, this becomes

$$\frac{V}{(2\pi\hbar)^3} \int d^3p \Theta\left(p_F - \left|\mathbf{p} - \frac{\mathbf{q}}{2}\right|\right) \Theta\left(p_F - \left|\mathbf{p} + \frac{\mathbf{q}}{2}\right|\right). \quad (3.104)$$

The integral runs over the common volume of two spheres of radius p_F in momentum space whose origins are separated by a distance $\mathbf{q}$ (see Fig. 3.3).



FIGURE 3.3 Common volume of two spheres at a distance $\mathbf{q}$ in momentum space. The right-hand drawing illustrates intermediate integration (3.105).

In units of p_F^3 , the volume is found by calculating the integral over the spherical shell $x^2 + (y - 1)^2 = 1$ (illustrated on the right-hand side of Fig. 3.3):

$$2\pi \int_0^{x_m} dx x^2 y = 2 \int_0^{y_m} dy y (1 - y) = 2\pi \left(\frac{y_m^2}{2} - \frac{y_m^3}{3} \right). \quad (3.105)$$

Subtracting this from the volume $\pi x_m^2 y_m = \pi (2y_m^2 - y_m^3)$ of a disk of thickness y_m , we find

$$\pi \left(y_m^2 - \frac{1}{3} y_m^3 \right), \quad y_m = 1 - \frac{q}{2p_F}. \quad (3.106)$$

This has to be multiplied by a factor $2 \times p_F^3$ to obtain the volume of overlap in Fig. 3.3:

$$\frac{4\pi p_F^3}{3} \left(1 - \frac{3}{2} x_q + \frac{1}{2} x_q^3 \right) \Theta(1 - x_q), \quad x_q \equiv \frac{q}{2p_F}. \quad (3.107)$$

Inserting this for the momenta $\mathbf{q}$ in Eq. (3.103), we arrive at

$$\begin{aligned}\Delta E^{(1)} &= -\frac{e^2}{2} \frac{1}{(2\pi\hbar)^3} \frac{4\pi p_F^3}{3} 2 \sum_{\mathbf{q} \neq 0} \frac{\hbar^2}{q^2} \left(1 - \frac{3}{2}x_q + \frac{1}{2}x_q^3\right) \\ &= -\frac{e^2}{2} \frac{V}{(2\pi\hbar)^6} \frac{4\pi p_F^3}{3} 2 \times 4\pi\hbar^2 2p_F \int_0^1 dx \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \\ &= -\frac{V}{(2\pi)^3} \frac{e^2}{4\pi} 2k_F^4.\end{aligned}\quad (3.108)$$

Replacing k_F^3 by $3\pi^2 N/V$ via (3.90) yields

$$\frac{\Delta E^{(1)}}{N} = -\frac{1}{4\pi} \frac{e^2}{2} \frac{3}{2\pi} k_F.\quad (3.109)$$

Inserting here p_F from (3.96), we obtain

$$\frac{\Delta E^{(1)}}{N} = -\frac{1}{4\pi} \frac{e^2}{2} \frac{3}{2\pi} \left(\frac{9\pi}{4}\right)^{1/3} \frac{\hbar}{r_s},\quad (3.110)$$

or, in terms of Rydberg units,

$$\frac{E^{(1)}}{N} = -\left(\frac{9\pi}{4}\right)^{1/3} \frac{3}{2\pi} \frac{a_H}{r_s} \text{ Ry} \approx -0.916 \frac{a_H}{r_s} \text{ Ry}.\quad (3.111)$$

The total energy per volume is then

$$\frac{E}{V} = \frac{1}{(2\pi)^3} \left(\frac{4\pi}{5m} k_F^5 - \frac{e^2}{4\pi} 2k_F^4 + \dots \right),\quad (3.112)$$

and the energy per particle has the high-density expansion

$$\begin{aligned}\frac{E}{N} &= \left[\frac{3}{5} \left(\frac{9\pi}{4}\right)^{2/3} \left(\frac{a_H}{r_s}\right)^2 - \left(\frac{9\pi}{4}\right)^{1/3} \frac{3}{2\pi} \frac{a_H}{r_s} + \dots \right] \frac{1}{4\pi} \frac{e^2}{2} \frac{3}{2\pi} \frac{\hbar}{r_s} \\ &\approx \left[2.21 \left(\frac{a_H}{r_s}\right)^2 - 0.916 \frac{a_H}{r_s} + \dots \right] \text{ Ry}.\end{aligned}\quad (3.113)$$

The leading term shows repulsion due to the exclusion principle. The second term represents the attraction due to the exchange interaction between the electrons. The curve is plotted in Fig. 3.4. It has a minimum at

$$\frac{r_s}{a_H} = \frac{4\pi}{5} \left(\frac{9\pi}{4}\right)^{1/3} \approx 4.823,\quad (3.114)$$

where

$$\frac{E_{\min}}{N} = -\frac{45}{48\pi^2} \approx -0.095 \text{ Ry}.\quad (3.115)$$

It is interesting to see that the minimum at $E/N \approx 0.095 \text{ Ry} \approx -1.29 \text{ eV}$ lies in

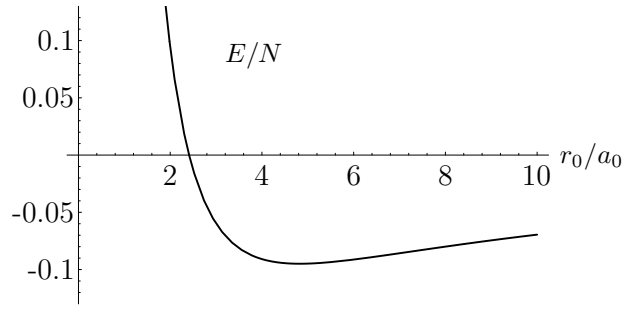


FIGURE 3.4 Energy density, in units Ry, of an electron gas in a uniform background of positive charge.

the neighborhood of the values found in metallic sodium:

$$\frac{r_s}{a_H} \approx 3.90, \quad \frac{E}{N} \approx -1.13Na. \quad (3.116)$$

This suggests that the main part of the metallic binding energy is due to the electrons in the lattice.

Improvements of this lowest-order result were given by Gell-Mann and Brueckner in 1957.² They derived the next term in the expansion, which Wigner³ called the *correlation energy*,

$$E^{(2)} = \left[\frac{2}{\pi^2} (1 - \log 2) \log \frac{r_s}{a_H} + C \right] \text{Ry} \approx \left[0.0622 \log \frac{r_s}{a_H} - 0.096 \right] \text{Ry}. \quad (3.117)$$

At metallic electron densities, the ratio r_s/a_H lies between 2 and 5. This regime can be described approximately by the above energies if $E^{(2)}$ is modified to⁴

$$E^{(2)} \approx \left[0.0622 \log \frac{r_s}{a_H} - 0.230 \right] \text{Ry}. \quad (3.118)$$

The further corrections vanish for $r_s \rightarrow 0$. For more details see the textbook by C. Kittel⁵.

Let us also remark that Wigner⁶ pointed out the possibility of an electron lattice (*Wigner lattice*) formed in the limit of low density. Such a gas has meanwhile been observed experimentally.

²M. Gell-Mann and K.A. Brueckner, Phys. Rev. *106*, 364 (1957),
M. Gell-Mann, Phys. Rev. *106*, 369, 367 (1957).

³E.P. Wigner, Phys. Rev. *46*, 1002 (1934). For the calculation see W. Macke, Z. Naturforsch. *5a*, 192 (1950), also A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, 1971, New York, Section 12.

⁴P. Nozières and D. Pines, Phys. Rev. *111*, 442 (1958).

⁵C. Kittel, *Quantum Theory of Solids*, John Wiley, New York, 1963, p. 115.

⁶E.P. Wigner, Phys. Rev. *46*, 1002 (1934).

3.3 Superconducting Electrons

In a metal, the Coulomb repulsion does not always dominate the behavior of the electrons. At low temperatures, the electron-phonon interactions may play an important role and lead to a completely new physical phenomenon, that of superconductivity.

Superconductors are materials without resistance to the flow of electricity. The first example was found in 1911 by the Dutch physicist Heike Kamerlingh Onnes at Leiden University. When he cooled mercury down to the temperature of liquid helium, which appears at about 4 degrees Kelvin (-269°C), its resistance suddenly vanished. Onnes won the Nobel Prize in physics in 1913 for this discovery.

Superconductors have an important property which distinguishes them from ordinary conductors of extremely low resistance: They are perfect diamagnets implying that they do not tolerate any magnetic fields on their inside. This is the so-called *Meissner-Ochsenfeld effect* discovered in 1933. This effect causes superconductive materials lying on top of a sufficiently strong magnetic field to be lifted if they are cooled below the critical temperature (levitation). A perfect conductor would only hover above the magnet if brought in from the outside due to induction generating a current with a magnetic moment opposite to the external field.

For the purpose of energy conservation, it is a challenging problem to find superconductive materials which can transport high currents without loss at room temperature. Since 1941, the record was held for a long time by niobium-nitride, which becomes superconducting at 16 K, surpassed in 1953 by vanadium-silicon with a critical temperature of 17.5 K. In 1962, a first commercial superconducting wire was manufactured from an alloy of niobium and titanium. First applications were made in 1987 in the Fermilab high-energy particle-accelerator Tevatron where magnetic fields were produced by supercurrents in copper-clad niobium-titanium. The magnets had been developed in 1960 at the Rutherford-Appleton Laboratory.

The first satisfactory theory of superconductivity was developed in 1957 by N.N. Bogoliubov and, independently, by J. Bardeen, L. Cooper, and J. Schrieffer [18], now called BCS, which won them the Nobel prize in 1972. This theory explains the early forms of superconductivity at temperatures close to absolute zero observed for elements and simple alloys.

New advances were made in the 1980s when the first organic superconductor was synthesized by the Danish researcher Klaus Bechgaard of the University of Copenhagen, together with three French team members. It turned out to become superconductive at 1.2 K transition. The possibility that this could happen had been pointed out in 1964 by Bill Little at Stanford University.

The latest major breakthrough was made in 1986 by Alex Müller and Georg Bednorz at the IBM Research Laboratory in Rüschlikon, Switzerland [17]. They synthesized a brittle ceramic compound that superconducted at the record temperature of 30 K. What made this discovery so remarkable was that ceramics are normally insulators. They don't conduct electricity well at all. So, researchers had not considered them as possible high-temperature superconductor candidates. The lanthanum, barium, copper, and oxygen compound that Müller and Bednorz syn-

thesized, behaved in a not-as-yet-understood way. Their discovery won them the Nobel Prize in 1987. It was later found that tiny amounts of this material were actually superconducting at 58 K.

Since then there has been a great deal of activity trying to find ceramics of many combinations with higher and higher critical temperatures. In 1987 superconductivity was reached in a material called YBCO at 92 K, a temperature which can simply be reached by cooling with liquid nitrogen.

The present world record was reached in 1994 at $T_c = 138$ K by a thallium-doped, mercuric-cuprate comprised of the elements mercury, thallium, barium, calcium, copper and oxygen. Under extreme pressure of 300 000 atmospheres, this critical temperature can be raised by 25 to 30 more degrees (see Fig. 3.5, from the Wikipedia page on Superconductivity).

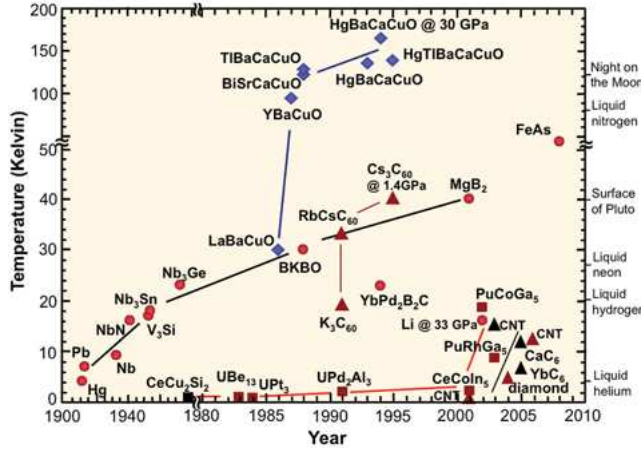


FIGURE 3.5 Historical evolution of critical temperatures of superconductivity (in units of Kelvin).

The phenomenon is based on an attraction between the electrons that move in momentum space close to the Fermi surface. An electron running through the lattice attracts the positive ions in its neighborhood. These, in turn, attract the other electrons. The relevant phonons are those with the highest frequency, which in the Debye model of the specific heat of the solid is called Debye frequency ω_D . This corresponds typically to a temperature of about 1000 K. If the electrons are near the Fermi surface, the phonon attraction can overcome the Coulomb repulsion, as was first suggested by Fröhlich in 1950, and later was brought to the level of a theory by Bardeen, Cooper, and Schrieffer (1957) (BCS) [18].

The effective electron Hamiltonian that emerges from an interaction like (3.10), after expressing it in terms of the momentum transfer $\mathbf{q} \equiv \mathbf{q}_3 - \mathbf{q}_1$ for the scattering process, reads

$$H_{\text{int}} = \frac{g}{2V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}, \sigma, \sigma'} a_{\mathbf{p}+\mathbf{q}, \sigma}^\dagger a_{\mathbf{p}'-\mathbf{q}, \sigma'}^\dagger a_{\mathbf{p}', \sigma} a_{\mathbf{p}, \sigma'}. \quad (3.119)$$

Assuming that there is an attractive δ -function interaction only between electrons with opposite spins, the total Hamiltonian in a grand-canonical ensemble coupled to a reservoir of chemical potential μ is written after the sum over the two spin states as

$$H = H_0 + H_{\text{int}} = \sum_{\mathbf{p}} \xi_{\mathbf{p}} a_{\mathbf{p},\sigma}^\dagger a_{\mathbf{p},\sigma} - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} a_{\mathbf{p}+\mathbf{q},\downarrow}^\dagger a_{\mathbf{p}'-\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}',\downarrow} a_{\mathbf{p},\uparrow}, \quad (3.120)$$

where

$$\xi_{\mathbf{p}} \equiv \varepsilon_{\mathbf{p}} - \mu \quad (3.121)$$

is the energy difference with respect to the chemical potential. If the potential is not $V(\mathbf{x} - \mathbf{x}') = g \delta^{(3)}(\mathbf{x} - \mathbf{x}')$ but

$$V(\mathbf{x} - \mathbf{x}') = \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q}\mathbf{x}} V(\mathbf{q}), \quad (3.122)$$

then the sum in the interaction contains an extra factor $V(\mathbf{q})$.

Since in the ground state, the main effect to be discussed will come from the attraction where the momenta are also opposite, BCS went further and approximated the interaction by the terms with $\mathbf{p}' = -\mathbf{p}$:

$$H_{\text{int}} \approx H_{\text{pair}} \equiv -\frac{g}{V} \sum_{\mathbf{p}, \mathbf{q}} a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{-\mathbf{p}-\mathbf{q},\downarrow}^\dagger a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow}. \quad (3.123)$$

The sum $H_0 + H_{\text{pair}}$ is the BCS pairing Hamiltonian.

The single-particle energies $\varepsilon_{\mathbf{p}}$ in H_0 are initially the free-particle kinetic energies $\mathbf{p}^2/2M$ of the electron in a metal, with an effective mass m different from the electron mass due to the effect of the crystal lattice. In order to find the phenomenon of superconductivity we must, however, study a grand-canonical ensemble of fluctuating total particle numbers in contact with a particle reservoir of chemical potential μ . At $T = 0$, this will be close to p_F , the Fermi surface of the free force electron gas. Instead of studying the gas at a fixed particle number, we shall investigate $H - \mu N$. In this Hamiltonian operator, spelled out in (3.120), the single-particle energies $\varepsilon_{\mathbf{p}}$ are replaced by $\xi_{\mathbf{p}} \equiv \varepsilon_{\mathbf{p}} - \mu$, as specified in (3.121).

Moreover, since the attractive interaction can be derived only for electrons near the Fermi surface, we can approximately replace $\xi_{\mathbf{p}} = \varepsilon_{\mathbf{p}} - \mu$ by $\xi_{\mathbf{p}} \approx (p_F/m)(|\mathbf{p}| - p_F)$ (see Fig. 3.6). After this, we treat the Hamiltonian following Bogoliubov's method [4] which goes as follows:

First one introduces two arbitrary real momentum-dependent parameters $\Sigma_{\mathbf{p}}$ and $\Delta_{\mathbf{p}}$ into the free Hamiltonian, changing it to

$$\bar{H}_0 \equiv \sum_{\mathbf{p}} (\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}) (a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\uparrow} - a_{-\mathbf{p},\downarrow} a_{-\mathbf{p},\downarrow}^\dagger) - \sum_{\mathbf{p}} \Delta_{\mathbf{p}}^\dagger a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} - \sum_{\mathbf{p}} \Delta_{\mathbf{p}} a_{\mathbf{p},\uparrow}^\dagger a_{-\mathbf{p},\downarrow}^\dagger + \xi_{\mathbf{p}}. \quad (3.124)$$

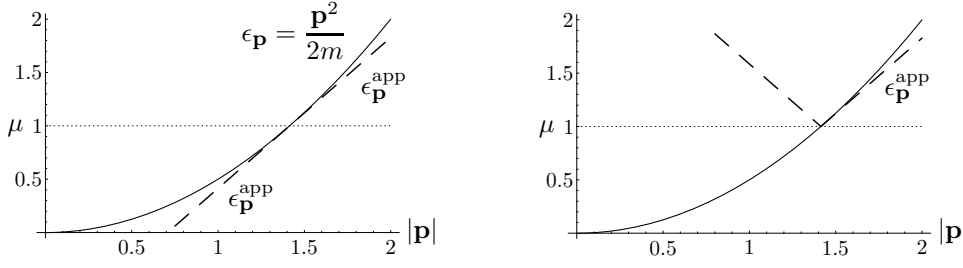


FIGURE 3.6 Dashed straight lines indicate the approximate energies $\xi_{\mathbf{p}} \approx (p_F/m)(|\mathbf{p}| - p_F)$ of a free electron near the Fermi surface in a grand-canonical ensemble. The right-hand plot shows the energies of the states below the Fermi surface. The hole excitations below the Fermi surface are filled and have approximate energies $\xi_{\mathbf{p}} \approx -(p_F/m)(|\mathbf{p}| - p_F)$.

The additional terms are subtracted from the interaction Hamiltonian, which becomes

$$\begin{aligned} \bar{H}_{\text{int}} \equiv & -\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} a_{\mathbf{p}+\mathbf{q}, \downarrow}^{\dagger} a_{\mathbf{p}'-\mathbf{q}, \uparrow}^{\dagger} a_{\mathbf{p}', \downarrow} a_{\mathbf{p}, \uparrow} + \sum_{\mathbf{p}} \Sigma_{\mathbf{p}} (a_{\mathbf{p}, \uparrow}^{\dagger} a_{\mathbf{p}, \uparrow} - a_{-\mathbf{p}, \downarrow} a_{-\mathbf{p}, \downarrow}^{\dagger}) \\ & + \sum_{\mathbf{p}} \Delta_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}, \downarrow} a_{\mathbf{p}, \uparrow} + \sum_{\mathbf{p}} \Delta_{\mathbf{p}} a_{\mathbf{p}, \uparrow}^{\dagger} a_{-\mathbf{p}, \downarrow}^{\dagger}. \end{aligned} \quad (3.125)$$

The total Hamiltonian

$$H = \bar{H}_0 + \bar{H}_{\text{int}} \quad (3.126)$$

has remained unchanged. The modified Hamiltonian $\bar{H}_0$ is bilinear in the creation and annihilation operators and can be written as

$$\bar{H}_0 = \sum_{\mathbf{p}} \mathcal{E}_{\mathbf{p}} (a_{\mathbf{p}, \uparrow}^{\dagger}, a_{-\mathbf{p}, \downarrow}) h_{\mathbf{p}} \begin{pmatrix} a_{\mathbf{p}, \uparrow} \\ a_{-\mathbf{p}, \downarrow}^{\dagger} \end{pmatrix} + \xi_{\mathbf{p}}, \quad (3.127)$$

with

$$\mathcal{E}_{\mathbf{p}} \equiv \sqrt{(\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}})^2 + \Delta_{\mathbf{p}}^2} \quad (3.128)$$

and the matrix

$$h_{\mathbf{p}} \equiv \frac{1}{\mathcal{E}_{\mathbf{p}}} \begin{pmatrix} \xi_{\mathbf{p}} - \Sigma_{\mathbf{p}} & -\Delta_{\mathbf{p}} \\ -\Delta_{\mathbf{p}} & -\xi_{\mathbf{p}} + \Sigma_{\mathbf{p}} \end{pmatrix}. \quad (3.129)$$

This matrix can be diagonalized by a similarity transformation due to Bogoliubov, leading to

$$h_{\mathbf{p}} = B_{\mathbf{p}}^{\dagger} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} B_{\mathbf{p}}, \quad B_{\mathbf{p}} \equiv \begin{pmatrix} u_{\mathbf{p}}^* & v_{\mathbf{p}}^* \\ -v_{\mathbf{p}} & u_{\mathbf{p}} \end{pmatrix}. \quad (3.130)$$

The matrix elements of $B_{\mathbf{p}}$ are determined, up to some phase factors $e^{i\gamma_{u_p}}$, $e^{i\gamma_{v_p}}$, to be

$$u_{\mathbf{p}} = \sqrt{\frac{\mathcal{E}_{\mathbf{p}} + \xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}}}, \quad v_{\mathbf{p}} = \sqrt{\frac{\mathcal{E}_{\mathbf{p}} - \xi_{\mathbf{p}} + \Sigma_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}}}. \quad (3.131)$$

Choosing the positive square-root, these satisfy

$$u_{\mathbf{p}}^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}} \right), \quad v_{\mathbf{p}}^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}} \right), \quad 2u_{\mathbf{p}}v_{\mathbf{p}} = -\frac{\Delta_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}}. \quad (3.132)$$

Due to their frequent occurrence we shall abbreviate the subtracted energy $\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}$ by

$$\tilde{\xi}_{\mathbf{p}} \equiv \xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}. \quad (3.133)$$

The similarity transformation of $h_{\mathbf{p}}$ amounts to a canonical transformation of the electrons to new quasiparticles, whose creation and annihilation operators are given by

$$\begin{aligned} \alpha_{\mathbf{p}} &= u_{\mathbf{p}} a_{\mathbf{p},\uparrow} - v_{\mathbf{p}} a_{-\mathbf{p},\downarrow}^{\dagger}, \\ \bar{\alpha}_{-\mathbf{p}} &= v_{\mathbf{p}} a_{\mathbf{p},\uparrow} + u_{\mathbf{p}} a_{-\mathbf{p},\downarrow}^{\dagger}. \end{aligned} \quad (3.134)$$

In terms of these, the diagonalized Hamiltonian (3.127) reads

$$\bar{H}_0 = \sum_{\mathbf{p}} \mathcal{E}_{\mathbf{p}} (\alpha_{\mathbf{p}}^{\dagger} \alpha_{\mathbf{p}} - \bar{\alpha}_{\mathbf{p}}^{\dagger} \bar{\alpha}_{\mathbf{p}}) + \xi_{\mathbf{p}}. \quad (3.135)$$

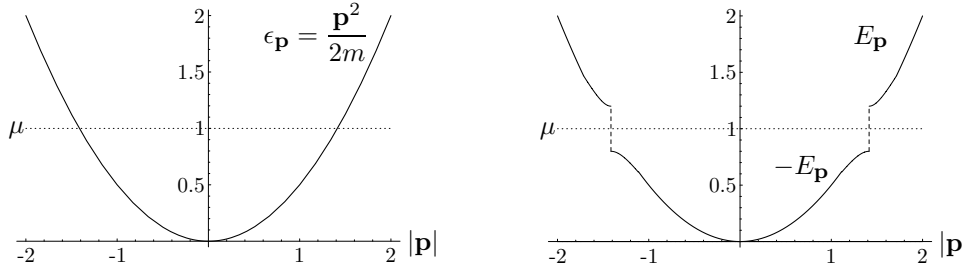


FIGURE 3.7 Gap in the energy spectrum caused by attraction of pairs of electrons with opposite spin and momenta.

The energy spectrum has a gap in comparison to the original energies in the first term in (3.124), as indicated in Fig. 3.7. The creation and annihilation operators $\alpha_{\mathbf{p}}^{\dagger}$, $\bar{\alpha}_{\mathbf{p}}^{\dagger}$ and $\alpha_{\mathbf{p}}$, $\bar{\alpha}_{\mathbf{p}}$ of the quasiparticles have the same anticommutation rules as the original particle operators $a_{\mathbf{p}}^{\dagger}$ and $a_{\mathbf{p}}$. The operators $\bar{\alpha}_{\mathbf{p}}^{\dagger}$ create states of negative energy. These can be turned into hole states of positive energy by replacing

$$\bar{\alpha}_{\mathbf{p}} \rightarrow \beta_{\mathbf{p}}^{\dagger}, \quad \bar{\alpha}_{\mathbf{p}}^{\dagger} \rightarrow \beta_{\mathbf{p}}. \quad (3.136)$$

This brings the Hamiltonian (3.135) to the form

$$\bar{H}_0 = \sum_{\mathbf{p}} \mathcal{E}_{\mathbf{p}} (\alpha_{\mathbf{p}}^{\dagger} \alpha_{\mathbf{p}} + \beta_{\mathbf{p}}^{\dagger} \beta_{\mathbf{p}}) + \sum_{\mathbf{p}} (\xi_{\mathbf{p}} - \mathcal{E}_{\mathbf{p}}). \quad (3.137)$$

The energies of quasiparticles and holes are shown in Fig. 3.8. The creation operators of the hole states have the same anticommutation rules as those of the particles. Altogether we have the anticommutation rules:

$$\{\alpha_{\mathbf{p}}, \alpha_{\mathbf{p}'}^{\dagger}\} = \delta_{\mathbf{p}\mathbf{p}'}, \quad \{\beta_{\mathbf{p}}, \beta_{\mathbf{p}'}^{\dagger}\} = \delta_{\mathbf{p},\mathbf{p}'}, \quad \{\alpha_{\mathbf{p}}, \beta_{\mathbf{p}'}^{\dagger}\} = 0. \quad (3.138)$$

The inverse transformation of (3.134) reads

$$\begin{aligned} a_{\mathbf{p},\uparrow} &= u_{\mathbf{p}}\alpha_{\mathbf{p}} + v_{\mathbf{p}}\beta_{-\mathbf{p}}^{\dagger}, \\ a_{-\mathbf{p},\downarrow}^{\dagger} &= -v_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + u_{\mathbf{p}}\beta_{-\mathbf{p}}. \end{aligned} \quad (3.139)$$

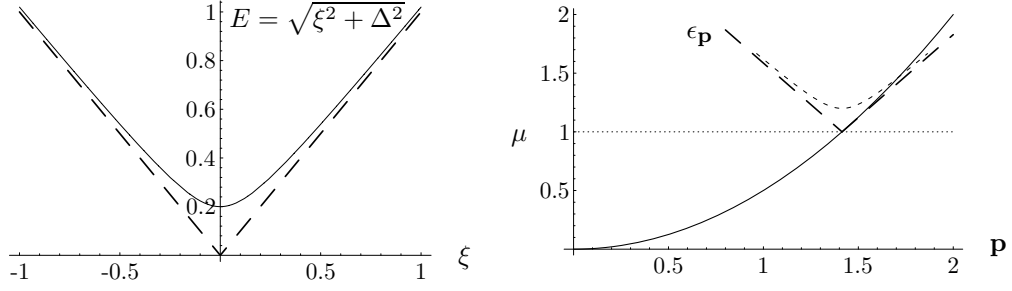


FIGURE 3.8 Details of the gap in energy spectrum. The straight dashed line is the same as in Fig. 3.6, but with a shifted origin. The right-hand side shows the position of these energy curves with respect to the free-particle energy in momentum space.

3.3.1 Zero Temperature

For zero temperature, we now use the vacuum state with respect to the quasiparticles as a trial ground state of the system. In it, the free part of the energy $\bar{H}_0$ has zero expectation. Consider now the expectation value of the interaction (3.125). For the pair terms, these are immediately calculated:

$$\langle a_{\mathbf{p},\uparrow}^{\dagger} a_{-\mathbf{p},\downarrow}^{\dagger} \rangle = \langle 0 | (u_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\beta_{-\mathbf{p}}) (-v_{\mathbf{p}}\alpha_{\mathbf{p}} + u_{\mathbf{p}}\beta_{-\mathbf{p}}^{\dagger}) | 0 \rangle = u_{\mathbf{p}}v_{\mathbf{p}} = \frac{\Delta_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}}, \quad (3.140)$$

$$\langle a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} \rangle = \langle 0 | (-v_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + u_{\mathbf{p}}\beta_{-\mathbf{p}}) (u_{\mathbf{p}}\alpha_{\mathbf{p}} + v_{\mathbf{p}}\beta_{-\mathbf{p}}^{\dagger}) | 0 \rangle = u_{\mathbf{p}}v_{\mathbf{p}} = \frac{\Delta_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}}. \quad (3.141)$$

Their momentum integrals will be denoted by δ and δ^* , respectively, i.e.,

$$\frac{1}{V} \sum_{\mathbf{p}} \langle a_{\mathbf{p},\uparrow}^{\dagger} a_{-\mathbf{p},\downarrow}^{\dagger} \rangle \equiv \delta^* = \frac{1}{V} \sum_{\mathbf{p}} \frac{\Delta_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}} \quad (3.142)$$

$$\frac{1}{V} \sum_{\mathbf{p}} \langle a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} \rangle \equiv \delta = \frac{1}{V} \sum_{\mathbf{p}} \frac{\Delta_{\mathbf{p}}}{2\mathcal{E}_{\mathbf{p}}}. \quad (3.143)$$

Note that the diagonal terms have the expectation values

$$\langle a_{\mathbf{p},\uparrow}^{\dagger} a_{\mathbf{p},\uparrow} \rangle = \langle 0 | (u_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + v_{\mathbf{p}}\beta_{-\mathbf{p}}) (u_{\mathbf{p}}\alpha_{\mathbf{p}} + v_{\mathbf{p}}\beta_{-\mathbf{p}}^{\dagger}) | 0 \rangle = v_{\mathbf{p}}^2 = \frac{1}{2} \left(1 - \frac{\tilde{\xi}_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}} \right), \quad (3.144)$$

$$\langle a_{-\mathbf{p},\downarrow}^{\dagger} a_{-\mathbf{p},\downarrow}^{\dagger} \rangle = \langle 0 | (-v_{\mathbf{p}}\alpha_{\mathbf{p}}^{\dagger} + u_{\mathbf{p}}\beta_{-\mathbf{p}}) (-v_{\mathbf{p}}\alpha_{\mathbf{p}} + u_{\mathbf{p}}\beta_{-\mathbf{p}}^{\dagger}) | 0 \rangle = u_{\mathbf{p}}^2 = \frac{1}{2} \left(1 + \frac{\tilde{\xi}_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}} \right). \quad (3.145)$$

The difference is compensated by the extra last term in (3.127). If we denote the expectation values (3.144) by

$$\langle a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\uparrow} \rangle \equiv n_{\mathbf{p},\uparrow} \equiv V \rho_{\mathbf{p},\uparrow}, \quad \langle a_{\mathbf{p},\downarrow}^\dagger a_{\mathbf{p},\downarrow} \rangle \equiv 1 - n_{\mathbf{p},\downarrow} \equiv 1 - V \rho_{\mathbf{p},\downarrow}, \quad (3.146)$$

and perform a sum over all momenta of these, we find

$$\sum_{\mathbf{p}} \langle a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\uparrow} \rangle = \sum_{\mathbf{p}} v_{\mathbf{p}}^2 = V \sum_{\mathbf{p}} \rho_{\mathbf{p},\uparrow} = V \rho_{\uparrow} = \frac{1}{2} N. \quad (3.147)$$

The expectation value of the interaction is more complicated to obtain. It requires evaluating

$$\langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger a_{\mathbf{p}',\downarrow} a_{\mathbf{p},\uparrow} | 0 \rangle. \quad (3.148)$$

This can be done by using the anticommutation rules⁷ (2.211) to expand (3.148) into the three pair terms:

$$\begin{aligned} \langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger a_{\mathbf{p}',\downarrow} a_{\mathbf{p},\uparrow} | 0 \rangle &= \langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger | 0 \rangle \langle 0 | a_{\mathbf{p}',\downarrow} a_{\mathbf{p},\uparrow} | 0 \rangle \\ &+ \langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p},\uparrow} | 0 \rangle \langle 0 | a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger a_{\mathbf{p}',\downarrow} | 0 \rangle \\ &- \langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}',\downarrow} | 0 \rangle \langle 0 | a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger a_{\mathbf{p},\uparrow} | 0 \rangle. \end{aligned} \quad (3.149)$$

Using (3.140)–(3.145), the first two terms on the right-hand side contribute the expectations

$$\langle 0 | a_{\mathbf{p}+\mathbf{q},\uparrow}^\dagger a_{\mathbf{p}'-\mathbf{q},\downarrow}^\dagger a_{\mathbf{p}',\downarrow} a_{\mathbf{p},\uparrow} | 0 \rangle = \delta_{\mathbf{p}',-\mathbf{p}} u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}+\mathbf{q}} v_{\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{q},0} v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2. \quad (3.150)$$

The last term in (3.149) gives no contribution due to the opposite spins, such that we obtain for the interaction in (3.120):

$$\langle 0 | H_{\text{int}} | 0 \rangle = -\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{q}} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}+\mathbf{q}} v_{\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{q},0} v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right) = -\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right), \quad (3.151)$$

and for the interaction (3.125):

$$\langle 0 | \bar{H}_{\text{int}} | 0 \rangle = -\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right) + \sum_{\mathbf{p}} \Sigma_{\mathbf{p}} \left(2v_{\mathbf{p}}^2 - 1 \right) + \sum_{\mathbf{p}} \Delta_{\mathbf{p}} 2u_{\mathbf{p}} v_{\mathbf{p}}. \quad (3.152)$$

Then the expectation value of the total energy $H = \bar{H}_0 + \bar{H}_{\text{int}}$ is, from (3.137) and (3.151):

$$\langle 0 | H | 0 \rangle = \sum_{\mathbf{p}} (\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}} - \mathcal{E}_{\mathbf{p}} + \Delta_{\mathbf{p}} 2u_{\mathbf{p}} v_{\mathbf{p}}) + \sum_{\mathbf{p}} \Sigma_{\mathbf{p}} 2v_{\mathbf{p}}^2 - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right). \quad (3.153)$$

⁷More elegantly we can use Wick's theorem to be derived in Section 7.17.1.

The first term can be simplified using Eq. (3.132), leading to

$$\langle 0|H|0\rangle = \sum_{\mathbf{p}} 2\xi_{\mathbf{p}} v_{\mathbf{p}}^2 - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right). \quad (3.154)$$

Let us vary this equation with respect to $v_{\mathbf{p}}$ under the constraint $u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2 = 1$, so that $\partial u_{\mathbf{p}} / \partial v_{\mathbf{p}} = -v_{\mathbf{p}} / u_{\mathbf{p}}$. This yields, for each momentum, an equation

$$2\xi_{\mathbf{p}} v_{\mathbf{p}} - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} u_{\mathbf{p}'} v_{\mathbf{p}'} \left(u_{\mathbf{p}} - v_{\mathbf{p}}^2 / u_{\mathbf{p}} \right) - 2\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} v_{\mathbf{p}'}^2 v_{\mathbf{p}} = 0. \quad (3.155)$$

Multiplying this with $u_{\mathbf{p}}$ and remembering the momentum sums (3.142) and (3.147), it becomes

$$2(\xi_{\mathbf{p}} - g\rho_{\downarrow}) u_{\mathbf{p}} v_{\mathbf{p}} - g\delta (u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2) = 0, \quad (3.156)$$

or

$$\rho_0 (\xi_{\mathbf{p}} - g\rho_{\downarrow}) \Delta_{\mathbf{p}} = g\delta (\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}). \quad (3.157)$$

This is solved by the constant variational parameters

$$\Sigma_{\mathbf{p}} = g\rho_{\uparrow}, \quad \Delta_{\mathbf{p}} = g\delta. \quad (3.158)$$

Inserting these into (3.143) and (3.145), we find the self-consistent gap equation

$$\Delta = g\delta = \frac{g}{V} \sum_{\mathbf{p}} \frac{\Delta}{2\xi_{\mathbf{p}}}, \quad (3.159)$$

and the self-consistent particle number equation

$$\rho_{\uparrow} = \frac{1}{2V} \sum_{\mathbf{p}} \left(1 - \frac{\xi_{\mathbf{p}} - g\rho_{\uparrow}}{\xi_{\mathbf{p}}} \right). \quad (3.160)$$

Inserting this into the energy (3.154) we obtain

$$\langle 0|H|0\rangle = \sum_{\mathbf{p}} 2(\xi_{\mathbf{p}} - g\rho_{\uparrow}) v_{\mathbf{p}}^2 - \frac{V}{g} \Delta^2. \quad (3.161)$$

The quantity δ is calculated from the gap equation, which is solved with the help of the modified chemical potential

$$\tilde{\mu}_{\uparrow} = \mu + g\rho_{\uparrow}, \quad (3.162)$$

which in turn is determined from the particle number equation (3.160). The result is simply the Hartree-Fock-Bogoliubov result.

Let us calculate this explicitly. First for repulsive $g < 0$, where the solution of the first gap equation in Eq. (3.159) is trivial: $\Delta = 0$. Then the momentum sum is carried out from zero to the place where $\tilde{\xi}_{\mathbf{p}}$ changes sign. If $T = 0$, this happens at the ρ -dependent modified Fermi momentum p_F^{ρ} determined by

$$p_F^{\rho} \equiv \sqrt{2M\tilde{\mu}}. \quad (3.163)$$

The sum yields

$$E^{(0)} = \sum_{\mathbf{p}} \xi_{\mathbf{p}} (\rho_{\mathbf{p},\uparrow} + \rho_{\mathbf{p},\downarrow}) = 2V \int_{p < p_F^\rho} \frac{d^3 p}{(2\pi)^3} \frac{\mathbf{p}^2}{2M}. \quad (3.164)$$

Recalling Eq. (3.89) this becomes

$$E^{(0)} = \frac{V}{(2\pi\hbar)^3} \frac{4\pi}{5m} p_F^\rho{}^5, \quad (3.165)$$

so that

$$\langle 0|H|0\rangle = \frac{V}{(2\pi\hbar)^3} \frac{4\pi}{5m} p_F^\rho{}^5 - V \frac{g}{2} \left(\frac{N}{V} \right)^2. \quad (3.166)$$

We now determine the size of ρ from the particle number by performing the sum at $T = 0$:

$$N = V \sum_{\mathbf{p}} (\rho_{\mathbf{p},\uparrow} + \rho_{\mathbf{p},\downarrow}) = 2V \int_{p < p_F^\rho} \frac{d^3 p}{(2\pi)^3}. \quad (3.167)$$

Recalling Eq. (3.90), this is equal to

$$\frac{N}{V} = \frac{1}{\hbar^3} \frac{p_F^\rho{}^3}{3\pi^2}. \quad (3.168)$$

The result (3.169) can also be expressed in a dimensionless equation with the help of (3.94) as

$$\langle 0|H|0\rangle = N \left(\frac{3}{5} \frac{p_F^\rho{}^2}{2m} - \frac{g}{2} \frac{1}{\hbar^3} \frac{p_F^\rho{}^3}{3\pi^2} \right) = N\varepsilon_F \left(\frac{3}{5} - \frac{g}{2} \frac{M}{\hbar^3} \frac{p_F^\rho}{3\pi^2} \right). \quad (3.169)$$

Expressing the attractive coupling strength g in terms of the s -wave phase shift by a formula $g = -4\pi\hbar^2 a_s/M$ to be derived later in Eq. (9.266), this becomes

$$\langle 0|H|0\rangle = N\varepsilon_F \left(\frac{3}{5} + \frac{2p_F}{3\pi^2\hbar} a_s \right). \quad (3.170)$$

For a repulsive interaction with $a_s > 0$, the total energy is increased above the free-particle energy. For an attractive interaction the chemical potential μ increases:

$$\mu \rightarrow \tilde{\mu} = \mu + g\rho/2. \quad (3.171)$$

From here on we shall assume that such a shift has been performed without exhibiting it in the notation.

For an attractive interaction with $g > 0$ the gap equation (3.159) has a nontrivial solution. It determines the gap by solving

$$\frac{1}{g} = \frac{1}{V} \sum_{\mathbf{p}} \frac{1}{2E_{\mathbf{p}}} = \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{2\sqrt{\xi_{\mathbf{p}}^2 + \Delta_0^2}}. \quad (3.172)$$

We have added a subscript 0 to the energy gap Δ to emphasize that this is the gap at *zero temperature*.

The integral diverges. In an old-fashioned weak-coupling superconductor, the attraction is caused by phonons whose energies are restricted to a thin layer $(-\omega_D, \omega_D)$ around the surface of the Fermi sphere where the momentum integral is restricted to $|p_F|\hat{\mathbf{p}} - p_F/m \lesssim \hbar\omega_D$. If we change variables from p to ξ by approximating

$$\int \frac{d^3p}{(2\pi\hbar)^3} \approx \mathcal{N}(0) \int_{-\omega_D}^{\omega_D} d\xi \quad (3.173)$$

with the density of states at the surface of the Fermi sea

$$\mathcal{N}(0) = \frac{mp_F}{2\pi^2\hbar^3} = \frac{3}{4\varepsilon_F} \frac{N}{V}, \quad (3.174)$$

(the right-hand part of (3.173) being valid only for one of the two spin components), we arrive at the gap equation

$$\frac{1}{g} \approx \mathcal{N}(0) \int_0^{\omega_D} d\xi \frac{1}{\sqrt{\xi^2 + \Delta_0^2}} = \mathcal{N}(0) \ln \frac{2\omega_D}{\Delta_0}. \quad (3.175)$$

Thus the energy gap is given by

$$\Delta_0 \approx 2\omega_D e^{-1/g\mathcal{N}(0)}. \quad (3.176)$$

This expression is non-perturbative in an essential way. It can obviously not be expanded in a power series in g .

3.4 Renormalized Theory at Strong Interactions

In modern high-temperature superconductors, where the attraction is strong, the restriction to the thin layer around the Fermi sphere is no longer valid, and the integral has to be done over the entire momentum space. Then the gap equation (3.159) reads

$$\Delta = \frac{g}{V} \sum_{\mathbf{p}} \frac{\Delta}{2\varepsilon_{\mathbf{p}}}. \quad (3.177)$$

This is a divergent quantity. The divergent part is

$$g\delta_{\text{div}} = \frac{g}{V} \sum_{\mathbf{p}} \frac{\Delta}{2\varepsilon_{\mathbf{p}}}. \quad (3.178)$$

It can be removed from the theory by adding a divergent so-called *mass counterterm* to the interaction Hamiltonian (3.125):

$$H_{\text{div}} = g\delta_{\text{div}} \sum_{\mathbf{p}} \left(a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} + a_{\mathbf{p},\uparrow}^\dagger a_{-\mathbf{p},\downarrow}^\dagger \right). \quad (3.179)$$

This term must be added to Eq. (3.154), changing it to

$$\langle 0|H|0\rangle = \sum_{\mathbf{p}} 2\xi_{\mathbf{p}} v_{\mathbf{p}}^2 - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} \left(u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \right) + g\delta_{\text{div}} \sum_{\mathbf{p}} u_{\mathbf{p}} v_{\mathbf{p}}. \quad (3.180)$$

Variation replaces the former equation (3.155) by

$$2\xi_{\mathbf{p}} v_{\mathbf{p}} - \frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} u_{\mathbf{p}'} v_{\mathbf{p}'} \left(u_{\mathbf{p}} - v_{\mathbf{p}}^2/u_{\mathbf{p}} \right) - 2\frac{g}{V} \sum_{\mathbf{p}, \mathbf{p}'} v_{\mathbf{p}'}^2 v_{\mathbf{p}} + g\delta_{\text{div}}(u_{\mathbf{p}} - v_{\mathbf{p}}^2/u_{\mathbf{p}}) = 0. \quad (3.181)$$

If this is multiplied by $u_{\mathbf{p}}$ and summed over $\mathbf{p}'$, it turns into

$$\rho_0 2(\xi_{\mathbf{p}} - g\rho_{\downarrow}) u_{\mathbf{p}} v_{\mathbf{p}} - g(\delta - \delta_{\text{div}}) (u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2) = 0, \quad (3.182)$$

and (3.156) becomes

$$\rho_0 (\xi_{\mathbf{p}} - g\rho_{\downarrow}) \Delta_{\mathbf{p}} = g(\delta - \delta_{\text{div}})(\xi_{\mathbf{p}} - \Sigma_{\mathbf{p}}). \quad (3.183)$$

Thus Eqs. (3.158) turn into the renormalized equations

$$\Sigma_{\mathbf{p}} = g\rho_{\uparrow}, \quad \Delta_{\mathbf{p}} = g(\delta - \delta_{\text{div}}) = g\delta_R, \quad (3.184)$$

and the self-consistent gap equation (3.159) turns into the renormalized gap equation

$$\Delta = g\delta_R = \frac{g}{V} \Delta \sum_{\mathbf{p}} \left(\frac{1}{2\varepsilon_{\mathbf{p}}} - \frac{1}{2\varepsilon_{\mathbf{p}}} \right), \quad (3.185)$$

so that Eq. (3.172) is renormalized to a finite equation:

$$\frac{1}{g} = \int \frac{d^3p}{(2\pi\hbar)^3} \left(\frac{1}{2\sqrt{\xi_{\mathbf{p}}^2 + \Delta_0^2}} - \frac{1}{2\varepsilon_{\mathbf{p}}} \right). \quad (3.186)$$

The total energy (3.180) becomes

$$\langle 0|H|0\rangle = \sum_{\mathbf{p}} 2(\xi_{\mathbf{p}} - g\rho_{\uparrow}) v_{\mathbf{p}}^2 - g\delta_R^2 + g\delta_{\text{div}}^2. \quad (3.187)$$

The last term must be removed at the end by an additive renormalization of the vacuum energy (see the discussion of this subtraction in Section 11.7).

It is worth emphasizing that the equation for $\Sigma_{\mathbf{p}}$ needs no mass counterterm since the momentum sum in (3.147) has no divergence.

The subtraction of a divergence as in (3.186) was encountered before in the Bose gas in Eq. (3.58), and it was pointed out that the renormalized coupling constant g_R can be observed experimentally via the s -wave scattering length a_s in the two-body scattering process, the relation being $1/g_R = -M/4\pi\hbar^2 a_s$ where $a_s < 0$ in the attractive case. This brings the subtracted gap equation (3.186) to the useful form

$$-\frac{M}{4\pi\hbar^2 a_s} = \int \frac{d^3p}{(2\pi\hbar)^3} \left(\frac{1}{2\sqrt{\xi_{\mathbf{p}}^2 + \Delta_0^2}} - \frac{1}{2\varepsilon_{\mathbf{p}}} \right). \quad (3.188)$$

3.4.1 Finite Temperature

It is easy to do the same calculation for a finite temperature T . Then the expectation values (3.140)–(3.145) become

$$\langle a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\uparrow} \rangle = \langle u_{\mathbf{p}}^2 \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + v_{\mathbf{p}}^2 \beta_{-\mathbf{p}}^\dagger \beta_{-\mathbf{p}} \rangle = v_{\mathbf{p}}^2 + \langle u_{\mathbf{p}}^2 \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} - v_{\mathbf{p}}^2 \beta_{-\mathbf{p}}^\dagger \beta_{-\mathbf{p}} \rangle, \quad (3.189)$$

$$\langle a_{\mathbf{p},\uparrow}^\dagger a_{-\mathbf{p},\downarrow}^\dagger \rangle = -u_{\mathbf{p}} v_{\mathbf{p}} \langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} - \beta_{-\mathbf{p}}^\dagger \beta_{-\mathbf{p}} \rangle = -u_{\mathbf{p}} v_{\mathbf{p}} \langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + \beta_{-\mathbf{p}}^\dagger \beta_{-\mathbf{p}} - 1 \rangle, \quad (3.190)$$

$$\langle a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} \rangle = -u_{\mathbf{p}} v_{\mathbf{p}} \langle \alpha_{-\mathbf{p}} \alpha_{-\mathbf{p}}^\dagger + \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} \rangle = -u_{\mathbf{p}} v_{\mathbf{p}} \langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + \beta_{-\mathbf{p}}^\dagger \beta_{-\mathbf{p}} - 1 \rangle. \quad (3.191)$$

The thermal expectation values of the quasiparticle densities $\alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}}$ and $\beta_{\mathbf{p}}^\dagger \beta_{\mathbf{p}}$ are given by the Bose occupation numbers

$$\langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} \rangle = \langle \beta_{\mathbf{p}}^\dagger \beta_{\mathbf{p}} \rangle = f^f(\mathcal{E}_{\mathbf{p}}) = \frac{1}{e^{\mathcal{E}_{\mathbf{p}}/T} + 1}, \quad (3.192)$$

so that

$$\langle a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\uparrow} \rangle = \langle a_{\mathbf{p},\downarrow}^\dagger a_{\mathbf{p},\downarrow} \rangle = v_{\mathbf{p}}^2 + (u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2) f^f(\mathcal{E}_{\mathbf{p}}), \quad (3.193)$$

$$\langle a_{\mathbf{p},\uparrow}^\dagger a_{\mathbf{p},\downarrow}^\dagger \rangle = \langle a_{-\mathbf{p},\downarrow} a_{\mathbf{p},\uparrow} \rangle = u_{\mathbf{p}} v_{\mathbf{p}} [1 - 2f^f(\mathcal{E}_{\mathbf{p}})]. \quad (3.194)$$

The momentum sums (3.160) and (3.159) are now given by

$$\rho_{\uparrow} = \rho_{\downarrow} = \frac{1}{V} \sum_{\mathbf{p}} \left[v_{\mathbf{p}}^2 + (u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2) f^f(\mathcal{E}_{\mathbf{p}}) \right], \quad (3.195)$$

$$\delta = \frac{1}{V} \sum_{\mathbf{p}} u_{\mathbf{p}} v_{\mathbf{p}} [1 - 2f^f(\mathcal{E}_{\mathbf{p}})]. \quad (3.196)$$

Inserting (3.192), these turn into the following $T \neq 0$ versions of $\rho_{\uparrow}$ and δ [compare (3.160) and (3.159)]:

$$\rho_{\uparrow} = \rho_{\downarrow} = \frac{1}{2} \int \frac{d^3 p}{(2\pi\hbar)^3} \left[1 - \frac{\xi_{\mathbf{p}} - g\rho_{\uparrow}}{\mathcal{E}_{\mathbf{p}}} \tanh\left(\frac{\mathcal{E}}{2T}\right) \right], \quad (3.197)$$

$$\delta = g\rho_{\uparrow} \frac{1}{2} \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\mathcal{E}_{\mathbf{p}}} \tanh\left(\frac{\mathcal{E}}{2T}\right). \quad (3.198)$$

With these, the energy (3.153) takes the form [respecting (3.158)]

$$\langle H \rangle_T = \sum_{\mathbf{p}} \left\{ \frac{2\mathcal{E}_{\mathbf{p}}}{e^{\mathcal{E}_{\mathbf{p}}/T} + 1} + \tilde{\xi}_{\mathbf{p}}(n_{\mathbf{p},\uparrow} + n_{\mathbf{p},\downarrow}) - \frac{V}{g} \Delta^2 \right\}. \quad (3.199)$$

For old-fashioned weak-coupling superconductors the gap equation (3.172) receives at nonzero temperature an extra factor $1 - f^f(\mathcal{E}_{\mathbf{p}})$ so that it becomes

$$\frac{1}{g} = \mathcal{N} \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \tanh \frac{E}{2T}. \quad (3.200)$$

It is solved by writing it as

$$\frac{1}{g} = \mathcal{N}(0) \left[\int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} + \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \left(\tanh \frac{E}{2T} - 1 \right) \right]. \quad (3.201)$$

The first integral gives

$$N(0) \ln \frac{2\omega_D}{\Delta} = \mathcal{N}(0) \left[\log \frac{2\omega_D}{\Delta_0} + \log \frac{\Delta_0}{\Delta} \right], \quad (3.202)$$

where Δ_0 is the zero-temperature gap and Δ the gap at finite temperature. In the second integral we expand

$$\tanh \frac{E}{T} - 1 = -2 \frac{e^{-E/T}}{e^{E/T} + 1} = -2 \sum_{n=1}^{\infty} (-)^{n+1} e^{-nE/T}. \quad (3.203)$$

The integrals over the terms in the series are all rapidly convergent so that we can take the upper limit ω_D to infinity in each of them. Then we may use the integral representation of the associated Bessel function $K_0(z)$:

$$\int_0^{\infty} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} e^{-E/T} = K_0(\Delta/T), \quad (3.204)$$

to obtain the gap equation at all temperatures

$$\ln \frac{\Delta_0}{\Delta(T)} = 2 \sum_1^{\infty} (-)^{n+1} K_0 \left(\frac{n\Delta(T)}{T} \right). \quad (3.205)$$

For large arguments, we approximate

$$2K_0 \left(\frac{\Delta_0}{T} \right) \approx \frac{1}{\Delta(0)} \sqrt{2\pi T \Delta_0} e^{-\Delta_0/T}, \quad (3.206)$$

so that the first correction to the low-temperature value of the gap is exponentially small:

$$\Delta(T) = \Delta_0 - \frac{1}{\Delta(0)} \sqrt{2\pi T \Delta_0} e^{-\Delta_0/T}. \quad (3.207)$$

For increasing T , the gap decreases. It vanishes at the *critical temperature* T_c . Near T_c , the gap equation is most conveniently studied by expanding

$$\begin{aligned} \frac{1}{2\sqrt{\xi^2 + \Delta^2}} \tanh \frac{\sqrt{\xi^2 + \Delta^2}}{2T} &= T \sum_m \frac{1}{\omega_m^2 + \xi^2 + \Delta^2} \\ &= T \sum_m \left[\frac{1}{\omega_m^2 + \xi^2} - \frac{\Delta^2}{(\omega_m^2 + \xi^2)^2} + \frac{\Delta^4}{(\omega_m^2 + \xi^2)^3} + \dots \right], \end{aligned} \quad (3.208)$$

where

$$\omega_m = 2\pi T m \quad (3.209)$$

are the Matsubara frequencies for the temperature T . Performing now the integrals over ξ in (3.201) gives the gap equation

$$\frac{1}{g} - \int_0^{\omega_D} \frac{d\xi}{\xi} \tanh \frac{\xi}{2T} = -\frac{\Delta^2}{(\pi T)^2} \sum_m \frac{1}{(2m+1)^3} + \frac{3}{8} \frac{\Delta^4}{(\pi T)^4} \sum_m \frac{1}{(2m+1)^5} + \dots \quad (3.210)$$

The integral is calculated as follows. A partial integration yields

$$\int_0^{\omega_D} \frac{d\xi}{\xi} \tanh \frac{\xi}{2T} = \log \frac{\xi}{T} \tanh \frac{\xi}{2T} \Big|_0^{\omega_D} - \frac{1}{2} \int_0^{\omega_D} d\frac{\xi}{T} \log \frac{\xi}{T} \cosh^{-2} \frac{\xi}{2T}. \quad (3.211)$$

Since $\omega_D/\pi T \gg 1$, the first term is equal to $\log(\omega_D/2T)$, with exponentially small corrections which can be ignored. In the second integral, we have taken the upper limit of integration to infinity since it converges. We may use the integral formula⁸

$$\int_0^{\infty} dx \frac{x^{\mu-1}}{\cosh^2(ax)} = \frac{4}{(2a)^\mu} (1 - 2^{2-\mu}) \Gamma(\mu) \zeta(\mu - 1), \quad (3.212)$$

set $\mu = 1 + \delta$, expand the formula to order δ , and insert the special values

$$\Gamma'(1) = -\gamma, \quad \zeta'(0) = -\frac{1}{2} \log(2\pi) \log(4e^\gamma/\pi), \quad (3.213)$$

to find from the linear terms in δ :

$$\int_0^{\infty} dx \frac{\log x}{\cosh^2(x/2)} = -2 \log(2e^\gamma/\pi), \quad (3.214)$$

so that we obtain

$$\int_0^{\omega_D} \frac{d\xi}{\xi} \tanh \frac{\xi}{2T} = \log \left(\frac{\omega_D}{T} \frac{2e^\gamma}{\pi} \right). \quad (3.215)$$

The sums over m in (3.210) can be expressed in terms of Riemann's zeta function (2.277) as

$$\sum_m \frac{1}{(2m+1)^z} = \frac{2^z - 1}{2^z} \zeta(z). \quad (3.216)$$

We now use the zero-temperature gap equation

$$\frac{1}{g} = \mathcal{N}(0) \frac{2\omega_D}{\Delta_0} \quad (3.217)$$

to eliminate $1/g$ in (3.210). This brings the left-hand side of (3.210) to the form $\log(T/T_c)$ so that the gap equation reads

$$\log \frac{T}{T_c} = -\frac{\Delta^2}{(\pi T)^2} \sum_m \frac{1}{(2m+1)^3} + \frac{3}{8} \frac{\Delta^4}{(\pi T)^4} \sum_m \frac{1}{(2m+1)^5} + \dots, \quad (3.218)$$

⁸See, for instance, I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980, Formula 3.527.3.

where we have set

$$T_c = \frac{e^\gamma}{\pi} \Delta_0 \approx \frac{\Delta_0}{1.76}, \quad (3.219)$$

which is the critical temperature where the gap vanishes. For T lying closely below the critical temperature T_c , we may keep only the first term on the right-hand side of (3.218) and find that the gap behaves like

$$\Delta^2(T) \approx \frac{8}{7\zeta(3)} \pi^2 T_c^2 \left(1 - \frac{T}{T_c}\right). \quad (3.220)$$

The full solution is plotted in Fig. 3.9. The existence of an energy gap in super-

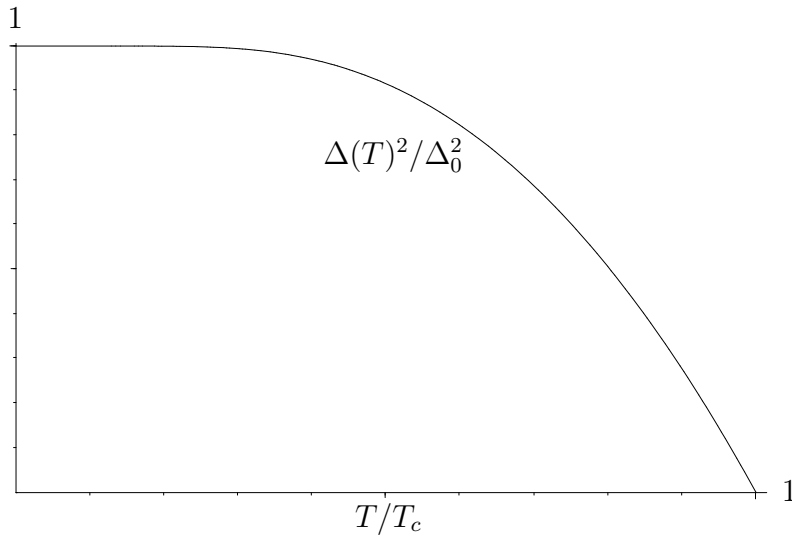


FIGURE 3.9 Solution of the gap equation for a weak attraction between electrons.

conductors was first confirmed experimentally by millimeter-microwave absorption in lead films below $T_c \approx 7.2^0$ K. The result was $2\Delta_0 \sim 3.4T_c$ which is in good agreement with the theoretical values 2×1.76 . The energy gap Δ is the reason behind the extraordinary stability of electric currents in a superconductor. In practical situations, the lifetime is often larger than 10^5 years. Superconductivity has not yet been exploited for long-distance transport of industrial electric currents because of the need to maintain wires at extremely low temperatures, for instance via liquid ^4He . Until a few years ago, the superconductor with the highest transition temperatures were alloys of Niob and Zirconion, or the compound Niobstannid Nb_3Sn , which has $T_c \approx 18.2^0\text{K}$, and remains superconductive up to magnetic fields of 20 Tesla. Superconductive coils have been used with great advantage in high-energy particle accelerators and in nuclear magnetic resonance devices, which have found important application in medicine (tomography). With the recent discovery of superconductivity at temperatures up to 100^0K , and with the possibility of more economic cooling via liquid nitrogen, superconductivity will become useful for broader industrial applications.

3.5 Crossover to Strong Couplings

If the coupling strength increases, the above approximation of integrating only over a thin shell around the surface of the Fermi sphere is no longer applicable, but the momentum integral must run over the entire momentum space. Then the subtracted gap equation (3.188) becomes

$$-\frac{1}{k_F a_s} = \frac{2}{\pi} \left[\frac{2}{3J_2(\hat{\mu})} \right]^{1/3} J_1(\hat{\mu}), \quad (3.221)$$

where $\hat{\mu} \equiv \tilde{\mu}/\Delta$ and

$$J_1(z) \equiv \int_0^\infty dx x^2 \left(\frac{1}{\sqrt{(x^2 - z)^2 + 1}} - \frac{1}{x^2} \right), \quad (3.222)$$

$$J_2(z) \equiv \int_0^\infty dx x^2 \left(1 - \frac{x^2 - z}{\sqrt{(x^2 - z)^2 + 1}} \right). \quad (3.223)$$

The particle number equation (3.160), that fixes the chemical potential $\tilde{\mu}$, takes the form

$$1 = \frac{3}{2} \left(\frac{\Delta}{\varepsilon_F} \right)^{3/2} J_2(\hat{\mu}). \quad (3.224)$$

The two equations can be solved numerically yielding the gap and the chemical potential $\tilde{\mu} = \mu + g\rho/2$ as a function of the inverse s -wave scattering length $1/k_F a_s$ from the weak-coupling (left) to the strong-coupling (BEC) limit as shown in Fig. 3.10.

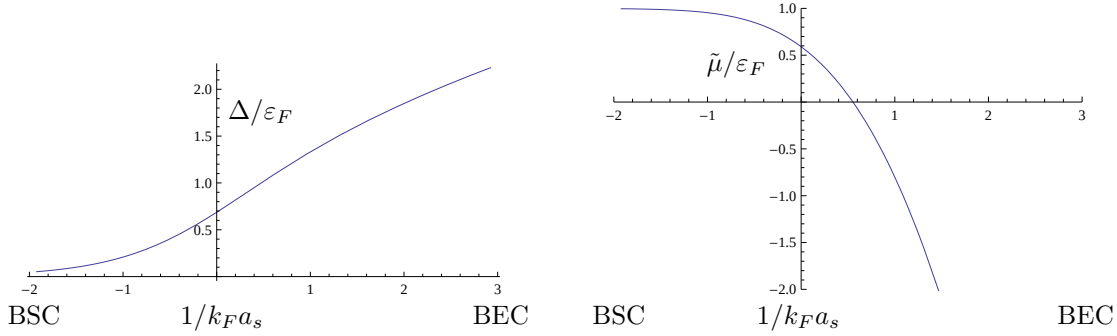


FIGURE 3.10 Plot of the gap function and of the chemical potential as functions of the inverse s -wave scattering length.

At finite temperature, we define the natural temperature $T_F \equiv \varepsilon_F/k_B$ and the reduced temperature $t \equiv T/T_F$, and the gap equation becomes

$$-\frac{1}{k_F a_s} = \frac{2}{\pi} \left[\frac{2}{3J_2(\hat{\mu}, t)} \right]^{1/3} J_1(\hat{\mu}, t), \quad (3.225)$$

where

$$J_1(z, t) \equiv \int_0^\infty dx x^2 \left(\frac{1}{\sqrt{(x^2 - z)^2 + 1}} \tanh \frac{x^2}{2t} - \frac{1}{x^2} \right), \quad (3.226)$$

$$J_2(z, t) \equiv \int_0^\infty d\kappa \kappa^2 \left(1 - \frac{\kappa^2 - z}{\sqrt{(\kappa^2 - z)^2 + 1}} \tanh \frac{\kappa^2}{2t} \right), \quad (3.227)$$

while the particle number equation (3.160), that fixes the chemical potential $\tilde{\mu}$, becomes simply

$$1 = \frac{3}{2} \left(\frac{\Delta}{\varepsilon_F} \right)^{3/2} J_2(\tilde{\mu}, t). \quad (3.228)$$

3.5.1 Bogoliubov Theory for Bose Gas at Finite Temperature

It is easy to extend Bogoliubov's weak-coupling theory to finite temperature T . There the expectation values (3.31) become

$$\langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle = v_{\mathbf{p}}^2 + \langle u_{\mathbf{p}}^2 \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + v_{\mathbf{p}}^2 \alpha_{-\mathbf{p}}^\dagger \alpha_{-\mathbf{p}} \rangle, \quad (3.229)$$

and

$$\langle a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \rangle = u_{\mathbf{p}} v_{\mathbf{p}} + u_{\mathbf{p}} v_{\mathbf{p}} \langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^\dagger \alpha_{-\mathbf{p}} \rangle. \quad (3.230)$$

The thermal expectation values of the quasiparticle densities $\alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}}$ are given by the Bose occupation numbers

$$\langle \alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} \rangle = f^b(\mathcal{E}_{\mathbf{p}}) = \frac{1}{e^{\mathcal{E}_{\mathbf{p}}/T} - 1}, \quad (3.231)$$

so that

$$\langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle = v_{\mathbf{p}}^2 + (u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) f^b(\mathcal{E}_{\mathbf{p}}), \quad (3.232)$$

$$\langle a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \rangle = u_{\mathbf{p}} v_{\mathbf{p}} [1 + 2f^b(\mathcal{E}_{\mathbf{p}})]. \quad (3.233)$$

The momentum sum of the first expectation value gives the temperature-dependent density of uncondensed particles

$$\rho_{\mathbf{u}} = \frac{1}{V} \sum_{\mathbf{p}} \left[v_{\mathbf{p}}^2 + (u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) f^b(\mathcal{E}_{\mathbf{p}}) \right]. \quad (3.234)$$

Inserting (3.231), this becomes

$$\rho_{\mathbf{u}} = \frac{1}{2} \int \frac{d^3 p}{(2\pi\hbar)^3} \left[\frac{\varepsilon_{\mathbf{p}} + g\rho_0}{\mathcal{E}_{\mathbf{p}}} \coth \left(\frac{\mathcal{E}_{\mathbf{p}}}{2T} \right) - 1 \right]. \quad (3.235)$$

Hence the density of uncondensed particles (3.47) is

$$\rho_{\mathbf{u}}(t) = k_{g\rho_0}^3 \frac{I_{\rho_{\mathbf{u}}}(t)}{4\pi^2}, \quad k_{g\rho_0} = \frac{\sqrt{2Mg\rho_0}}{\hbar} = 2\sqrt{2\pi a_s \rho_0}, \quad (3.236)$$

where $I_{\rho_{\mathbf{u}}}(t)$ is the integral

$$I_{\rho_{\mathbf{u}}}(t) \equiv \int_0^\infty d\kappa \kappa^2 \left[\frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \coth \left(\frac{\sqrt{(\kappa^2 + 1)^2 - 1}}{2t} \right) - 1 \right] = \frac{\sqrt{2}}{3} h_{\rho_{\mathbf{u}}}(t). \quad (3.237)$$

Here t is the reduced temperature

$$t \equiv k_B T / \varepsilon_{g\rho_0}, \quad (3.238)$$

and

$$\varepsilon_{g\rho_0} \equiv \frac{\hbar^2 k_{g\rho_0}^2}{2M} = \frac{4\pi\hbar^2}{M} (a_s \rho_0)^2. \quad (3.239)$$

We may also write

$$\rho_{\mathbf{u}}(t) = \rho_{\mathbf{u}}(0) h_{\rho_{\mathbf{u}}}(t) = k_{g\rho_0}^3 \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2} h_{\rho_{\mathbf{u}}}(t) = \frac{8\rho_0}{3\sqrt{\pi}} \sqrt{a_s^3 \rho_0}^{1/2} h_{\rho_{\mathbf{u}}}(t), \quad (3.240)$$

where

$$h_{\rho_{\mathbf{u}}}(t) = \frac{3}{\sqrt{2}} \int_0^\infty d\kappa \kappa^2 \left[\frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \left(1 + \frac{2}{e^{\sqrt{(\kappa^2 + 1)^2 - 1}/t} - 1} \right) - 1 \right]. \quad (3.241)$$

This can be split as

$$h_{\rho_{\mathbf{u}}}(t) \equiv 1 + \Delta h_{\rho_{\mathbf{u}}}(t) = 1 + \frac{3}{\sqrt{2}} \int_0^\infty d\kappa \kappa^2 \frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \frac{2}{e^{\sqrt{(\kappa^2 + 1)^2 - 1}/t} - 1}. \quad (3.242)$$

After introducing new variables $y \equiv \kappa^2/t$ and $x \equiv \sqrt{(\kappa^2 + 1)^2 - 1}/t$, $yt \equiv \sqrt{(xt)^2 + 1} - 1$, so that $d\kappa \kappa^2 = t dy (ty)^{1/2}/2$ and $dy = dx xt/(yt + 1)$, we may rewrite $h_{\rho_{\mathbf{u}}}(t)$ in the following form:

$$h_{\rho_{\mathbf{u}}}(t) = 1 + \frac{\sqrt{3}}{2} t \int_0^\infty dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{e^x - 1}. \quad (3.243)$$

The corresponding formula for the full uncondensed density (3.236) is

$$\rho_{\mathbf{u}}(t) = \frac{k_{g\rho_0}^3}{4\pi^2} \frac{\sqrt{2}}{3} h_{\rho_{\mathbf{u}}}(t) = \frac{k_{g\rho_0}^3}{4\pi^2} \left(\frac{\sqrt{2}}{3} + t \int_0^\infty dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{e^x - 1} \right). \quad (3.244)$$

For weak couplings, $\varepsilon_{g\rho_0}$ becomes very small, so that the integral (3.242) is dominated by the large- κ regime, and we find

$$\Delta h_{\rho_u}(t) \rightarrow \frac{6}{\sqrt{2}} \int_0^\infty d\kappa \kappa^2 \frac{1}{e^{\kappa^2/t} - 1} = \frac{3}{2} \sqrt{\frac{\pi}{2}} t^{3/2} \zeta(3/2). \quad (3.245)$$

This implies that

$$\rho_u(t) \underset{T \approx 0}{=} \rho_u(0) + \frac{k_{g\rho_0}^3}{4\pi^2} I_{\rho_u} \Delta h_{\rho_u}(t) = \frac{8\rho_0}{3\sqrt{\pi}} \sqrt{a_s \rho_0}^{3/2} + \rho \left(\frac{T}{T_c} \right)^{3/2}, \quad (3.246)$$

with

$$T_c \equiv [\zeta(3/2)]^{-2/3} 4\pi T_a, \quad (3.247)$$

and

$$T_a \equiv \varepsilon_a/k_B, \quad \varepsilon_a \equiv \hbar^2/2Ma^2. \quad (3.248)$$

The ratio $\hat{T} \equiv T/T_a$ is the temperature measured in units of the fundamental temperature T_a , so that $s/\hat{T} = \bar{\Sigma}/k_B T = 1/t$.

The temperature T_c at zero coupling strength agrees with the condensation temperature of free Bose gases determined in Eq. (2.338).

To plot the full temperature behavior it is convenient to introduce the dimensionless parameter $s \equiv g\rho_0/\varepsilon_a$. Now we rescale the momentum integration, and obtain

$$\Delta h_{\rho_u}(t) = \frac{1}{s^{3/2}} \frac{3}{\sqrt{2}} \int_0^\infty d\kappa \kappa^2 \frac{\kappa^2 + s}{\sqrt{(\kappa^2 + s)^2 - s^2}} \frac{2}{e^{\sqrt{(\kappa^2 + s)^2 - s^2}/\hat{T}} - 1}, \quad (3.249)$$

where $\hat{T} \equiv T/T_a$ is the temperature measured in units of the fundamental temperature T_a . The plots are shown in Fig. 3.11.

3.6 Bose Gas at Strong Interactions

We are now prepared to carry the Bogoliubov theory of a weakly interacting spinless Bose gas to strong couplings. For this we proceed as in Eq. (3.124) and add, to the free Hamiltonian (3.4), variational energy terms with real $\Delta_{\mathbf{p}}$

$$\bar{H}_{\text{trial}} \equiv \frac{1}{2} \sum_{\mathbf{p}} \left[\Sigma_{\mathbf{p}} (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}} a_{-\mathbf{p}}^\dagger) + \Delta_{\mathbf{p}} a_{-\mathbf{p}} a_{\mathbf{p}} + \Delta_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \right]. \quad (3.250)$$

In contrast to the Bogoliubov theory, we work in a grand-canonical ensemble and allow for a chemical potential $\mu \neq 0$, to rewrite the free part of the Hamiltonian as

$$\bar{H}_0 \equiv \frac{1}{2} \sum_{\mathbf{p}} \left[(\varepsilon_{\mathbf{p}} - \mu + \Sigma_{\mathbf{p}}) (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}} a_{-\mathbf{p}}^\dagger) + \Delta_{\mathbf{p}}^\dagger a_{-\mathbf{p},\alpha} a_{\mathbf{p},\alpha} + \Delta_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \right]. \quad (3.251)$$

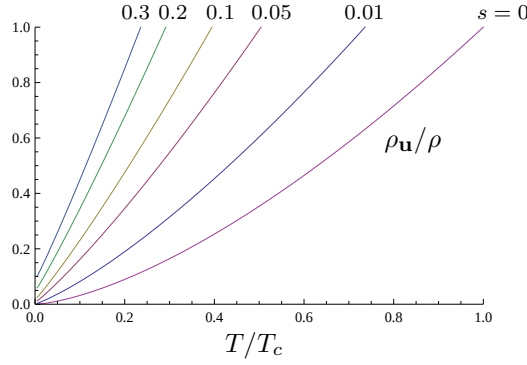


FIGURE 3.11 Temperature dependence of the uncondensed fraction ρ_u/ρ in a Bose gas. The temperature $\hat{T}$ is measured in units of the natural temperature $T_a \equiv \varepsilon_a/k_B = \hbar^2/2Ma^2k_B$. The critical temperature of the free Bose gas lies at $\hat{T}_c = T_c/T_a = [\zeta(3/2)]^{-2/3}4\pi$. The parameter s on the various curves is the dimensionless ratio $s \equiv g\rho_0/\varepsilon_a$ of the quasiparticle energies $\mathcal{E}_{\mathbf{p}} = \sqrt{(\varepsilon_{\mathbf{p}} + g\rho_0)^2 - g^2\rho_0^2}$. The transition to the normal phase takes place when the curves reach unity. Note the nonzero intercepts on the vertical axis, showing the depletion of the condensate at zero temperature.

To this we add the zero-momentum part (3.17) of the free Hamiltonian (3.17), so that we are faced with

$$H'_0 \equiv -V \frac{\mu}{g} \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + \sum_{\mathbf{p} \neq 0} (\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}}) a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{1}{2} (\Sigma_0 + \Delta_{\mathbf{p}}) \sum_{\mathbf{p} \neq 0} (a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + \text{h.c.}). \quad (3.252)$$

An important difference with respect to Bogoliubov's theory, the zero-momentum operator a_0 is *not* approximated by a scalar A_0 that is identified as $\sqrt{V\rho_0}$, where ρ_0 is the condensate density. Instead, we shall take the expectation value $A_0 \equiv \langle \psi(\mathbf{x}) \rangle$ of the field $\psi(\mathbf{x}) = \sum_{\mathbf{p}} e^{i\mathbf{p}\mathbf{x}/\hbar} a_{\mathbf{p}}$ and introduce a parameter

$$\Sigma_0 \equiv gA_0^2/V, \quad (3.253)$$

leaving its physical meaning open, and considering it as a variational parameter to be determined in each order in perturbation theory by optimization. Optimization will mostly succeed by extremizing the energy with respect to Σ_0 . Only after that, Σ_0 will acquire a physical meaning. To lowest order, Σ_0 will turn out to be equal to g times the condensate density ρ_0 , as in Bogoliubov's theory. Correction To higher orders, there will be corrections.

After a Bogoliubov transformation we arrive at the Hamiltonian

$$\begin{aligned} H'_0 = & -V \frac{\mu}{g} \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + \sum_{\mathbf{p} \neq 0} \left(\{ [\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}}] v_{\mathbf{p}}^2 + (\Sigma_0 + \Delta_{\mathbf{p}}) u_{\mathbf{p}} v_{\mathbf{p}} \} \right. \\ & + \frac{1}{2} \{ [\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}}] (u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) + (\Sigma_0 + \Delta_{\mathbf{p}}) 2u_{\mathbf{p}} v_{\mathbf{p}} \} (\alpha_{\mathbf{p}}^\dagger \alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^\dagger \alpha_{-\mathbf{p}}) \\ & \left. + \frac{1}{2} \{ [\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}}] 2u_{\mathbf{p}} v_{\mathbf{p}} + (\Sigma_0 + \Delta_{\mathbf{p}}) (u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2) \} (\alpha_{\mathbf{p}}^\dagger \alpha_{-\mathbf{p}}^\dagger + \alpha_{\mathbf{p}} \alpha_{-\mathbf{p}}) \right). \end{aligned} \quad (3.254)$$

At zero temperature, all quasiparticles are frozen out and only the first line of this energy survives. This will be denoted by W_0 and provides us with the lowest-order variational energy of the system. The energy W_0 is now extremized with respect to the Bogoliubov coefficients $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ while maintaining the constraint $u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2 = 1$ for every momentum $\mathbf{p}$, so that $\delta u_{\mathbf{p}} = \delta v_{\mathbf{p}} v_{\mathbf{p}} / u_{\mathbf{p}}$, as in the previous treatment of Eq. (3.41). To this we must add the expectation value of the interaction energy (3.15):

$$\langle H'_{\text{int}} \rangle = \frac{g}{2V} \sum_{\mathbf{p} \neq 0, \mathbf{p}' \neq 0, \mathbf{q} \neq 0} \langle a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} a_{\mathbf{p}} \rangle. \quad (3.255)$$

As in Eq. (3.149) we can use the commutation rules⁹ (2.211) to expand the right-hand side into the three pair terms

$$\begin{aligned} \langle 0 | a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} a_{\mathbf{p}} | 0 \rangle &= \langle 0 | a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger | 0 \rangle \langle 0 | a_{\mathbf{p}'} a_{\mathbf{p}} | 0 \rangle \\ &+ \langle 0 | a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}} | 0 \rangle \langle 0 | a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} | 0 \rangle \\ &+ \langle 0 | a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'} | 0 \rangle \langle 0 | a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}} | 0 \rangle. \end{aligned} \quad (3.256)$$

Note the opposite sign of the last term with respect to the fermion expression (3.152). Inserting the expectation values (3.31), this becomes

$$\langle 0 | a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{p}'-\mathbf{q}}^\dagger a_{\mathbf{p}'} a_{\mathbf{p}} | 0 \rangle = \delta_{\mathbf{p},-\mathbf{p}'} u_{\mathbf{p}+\mathbf{q}} v_{\mathbf{p}+\mathbf{q}} u_{\mathbf{p}} v_{\mathbf{p}} + 2\delta_{\mathbf{q},0} v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2 \quad (3.257)$$

and we find

$$\langle H'_{\text{int}} \rangle = \frac{g}{2V} \sum_{\mathbf{p} \neq 0, \mathbf{p}' \neq 0} (u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + 2v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2). \quad (3.258)$$

Finally we must subtract the expectation value of the trial Hamiltonian $\bar{H}_{\text{trial}}$. The total variational ground state energy $E'_{\text{tot}} = E'_0 + \langle H'_{\text{int}} \rangle - \langle H'_{\text{trial}} \rangle$ is now

$$\begin{aligned} E'_{\text{tot}} &= -V \frac{\mu}{g} \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + \sum_{\mathbf{p} \neq 0} [(\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}}) v_{\mathbf{p}}^2 + (\Sigma_0 + \Delta_{\mathbf{p}}) u_{\mathbf{p}} v_{\mathbf{p}}] \\ &+ \frac{g}{2V} \sum_{\mathbf{p} \neq 0, \mathbf{p}' \neq 0} (u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{p}'} v_{\mathbf{p}'} + 2v_{\mathbf{p}}^2 v_{\mathbf{p}'}^2) - \sum_{\mathbf{p} \neq 0} (\Sigma_{\mathbf{p}} v_{\mathbf{p}}^2 + \Delta_{\mathbf{p}} u_{\mathbf{p}} v_{\mathbf{p}}). \end{aligned} \quad (3.259)$$

According to the rules of Variational Perturbation Theory (VPT) we shall write this as $W_1 = W_0 + W_{11} + W_{12}$, where W_0 denotes, in the first line of (3.259), the zeroth-order variational energy, whereas $W_{11} + W_{12}$ are the two terms in the second line. It is important to treat the energy W_{12} as a first-order perturbation. Otherwise the variational parameters $\Sigma_{\mathbf{p}}$ and $\Delta_{\mathbf{p}}$ cancel completely and do not improve the ground-state results.¹⁰

⁹More elegantly we can use Wick's theorem to be derived in Section 7.17.1.

¹⁰The first term in W_{11} can be split into two parts $\alpha_0 W_{11} + (1 - \alpha_0) W_{11}$, considering the first part as belonging to W_0 and the second part to the perturbation. The results of this will be independent of α_0 .

By differentiating the energy with respect to $-\mu$ and setting the result equal to N , we find for the density $\rho = N/V$:

$$\rho = \frac{\Sigma_0}{g} + \sum_{\mathbf{p} \neq 0} v_{\mathbf{p}}^2. \quad (3.260)$$

As in Eq. (3.47), the second term is the density of excited, uncondensed particles $\rho_{\mathbf{u}}$, so that (3.260) reveals Σ_0/g as the condensate density ρ_0 :

$$\frac{\Sigma_0}{g} = \rho_0 = \rho - \rho_{\mathbf{u}}, \quad (3.261)$$

as before in Bogoliubov's theory.

Next we extremize W_1 with respect to the variational parameter Σ_0 , which yields the equation

$$\frac{\mu - \Sigma_0}{g} = \sum_{\mathbf{p} \neq 0} (2v_{\mathbf{p}}^2 + u_{\mathbf{p}}v_{\mathbf{p}}) = 2\rho_{\mathbf{u}} + \sum_{\mathbf{p} \neq 0} u_{\mathbf{p}}v_{\mathbf{p}} = 2\rho_{\mathbf{u}} + \delta, \quad (3.262)$$

so that

$$\frac{\mu}{g} = \rho + \rho_{\mathbf{u}} + \delta. \quad (3.263)$$

We are now able to fix the size of the Bogoliubov coefficients $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$. The original way of doing this is algebraic, based on the elimination of the off-diagonal elements of the transformed Hamiltonian operator. In the framework of our variational approach it is more natural to use the equivalent procedure of *extremizing* the energy W_0 with respect to $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ under the constraint $u_{\mathbf{p}}^2 - v_{\mathbf{p}}^2 = 1$, so that $\partial u_{\mathbf{p}} / \partial v_{\mathbf{p}} = v_{\mathbf{p}} / u_{\mathbf{p}}$. For each nonzero momentum, this yields the equation

$$2(\varepsilon_{\mathbf{p}} - \mu + 2\Sigma_0 + \Sigma_{\mathbf{p}})v_{\mathbf{p}} + (\Sigma_0 + \Delta_{\mathbf{p}})(u_{\mathbf{p}} + v_{\mathbf{p}}^2/u_{\mathbf{p}}) = 0. \quad (3.264)$$

In order to solve this, we assume $\Sigma_{\mathbf{p}} \equiv \Sigma$ to be independent of $\mathbf{p}$ so that we may introduce a constant

$$\bar{\Sigma} \equiv -\mu + 2\Sigma_0 + \Sigma. \quad (3.265)$$

In the prefactor of the second term of (3.264), we assume that $\Delta_{\mathbf{p}}$ is also independent of $\mathbf{p}$, so that it may be set equal to a constant Δ . After this, we may define a constant

$$\bar{\Delta} \equiv \Sigma_0 + \Delta, \quad (3.266)$$

and rewrite (3.264) in the simple form

$$2(\varepsilon_{\mathbf{p}} + \bar{\Sigma})v_{\mathbf{p}} + \bar{\Delta}(u_{\mathbf{p}} + v_{\mathbf{p}}^2/u_{\mathbf{p}}) = 0, \quad (3.267)$$

which is solved for all $\mathbf{p}$ by a new Bogoliubov transformation with coefficients:

$$u_{\mathbf{p}}^2 = \frac{1}{2} \left(1 + \frac{\varepsilon_{\mathbf{p}} + \bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}} \right), \quad v_{\mathbf{p}}^2 = -\frac{1}{2} \left(1 - \frac{\varepsilon_{\mathbf{p}} + \bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}} \right), \quad (3.268)$$

where $u_{\mathbf{p}}v_{\mathbf{p}} = -\bar{\Delta}/2\mathcal{E}_{\mathbf{p}}$, and the quasiparticle energies are now

$$\mathcal{E}_{\mathbf{p}} = \sqrt{(\varepsilon_{\mathbf{p}} + \bar{\Sigma})^2 - \bar{\Delta}^2}. \quad (3.269)$$

According to the Nambu-Goldstone theorem, these have to vanish linearly for $\mathbf{p} \rightarrow 0$. This forces us to set $\bar{\Delta} = \bar{\Sigma}$, or

$$\Delta = \bar{\Sigma} - \Sigma_0, \quad (3.270)$$

thus avoiding the main hurdle in previous attempts to go beyond the Bogoliubov theory [28].

Having determined the Bogoliubov coefficients we may now calculate the momentum sums in Eq. (3.263). First, there is the density of uncondensed particles which is evaluated in the same way as before the expression (3.47) of Bogoliubov's theory. We insert $v_{\mathbf{p}}^2$ of (3.268) into the momentum sum and arrive at

$$\rho_{\mathbf{u}} = \sum_{\mathbf{p} \neq 0} \langle a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \rangle = \frac{1}{V} \sum_{\mathbf{p} \neq 0} v_{\mathbf{p}}^2 = \int \frac{d^3p}{(2\pi\hbar)^3} v_{\mathbf{p}}^2 = \frac{1}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \left(\frac{\varepsilon_{\mathbf{p}} + \bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}} - 1 \right). \quad (3.271)$$

Performing variable substitutions as before in (3.47), we obtain

$$\rho_{\mathbf{u}} = k_{\bar{\Sigma}}^3 \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2}, \quad (3.272)$$

where $I_{\rho_{\mathbf{u}}} = \sqrt{2}/3$ is the same number as before in (3.52), whereas $k_{\bar{\Sigma}}$ is defined as in (3.49), except that the energy $g\rho_0$ is replaced by the new energy $\bar{\Sigma}$:

$$k_{\bar{\Sigma}} = \frac{\sqrt{2M\bar{\Sigma}}}{\hbar}. \quad (3.273)$$

The other momentum sum in Eq. (3.263) becomes, due to (3.268),

$$\delta = \sum_{\mathbf{p} \neq 0} \langle a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}^{\dagger} \rangle = \frac{1}{V} \sum_{\mathbf{p}} u_{\mathbf{p}}v_{\mathbf{p}} = \int \frac{d^3p}{(2\pi\hbar)^3} u_{\mathbf{p}}v_{\mathbf{p}} = -\frac{\bar{\Sigma}}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{\mathcal{E}_{\mathbf{p}}}. \quad (3.274)$$

This is a divergent quantity. The divergence can be removed in the same way as before the divergence in the energy (3.57), by absorbing it into the inverse coupling constant of the model using Formula (3.58). Thus we introduce the finite renormalized quantity

$$\delta_R = \frac{1}{V} \sum_{\mathbf{p}} u_{\mathbf{p}}v_{\mathbf{p}} = \int \frac{d^3p}{(2\pi\hbar)^3} u_{\mathbf{p}}v_{\mathbf{p}} = -\frac{\bar{\Sigma}}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \left(\frac{1}{\mathcal{E}_{\mathbf{p}}} - \frac{1}{\varepsilon_{\mathbf{p}}} \right), \quad (3.275)$$

and write

$$\delta = \delta_R + \delta_{\text{div}}, \quad (3.276)$$

where the infinity is contained in the momentum sum

$$\delta_{\text{div}} \equiv -\frac{\bar{\Sigma}}{V} \sum_{\mathbf{p}} \frac{1}{2\varepsilon_{\mathbf{p}}} = -\frac{\bar{\Sigma}}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{\varepsilon_{\mathbf{p}}}. \quad (3.277)$$

Let us denote the divergence by

$$\frac{1}{Vv} = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{\varepsilon_{\mathbf{p}}}. \quad (3.278)$$

Then we have

$$\delta = -\frac{\bar{\Sigma}}{g} = \delta_R + \delta_{\text{div}} = \delta_R - \frac{\bar{\Sigma}}{2Vv}, \quad \delta_R \equiv -\frac{\bar{\Sigma}}{g_R}. \quad (3.279)$$

Inserting (3.276) together with (3.276) into (3.263), we find

$$\frac{\mu}{g} - \frac{\Sigma_0}{g} = 2\rho_{\mathbf{u}} + \delta_R + \delta_{\text{div}}. \quad (3.280)$$

Recalling (3.261), this implies

$$\frac{\mu}{g} = \rho_{\mathbf{0}} + 2\rho_{\mathbf{u}} + \delta_R + \delta_{\text{div}} = \rho + \rho_{\mathbf{u}} + \delta_R + \delta_{\text{div}}. \quad (3.281)$$

We evaluate the convergent momentum sum (3.275) in the same way as in (3.271) and find

$$\delta_R = k_{\Sigma}^3 \frac{I_{\delta}}{4\pi^2} \quad (3.282)$$

where I_{δ} is given by an integral similar to (3.52):

$$I_{\delta} \equiv -\int_0^{\infty} d\kappa \kappa^2 \left(\frac{1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - \frac{1}{\kappa^2} \right) = \sqrt{2}. \quad (3.283)$$

Hence we see that

$$\delta_R = 3\rho_{\mathbf{u}}. \quad (3.284)$$

Before we continue, we may simplify *all* diverging expressions by making use of the renormalizability of the theory. Since we have added and subtracted only terms in the Hamiltonian (3.259) which are quadratic in the fields, and contain at most two spatial derivatives (the latter if $\Sigma_{\mathbf{p}}$ and $\Delta_{\mathbf{p}}$ contain a nonzero term $\Sigma'_{\mathbf{p}}$ and $\Delta'_{\mathbf{p}}$), all infinities can be absorbed in the initial parameters of the Hamiltonian. This property will be discussed in more detail in Chapters 11 and 20. In such theories,

we may eliminate all divergencies simply by using *Veltman's rule* (11A.1), which amounts here to setting

$$\int d^3p \frac{1}{\varepsilon_{\mathbf{p}}} = 0, \quad (3.285)$$

and thus $\delta_{\text{div}} = 0$. After this we may identify all quantities directly with the renormalized, observable ones.

It is further useful to introduce a natural length scale, the average distance per particle a , that makes the particle density equal to $\rho = 1/a^3$. We also introduce a corresponding energy scale:

$$\varepsilon_a \equiv \frac{\hbar^2}{2Ma^2}, \quad (3.286)$$

and an associated reduced s -wave scattering length

$$\hat{a}_s \equiv 8\pi \frac{a_s}{a}. \quad (3.287)$$

In terms of this, the renormalized coupling constant is

$$g_R = \frac{4\pi\hbar^2}{M}a_s = 8\pi\varepsilon_a a^2 a_s = \varepsilon_a a^3 \hat{a}_s. \quad (3.288)$$

After this, we re-express all equations in a dimensionless form, for instance

$$\bar{\Sigma} \equiv s \varepsilon_a, \quad (3.289)$$

which leads to

$$k_{\bar{\Sigma}} = \frac{\sqrt{s}}{a}, \quad \frac{\bar{\Sigma}}{g_R} = \frac{s}{8\pi a^2 a_s} = \frac{s}{a^3 \hat{a}_s}. \quad (3.290)$$

From the quasiparticle spectrum (3.291) with $\bar{\Sigma} = \bar{\Delta}$ we see that the parameter $\bar{\Sigma}$ determines the *slope* in the gapless energy spectrum, which we may write as

$$\mathcal{E}_{\mathbf{p}} = \sqrt{2\bar{\Sigma}\varepsilon_{\mathbf{p}} + \varepsilon_{\mathbf{p}}^2}. \quad (3.291)$$

This fixes the velocity of second sound to

$$c \equiv \sqrt{\frac{\bar{\Sigma}}{M}}, \quad (3.292)$$

thereby generalizing (3.64). Inserting (3.289) and (3.286), we find its dimensionless form

$$c = \sqrt{\frac{s}{2}} v_a, \quad v_a \equiv \frac{p_a}{M} \equiv \frac{\hbar}{aM}. \quad (3.293)$$

In these units, the uncondensed particle density (3.272) reads

$$\frac{\rho_{\mathbf{u}}}{\rho} = s^{3/2} \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2}. \quad (3.294)$$

As a result, we can write the Bogoliubov-transformed energy (3.259) as

$$W_1 = -V \frac{\mu}{g} \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + V w(\bar{\Sigma}) - \frac{1}{4} \frac{\bar{\Sigma}^2}{Vv} + \frac{gV}{2} (2\rho_{\mathbf{u}}^2 + \delta^2) - V(\Sigma \rho_{\mathbf{u}} + \Delta \delta), \quad (3.295)$$

where we have abbreviated

$$w(\bar{\Sigma}) \equiv \frac{1}{2V} \sum_{\mathbf{p} \neq 0} \left[(\mathcal{E}_{\mathbf{p}} - \varepsilon_{\mathbf{p}} - \bar{\Sigma}) + \frac{\bar{\Sigma}^2}{2\varepsilon_{\mathbf{p}}} \right]. \quad (3.296)$$

The subtracted term is the analog of the last term in the original Bogoliubov energy (3.57), which was performed to make the momentum sum convergent. It can be evaluated in the same way as in (3.59), yielding a similar result as in (3.297):

$$w(\bar{\Sigma}) = \bar{\Sigma} k_{\bar{\Sigma}}^3 \frac{I_E}{4\pi^2}, \quad (3.297)$$

where $I_E = 8\sqrt{2}/15$ is the previous integral (3.61).

The parameter Σ still needs to be determined. For this we must extremize W_1 with respect to Σ . This is done most easily by inserting $\Sigma \equiv \bar{\Sigma} + \mu - 2\Sigma_0$ from (3.265), and $\Delta \equiv \bar{\Sigma} - \Sigma_0$ from (3.270) into (3.295) to write W_1 as

$$\begin{aligned} W_1 = & -V \frac{\mu}{g} \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + V \bar{\Sigma} k_{\bar{\Sigma}}^3 \frac{I_E}{4\pi^4} - \frac{1}{4} \frac{\bar{\Sigma}^2}{Vv} \\ & + \frac{gV}{2} (2\rho_{\mathbf{u}}^2 + \delta^2) - V[(\bar{\Sigma} + \mu - 2\Sigma_0)\rho_{\mathbf{u}} + (\bar{\Sigma} - \Sigma_0)\delta], \end{aligned} \quad (3.298)$$

and extremizing this with respect to $\bar{\Sigma}$. To do this, we use the fact that at zero temperature

$$\partial_{\bar{\Sigma}} w(\bar{\Sigma}) = \partial_{\bar{\Sigma}} \bar{\Sigma} k_{\bar{\Sigma}}^3 \frac{I_E}{4\pi^2} = k_{\bar{\Sigma}}^3 \left(\frac{I_{\rho_{\mathbf{u}}}}{4\pi^2} + \frac{I_{\delta}}{4\pi^2} \right) = \rho_{\mathbf{u}} + \delta, \quad (3.299)$$

so that we obtain the derivative with respect to $\bar{\Sigma}$, denoted by a prime:

$$W'_1 = gV(2\rho_{\mathbf{u}}\rho'_{\mathbf{u}} + \delta\delta') - V[(\bar{\Sigma} + \mu - 2\Sigma_0)\rho'_{\mathbf{u}} + (\bar{\Sigma} - \Sigma_0)\delta']. \quad (3.300)$$

Setting W'_1 equal to zero, this yields

$$(\bar{\Sigma} + \mu - 2\Sigma_0 - 2g\rho_{\mathbf{u}})\rho'_{\mathbf{u}} + (\bar{\Sigma} - \Sigma_0 - g\delta)\delta' = 0. \quad (3.301)$$

Inserting Σ_0 and μ from Eqs. (3.261) and (3.281), the latter after having applied Veltman's rule that will be derived in Chapter 7 (see p. 589), we obtain the equation for $\bar{\Sigma}$ at $T = 0$:

$$[\bar{\Sigma} - g(\rho - \rho_{\mathbf{u}} + \delta)]\rho'_{\mathbf{u}} + [\bar{\Sigma} - g(\rho - \rho_{\mathbf{u}} - \delta)]\delta' = 0, \quad (3.302)$$

which is solved by

$$\frac{\bar{\Sigma}}{g} = \rho - \rho_{\mathbf{u}} - \delta \frac{\rho'_{\mathbf{u}} - \delta'}{\rho'_{\mathbf{u}} + \delta'} = 0. \quad (3.303)$$

Inserting $\rho_{\mathbf{u}}$ from (3.272) and δ from (3.282), and using (3.284), this reduces to

$$\frac{\bar{\Sigma}}{g} = \rho + \frac{1}{2}\rho_{\mathbf{u}}. \quad (3.304)$$

In natural units, this amounts to the equation

$$\frac{s}{\hat{a}_s} = 1 + \frac{1}{2} \frac{I_{\rho_{\mathbf{u}}}}{4\pi^2}, \quad (3.305)$$

which is solved explicitly by

$$\hat{a}_s = \frac{s}{1 + \frac{1}{2}s^{3/2}\frac{\sqrt{2}}{3}\frac{1}{4\pi^2}}. \quad (3.306)$$

For a plot of this relation see Fig. 3.12a.

Equation (3.305) can be solved for s as a function of the reduced s -wave scattering length $\hat{a}_s \equiv 8\pi a_s/a$ by

$$s = \hat{a}_s + \frac{1}{12\sqrt{2}}\hat{a}_s^{5/2} + \frac{1}{192\pi^4}\hat{a}_s^4 + \frac{7}{9216\sqrt{2}\pi^6}\hat{a}_s^{11/2} + \mathcal{O}(\hat{a}_s^7). \quad (3.307)$$

Inserting this into (3.294) yields

$$\frac{\rho_{\mathbf{u}}}{\rho} = \frac{1}{6\sqrt{2}\pi^2}\hat{a}_s^{3/2} + \frac{1}{96\pi^4}\hat{a}_s^3 + \frac{7}{4608\sqrt{2}\pi^6}\hat{a}_s^{9/2} + \mathcal{O}(\hat{a}_s^6). \quad (3.308)$$

The first term agrees with Bogoliubov's weak-coupling calculation (3.54) of the depletion of the condensate due to interactions. The general behavior up to strong couplings is shown in Fig. 3.12b.

We now calculate the total energy (3.298) at $T = 0$. We go to natural units and introduce the reduced quantities $\hat{\rho}_{\mathbf{u}} \equiv \rho_{\mathbf{u}}/\rho = s^{3/2}\bar{I}_{\rho_{\mathbf{u}}}$ and $\hat{\delta} \equiv \delta_R/\rho = s^{3/2}\bar{I}_{\delta}$, to obtain the reduced variational energy $w_1 \equiv W_1/N\varepsilon_a$ in the form:

$$\begin{aligned} w_1 = & -\hat{a}_s(1+\hat{\rho}_{\mathbf{u}}+\hat{\delta})(1-\hat{\rho}_{\mathbf{u}}) + \frac{\hat{a}_s}{2}(1-\hat{\rho}_{\mathbf{u}})^2 + s^{5/2}\bar{I}_E \\ & + \frac{\hat{a}_s}{2}(2\hat{\rho}_{\mathbf{u}}^2 + \hat{\delta}^2) - \hat{a}_s(\sigma_{\Sigma}\hat{\rho}_{\mathbf{u}} + \sigma_{\Delta}\hat{\delta}), \end{aligned} \quad (3.309)$$

with $\sigma_{\Sigma} \equiv s/\hat{a}_s - 1 + 3\hat{\rho}_{\mathbf{u}} + \delta$ and $\sigma_{\Delta} \equiv s/\hat{a}_s - 1 + \hat{\rho}_{\mathbf{u}}$. Inserting $\hat{\rho}_{\mathbf{u}}$ and $\hat{\delta}$, and going from the grand-canonical to the true proper energies by adding μN to W_1 and forming $W^e = W_1 + \mu V\rho$, we obtain the reduced energy

$$w_1^e = \frac{\hat{a}_s}{2} + \frac{\sqrt{2}}{3\pi^2}\hat{a}_s s^{3/2} - \frac{\sqrt{2}}{5\pi^2}s^{5/2} + \frac{\hat{a}_s}{72\pi^4}s^3. \quad (3.310)$$

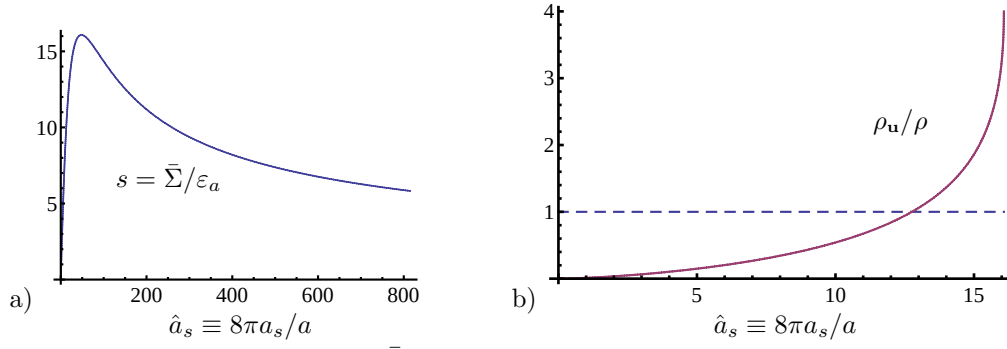


FIGURE 3.12 Reduced gap $s \equiv \bar{\Sigma}/\epsilon_a$ and uncondensed particle fraction as functions of the reduced s -wave scattering length $\hat{a}_s = 8\pi a_s/a = 8\pi a_s \rho^{1/3}$. At a_s where $\rho_u/\rho = 1$, the gas becomes normal.

Inserting here the expansion (3.307), we find that up to the term $\hat{a}_s^4$ the energy has the expansion

$$w_1^e = \frac{\hat{a}_s}{2} + \frac{2\sqrt{2}}{15\pi^2} \hat{a}_s^{5/2} + \frac{1}{72\pi^4} \hat{a}_s^4 + \dots \quad (3.311)$$

The first two terms agree with the corresponding terms in Bogoliubov's weak-coupling result (3.62):

$$w_{\text{Bog}} = \frac{\hat{a}_s}{2} + \frac{2\sqrt{2}}{15\pi^2} \hat{a}_s^{5/2} \quad (3.312)$$

The result is plotted in Fig. 3.13.

The accuracy can be increased to any desired level, with an exponentially fast convergence, as was demonstrated by the calculation of critical exponents in all euclidean φ^4 theories with N components in D dimensions [3]. The fact that the theory is renormalizable, so that all divergencies can be removed by Veltman's rule,

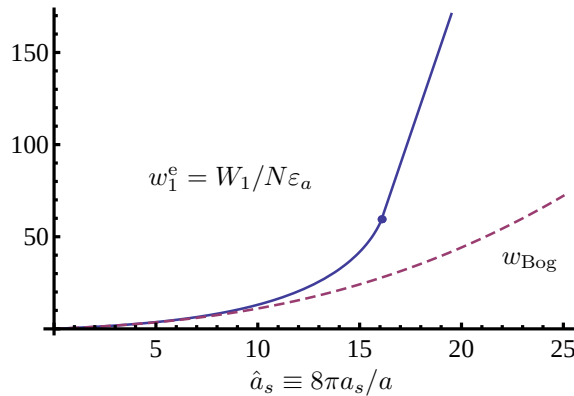


FIGURE 3.13 Reduced energy per particle $w_1^e = W_1/N\epsilon_a$ as a function of the reduced s -wave scattering length $\hat{a}_s = 8\pi a_s/a$ compared with Bogoliubov's weak-coupling result (3.312). There is a continuous phase transition at $(\hat{a}_s, s) \approx (16.08, 48.23)$, where the condensate becomes depleted and the ratio ρ_u/ρ reaches unity.

is an essential advantage of the present theory over any previous strong-coupling scheme.¹¹

Let us also study the temperature dependence of the depletion equation (3.294) and of Eq. (3.271). For this we proceed as in Eqs. (3.235), and introduce the temperature-dependent integral (3.237) to find, instead of (3.236), the result

$$\rho_{\mathbf{u}}(t) = k_{\bar{\Sigma}}^3 \frac{I_{\rho_{\mathbf{u}}}(t)}{4\pi^2}, \quad k_{\bar{\Sigma}} = \frac{\sqrt{2M\bar{\Sigma}}}{\hbar} = \frac{\sqrt{s}}{a}, \quad (3.313)$$

and t is now the reduced temperature

$$t \equiv k_B T / \bar{\Sigma} = k_B T / s \varepsilon_a. \quad (3.314)$$

It will be useful to rewrite $I_{\rho_{\mathbf{u}}}(t)$ in a form analogous to (3.237), (3.241) as

$$I_{\rho_{\mathbf{u}}}(t) = \frac{\sqrt{2}}{3} h_{\rho_{\mathbf{u}}}(t) = \frac{\sqrt{2}}{3} + t \int_0^\infty dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{e^x - 1}, \quad (3.315)$$

and

$$\hat{\rho}_{\mathbf{u}}^s(t) \equiv \frac{\rho_{\mathbf{u}}}{\rho} = \frac{s^{3/2}}{4\pi^2} I_{\rho_{\mathbf{u}}}(t). \quad (3.316)$$

In addition, we need a nonzero temperature version of the integral I_δ of (3.275) and (3.283):

$$I_\delta(t) \equiv - \int_0^\infty d\kappa \kappa^2 \left[\frac{1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \coth \left(\frac{\sqrt{(\kappa^2 + 1)^2 - 1}}{2t} \right) - \frac{1}{\kappa^2} \right], \quad (3.317)$$

to find

$$\hat{\delta}_R^s(t) \equiv \frac{\delta_R}{\rho} = \frac{s^{3/2}}{4\pi^2} I_\delta(t). \quad (3.318)$$

Here we write alternatively:

$$I_\delta(t) \equiv \sqrt{2} h_\delta(t) = - \int_0^\infty d\kappa \kappa^2 \left[\frac{1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \left(1 + \frac{2}{e^{\sqrt{(\kappa^2 + 1)^2 - 1}/t} - 1} \right) - \frac{1}{\kappa^2} \right], \quad (3.319)$$

or

$$I_\delta(t) \equiv \sqrt{2} + \Delta I_\delta(t) = \sqrt{2} - \int_0^\infty d\kappa \kappa^2 \frac{1}{\sqrt{(\kappa^2 + 1)^2 - 1}} \frac{2}{e^{\sqrt{(\kappa^2 + 1)^2 - 1}/t} - 1}. \quad (3.320)$$

¹¹Our results can be made more reliable by calculating the contribution of the still-missing second two-loop diagram, the second in Eq. (3.741) of the textbook [6]. Its contribution would be the 3 + 1-dimensional version of the last term in Eq. (3.767) that is essential in the $X \neq 0$ phase. Without this term, the slope of the quantum-mechanical energy as a function of the coupling constant is missed by 25%, as discussed in the heading of Fig. 5.24.

A convenient formula of the type (3.315) is

$$I_\delta(t) = \sqrt{2} - t \int_0^\infty dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{\sqrt{(xt)^2 + 1}(e^x - 1)}, \quad (3.321)$$

from which we obtain

$$\hat{\delta}(t) \equiv \frac{\delta_R(t)}{\rho} = \frac{s^{3/2}}{4\pi^2} I_\delta(t). \quad (3.322)$$

Finally we must calculate the nonzero temperature version of the energy (3.296), which replaces (3.297) by

$$w(\bar{\Sigma}, t) \equiv V \bar{\Sigma} k_\Sigma^3 \frac{I_E(t)}{4\pi^2}, \quad (3.323)$$

which amounts to the reduced energy

$$\hat{w}^s(s, t) \equiv \frac{w(\bar{\Sigma}, t)}{\varepsilon_a} = \frac{s^{5/2}}{4\pi^2} I_E(t), \quad (3.324)$$

where $I_E(t)$ is the integral

$$I_E(t) \equiv \int_0^\infty d\kappa \kappa^2 \left[\sqrt{(\kappa^2 + 1)^2 - 1} \coth \left(\frac{\sqrt{(\kappa^2 + 1)^2 - 1}}{2t} \right) - \kappa^2 - 1 + \frac{1}{2\kappa^2} \right], \quad (3.325)$$

with

$$I_E(t) \equiv \frac{8\sqrt{2}}{15} + \Delta I_E(t) = \frac{8\sqrt{2}}{15} + \int_0^\infty d\kappa \kappa^2 \sqrt{(\kappa^2 + 1)^2 - 1} \frac{2}{e^{\sqrt{(\kappa^2 + 1)^2 - 1}/t} - 1}. \quad (3.326)$$

A formula of the type (3.315) for $I_E(t)$ is:

$$I_E(t) = \frac{8\sqrt{2}}{15} + t \int_0^\infty dx (xt)^2 \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{\sqrt{(xt)^2 + 1}(e^x - 1)}. \quad (3.327)$$

Now we can derive the finite-temperature version of Eq. (3.303). For this we must calculate the $\bar{\Sigma}$ -derivatives of (3.313) and (3.318), and using (3.315) and (3.321), we find the expression

$$\rho'_{\mathbf{u}}(s, t) = \frac{\rho}{\varepsilon_a} \frac{s^{1/2}}{4\pi^2} \left[\frac{3}{2} I_{\rho_{\mathbf{u}}}(t) - t \dot{I}_{\rho_{\mathbf{u}}}(t) \right], \quad (3.328)$$

where

$$\dot{I}_{\rho_{\mathbf{u}}}(t) \equiv \frac{d}{dt} I_{\rho_{\mathbf{u}}}(t) = \int dx \frac{3(xt)^2 + 2 - 2\sqrt{(xt)^2 + 1}}{2\sqrt{(xt)^2 + 1}(\sqrt{(xt)^2 + 1} - 1)^{1/2}(e^x - 1)} \quad (3.329)$$

and

$$\delta'_R(s, t) = \frac{\rho}{\varepsilon_a} \frac{s^{1/2}}{4\pi^2} \left[\frac{3}{2} I_\delta(t) + t \dot{I}_\delta(t) \right], \quad (3.330)$$

with

$$\dot{I}_\delta(t) \equiv \frac{d}{dt} I_\delta(t) = \int dx \frac{[(xt)^2 + 2] \sqrt{(xt)^2 + 1} - 2}{2 \sqrt{(xt)^2 + 1}^3 (\sqrt{(xt)^2 + 1} - 1)^{1/2} (e^x - 1)}. \quad (3.331)$$

Similarly we find

$$\hat{w}'(s, t) = \frac{1}{\varepsilon_a} \frac{s^{3/2}}{4\pi^2} \left[\frac{5}{2} I_E(t) - t \dot{I}_E(t) \right], \quad (3.332)$$

with

$$\dot{I}_E(t) \equiv \frac{d}{dt} I_E(t) = \int dx \frac{3(xt)^2 (\sqrt{(xt)^2 + 1} - 1) + (xt)^4 \left(\frac{5}{2} \sqrt{(xt)^2 + 1} - 2 \right)}{[(xt)^2 + 1]^{3/2} (\sqrt{(xt)^2 + 1} - 1)^{1/2} (e^x - 1)}. \quad (3.333)$$

At finite temperature, the relations (3.284) and (3.299) are no longer true. The latter relation must be replaced by the frequency sum

$$\frac{1}{V} \partial_{\bar{\Sigma}} w(\bar{\Sigma}, t) = \partial_{\bar{\Sigma}} \bar{\Sigma} k_{\bar{\Sigma}}^3 \frac{I_E(t)}{4\pi^2} = k_{\bar{\Sigma}}^3 \frac{I_{\rho_{\mathbf{u}}}(t) + I_\delta(t)}{4\pi^2} - \alpha(s, t) = \rho_{\mathbf{u}}(s, t) + \delta(s, t) - \alpha(s, t), \quad (3.334)$$

where α is yet another frequency sum

$$\alpha(s, t) = \frac{1}{4V} \sum_{\mathbf{p}} \frac{\varepsilon_{\mathbf{p}}}{k_B T} \frac{1}{\sinh^2(E_{\mathbf{p}}/2k_B T)} = \rho \frac{s^{3/2}}{2t} \int d\kappa \frac{\kappa^4}{\sinh^2(\sqrt{(\kappa^2 + 1)^2 - 1}/2t)}. \quad (3.335)$$

Using these we calculate the finite-temperature relation between $\bar{\Sigma}$ and g

$$\frac{\bar{\Sigma}}{g} + \frac{\alpha}{g} \frac{1}{\rho'_{\mathbf{u}} + \delta'} = \rho - \rho_{\mathbf{u}} - \delta \frac{\rho'_{\mathbf{u}} - \delta'}{\rho'_{\mathbf{u}} + \delta'}. \quad (3.336)$$

instead of (3.303). The corresponding dimensionless relation between s and $\hat{a}_s$ is

$$\hat{a}_s = \left[s + \frac{\hat{\alpha}}{\hat{\rho}'_{\mathbf{u}} + \hat{\delta}'} \right] \bigg/ \left[1 - \hat{\rho}_{\mathbf{u}} - \hat{\delta} \frac{\hat{\rho}'_{\mathbf{u}} - \hat{\delta}'}{\hat{\rho}'_{\mathbf{u}} + \hat{\delta}'} \right], \quad (3.337)$$

where

$$\hat{\alpha} \equiv \frac{\alpha}{\rho} = s^{3/2} \frac{I_\alpha(t)}{4\pi^2}, \quad (3.338)$$

with

$$I_\alpha(t) = \frac{1}{2t} \int d\kappa \frac{\kappa^4}{\sinh^2(\sqrt{(\kappa^2 + 1)^2 - 1}/2t)} = \frac{1}{4} \int dx \frac{xt}{\sqrt{(xt)^2 + 1}} \frac{(\sqrt{(xt)^2 + 1} - 1)^{3/2}}{\sinh^2(x/2)}. \quad (3.339)$$

The primes in (3.337) now denote the derivatives with respect to s .

Let us evaluate this for small s where $t = k_B T / s \varepsilon_a$ is large so that (3.339) becomes¹²

$$I_\alpha(t) \approx \frac{t^{3/2}}{4} \int dx \frac{x^{3/2}}{\sinh^2(x/2)} = t^{3/2} \frac{3}{4} \sqrt{\pi} \zeta(3/2) = \frac{6\pi^2}{s^{3/2}} \left(\frac{T_a}{T_c} \right)^{3/2}. \quad (3.340)$$

Here we have used the ideal-gas critical temperature $T_c \equiv [\zeta(3/2)]^{-2/3} 4\pi T_a$ [recall (3.247)] to equate $t = s^{-1} (T/T_c) [\zeta(3/2)]^{-2/3} 4\pi$. Hence we find that $\hat{\alpha}$, for $s \rightarrow 0$, is equal to

$$\hat{\alpha} = s^{3/2} \frac{I_\alpha(t)}{4\pi^2} = \left(\frac{k_B T}{\varepsilon_a} \right)^{3/2} \frac{3}{2} \left(\frac{T_a}{T_c} \right)^{3/2} = \frac{3}{2} \left(\frac{T}{T_c} \right)^{3/2}. \quad (3.341)$$

The phase transition lies at the temperature where $\rho_{\mathbf{u}} = \rho$. For weak couplings, this can be calculated analytically. The calculation is somewhat subtle since the small- s region of the integral cannot simply be obtained by expanding the integrand in powers of s . Instead, the first correction starts with the power $\sqrt{s}$. To see this, we must proceed as in the derivation of the Robinson expansion of the Bose-Einstein integral function [20]. Recalling (3.249), we study the integral

$$\frac{\Delta \rho_{\mathbf{u}}}{\rho} = \frac{1}{4\pi^2} \int_0^\infty d\kappa \kappa^2 \frac{\kappa^2 + s}{\sqrt{(\kappa^2 + s)^2 - s^2}} \frac{2}{e^{\sqrt{(\kappa^2 + s)^2 - s^2}/\hat{T}} - 1} \quad (3.342)$$

for small s . The integral can be done immediately for $s = 0$ where we find, as in (3.246),

$$\frac{\Delta \rho_{\mathbf{u}}}{\rho} \underset{s \rightarrow 0}{=} \frac{\Delta \rho_{\mathbf{u}}^0}{\rho} = \left(\frac{T}{T_c} \right)^{3/2}. \quad (3.343)$$

For small s , we are left with the subtracted expression

$$\frac{\Delta \rho_{\mathbf{u}}'}{\rho} = \frac{1}{4\pi^2} \int_0^\infty d\kappa \kappa^2 \left[\frac{\kappa^2 + s}{\sqrt{(\kappa^2 + s)^2 - s^2}} \frac{2}{e^{\sqrt{(\kappa^2 + s)^2 - s^2}/\hat{T}} - 1} - \frac{2}{e^{\kappa^2/\hat{T}} - 1} \right]. \quad (3.344)$$

The first term can be expanded in powers of s , but the integral takes its leading behavior from linear momentum behavior of the sound à la Nambu-Goldstone, leaving

$$\frac{\Delta \rho_{\mathbf{u}}'}{\rho} \approx \frac{\hat{T}}{2\pi^2} \int_0^\infty d\kappa \kappa^2 \left(\frac{\kappa^2 + s}{\kappa^4 + 2s\kappa^2} - \frac{1}{\kappa^2} \right) = -\frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}}, \quad (3.345)$$

so that

$$\frac{\rho_{\mathbf{u}}}{\rho} = \frac{s^{3/2}}{4\pi^2} \frac{\sqrt{2}}{3} + \left(\frac{T}{T_c} \right)^{3/2} - \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}} + \dots \quad (3.346)$$

¹²I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980, Formula 3.527.

Thus we obtain, for small s , the leading terms

$$\frac{\rho_{\mathbf{u}}}{\rho} = \frac{s^{3/2}}{4\pi^2} \frac{\sqrt{2}}{3} + \left(\frac{T}{T_c}\right)^{3/2} - \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}} + \dots \quad (3.347)$$

The second frequency sum has the small- s -behavior

$$\frac{\delta}{\rho} = s^{3/2} \frac{I_\delta(t)}{4\pi^2} = \frac{s^{3/2}}{4\pi^2} \sqrt{2} + \frac{\sqrt{2}}{4\pi^2} s^{3/2} \Delta h_\delta(t), \quad (3.348)$$

where the correction term is [compare (3.242)]

$$\frac{\sqrt{2}}{4\pi^2} s^{3/2} \Delta h_\delta(t) \equiv -\frac{s}{4\pi^2} \int_0^\infty d\kappa \kappa^2 \frac{1}{\sqrt{(\kappa^2 + s)^2 - s^2}} \frac{2}{e^{\sqrt{(\kappa^2 + s)^2 - s^2}/\hat{T}} - 1}, \quad (3.349)$$

so that

$$\frac{\delta}{\rho} = \frac{s^{3/2}}{4\pi^2} \sqrt{2} - \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}} + \dots \quad (3.350)$$

We can now evaluate Eq. (3.336) at small s near the phase transition. Since $\hat{\alpha}$ is constant for $s = 0$, the last term in Eq. (3.336) is of the order of $s^{3/2}/\hat{\alpha}_s$ and can be neglected in comparison with the left-hand side, so that we obtain

$$\frac{s}{\hat{\alpha}_s} \approx 1 - \left(\frac{T}{T_c}\right)^{3/2} + \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}} + O(s^{3/2}) + \dots \quad (3.351)$$

The integral is once more treated with care (3.249), approximating it by

$$\int_0^\infty d\kappa \frac{2\hat{T}}{\kappa^2 + 2s} = \frac{\hat{T}}{4\pi\sqrt{2s}}, \quad (3.352)$$

and we find

$$s^{3/2} \frac{I_\delta(t)}{4\pi^2} = s^{3/2} \frac{\sqrt{2}}{4\pi^2} - \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}}. \quad (3.353)$$

The last terms in (3.347) and (3.353) are dominant for small s . They have a dramatic effect upon the phase diagram, with the consequence observed in earlier publications that, for small coupling, the critical temperature *increases* above the free Bose gas value [21]. Let us see how this happens. We insert (3.347) and (3.353) into (3.337) and find for small s :

$$\frac{s}{\hat{\alpha}_s} = 1 - \left(\frac{T}{T_c}\right)^{3/2} + \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}} + \mathcal{O}(s^{3/2}) + \dots, \quad (3.354)$$

the last term in (3.337) being exponentially small for small s .

Hence we obtain for small s , and on the phase transition line, the relation between s and $\hat{a}_s$:

$$\sqrt{\frac{s}{2}} = \hat{a}_s \frac{\hat{T}}{8\pi} + \mathcal{O}(\hat{a}_s^2). \quad (3.355)$$

Inserting this into (3.347), we obtain on the phase transition line where $\rho_{\mathbf{u}} = \rho$, the relation

$$1 \approx \left(\frac{T}{T_c}\right)^{3/2} - \frac{\hat{T}}{4\pi} \sqrt{\frac{s}{2}}, \quad (3.356)$$

or

$$\frac{T}{T_c} \approx 1 + \frac{2}{3} \frac{\hat{T}_c^2}{32\pi^2} \hat{a}_s + \dots \quad (3.357)$$

Inserting $\hat{T}_c = [\zeta(3/2)]^{-2/3} 4\pi$ from (3.247), this becomes

$$\frac{T}{T_c} = 1 + \frac{1}{3\zeta(3/2)^{4/3}} \hat{a}_s + \dots \quad (3.358)$$

This is the surprising initial increase of the critical temperature for small repulsion between the bosons observed in [21].

Numerically, the prefactor c of the initially linear relation

$$\frac{T}{T_c} = 1 + c \frac{a_s}{a} + \dots \quad (3.359)$$

is $c \approx 3\zeta(3/2)^{4/3} \approx 1.03$. This agrees reasonably well with the values $c_{\text{VPT}}^{\text{5loop}} = 0.93 \pm 0.13$ predicted from 5-loop variational perturbation theory in Ref. [22], and with its extension to seven-loops [23] which gave $c = 1.27 \pm 0.11$. It happens to be exactly equal to the value derived by Baym et al. from large- N calculations [24].

Let us now calculate the superfluid density of the condensate. Recalling the remarks made about superfluid ^4He on p. 185, this must be distinguished from the condensate density. The general formula in D dimensions is [25]

$$\begin{aligned} \rho_s &= \rho - \rho_n = \rho + \frac{2}{DV} \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} \partial_{\varepsilon_{\mathbf{p}}} \frac{1}{e^{\varepsilon_{\mathbf{p}}/k_B T} - 1} \\ &= \rho - \frac{2}{Dk_B TV} \sum_{\mathbf{p}} \frac{\varepsilon_{\mathbf{p}} e^{\varepsilon_{\mathbf{p}}/k_B T}}{(e^{\varepsilon_{\mathbf{p}}/k_B T} - 1)^2}. \end{aligned} \quad (3.360)$$

Using the surface of the unit sphere in D dimensions $S_D = 2\pi^{D/2}/\Gamma(D/2)$, this can be written as

$$\rho_n = \frac{2}{D} \frac{S_D}{(2\pi)^D} \int_0^\infty dk k^{D-1} \frac{ye^x}{(e^x - 1)^2}, \quad (3.361)$$

where $y \equiv \varepsilon_{\mathbf{p}}/k_B T$ and $x \equiv \mathcal{E}_{\mathbf{p}}/k_B T$. Setting $k = k_{\Sigma}\kappa$ this is equal to

$$\rho_n = \frac{2}{D} \frac{S_D}{(2\pi)^D} k_{\Sigma}^D \int_0^{\infty} d\kappa \kappa^{D-1} \frac{ye^x}{(e^x - 1)^2}. \quad (3.362)$$

Since $y \equiv \kappa^2/t$ and $x \equiv \sqrt{(\kappa^2 + 1)^2 - 1}/t$, we have $d\kappa \kappa^{D-1} = t^{D/2} dy y^{D/2-1}/2$ so that we obtain

$$\rho_n = \frac{1}{D} \frac{S_D}{(2\pi)^D} k_{\Sigma}^D t^{D/2} \int_0^{\infty} dy y^{D/2} \frac{e^x}{(e^x - 1)^2}, \quad (3.363)$$

where $dy = dx x/(ty + 1) = dx tx/\sqrt{(xt)^2 + 1}$, implying that

$$\rho_n = \frac{1}{D} \frac{S_D}{(2\pi)^D} k_{\Sigma}^D t \int_0^{\infty} dx x \frac{(\sqrt{(xt)^2 + 1} - 1)^{D/2}}{\sqrt{(xt)^2 + 1}} \frac{e^x}{(e^x - 1)^2}. \quad (3.364)$$

For large t , the integral can be approximated by

$$t^{D/2} \int_0^{\infty} dx \frac{x^{D/2} e^x}{(e^x - 1)^2} = t^{D/2} \frac{D}{2} \Gamma(D/2) \zeta(D/2), \quad (3.365)$$

so that ρ_n has the large- t behavior

$$\rho_n = \frac{\pi^{D/2} \zeta(D/2)}{(2\pi)^D} k_{\Sigma}^D t^{D/2}, \quad (3.366)$$

which yields in $D = 3$ dimensions

$$\rho_n = \frac{\zeta(3/2) k_{\Sigma}^3}{(4\pi^2)^{3/2}} \left(\frac{T}{\bar{\Sigma}} \right)^{3/2} = \left(\frac{T}{T_c^0} \right)^{3/2} \rho = \tau^{3/2} \rho. \quad (3.367)$$

At finite t , the right-hand side is multiplied by the function:

$$h(t) \equiv \frac{2t}{D \Gamma(D/2) \zeta(D/2) t^{D/2}} \times \int_0^{\infty} dx x \frac{(\sqrt{(xt)^2 + 1} - 1)^{D/2}}{\sqrt{(xt)^2 + 1}} \frac{e^x}{(e^x - 1)^2}. \quad (3.368)$$

The function $h(t)$ is plotted in Fig. 3.14.

The result may be compared with an analogous expression for the uncondensed particle density (3.271), which can be written in a form like in Eq. (3.361) as

$$\rho_u = \frac{k_{\Sigma}^3}{4\pi^2} \left(\frac{\sqrt{2}}{3} + t \int_0^{\infty} dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{e^x - 1} \right). \quad (3.369)$$

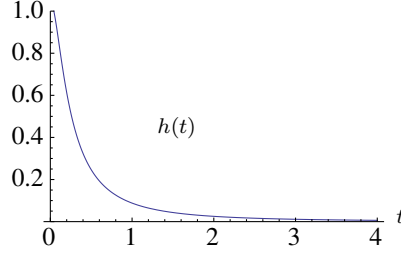


FIGURE 3.14 Temperature dependence of the normal particle density, where $t \equiv k_B T / \bar{\Sigma} = k_B T / s \varepsilon_a = \hat{T}_c^0 T / T_c^0 s = \hat{T}_c^0 \tau / s$ is the reduced temperature.

Similarly we can write (3.275) as

$$\delta_R = \frac{k_{\bar{\Sigma}}^3}{4\pi^2} \left(\sqrt{2} - t \int_0^\infty dx \frac{(\sqrt{(xt)^2 + 1} - 1)^{1/2}}{\sqrt{(xt)^2 + 1} (e^x - 1)} \right). \quad (3.370)$$

There is no problem to raise the accuracy to any desired level, with exponentially fast convergence, as was demonstrated by the calculation of critical exponents in all euclidean φ^4 theories with N components in D dimensions [21]. The procedural rules were explained in paper [27]. We merely have to calculate higher-order diagrams using the harmonic Hamiltonian (3.252) as the free theory that determines the Feynman diagrams, and

$$H_{\text{int}}^{\text{var}} = H_{\text{int}}'' - \bar{H}_{\text{trial}} \quad (3.371)$$

as the interaction Hamiltonian from which to calculate the vertices. At any given order, the results are optimized in the variational parameters Σ_0 , Σ , and $\bar{\Sigma}$. The theory is renormalizable, so that all divergencies can be absorbed in a redefinition of the parameters of the original action, order by order. This is the essential advantage of the present theory over any previous strong-coupling scheme published so far in the literature, in particular over those based on Hubbard-Stratonovich transformations of the interaction, which are applicable only in some large- N limit as explained in [27], and for which no higher-loop calculations are renormalizable.

3.7 Corrections Due to Omitted Interaction Hamiltonian

Let us now calculate the changes of this result caused by the omitted interaction Hamiltonian H_{int}'' in Eq. (3.16). It contributes to the energy a term¹³

$$\Delta_2 E = - \lim_{t_b - t_a \rightarrow \infty} \frac{i\hbar}{t_b - t_a} \frac{1}{2\hbar^2} \int_{t_a}^{t_b} dt dt' \langle \hat{T} H_{\text{int}}''(t) H_{\text{int}}''(t') \rangle, \quad (3.372)$$

where $H_{\text{int}}''(t)$ is the time-dependent operator

$$H_{\text{int}}''(t) \equiv e^{iH_0 t/\hbar} H_{\text{int}}''(t) e^{-iH_0 t/\hbar}, \quad (3.373)$$

¹³See Formula (1.305) in Chapter 1.

and $\hat{T}$ is the time-ordering operator (2.231).

In order to calculate this, we split the creation and annihilation operators into a Hermitian and an antihermitian part:

$$a_{\mathbf{p}} \equiv \frac{1}{\sqrt{2}}(\xi_{\mathbf{p}} + i\eta_{\mathbf{p}}), \quad a_{\mathbf{p}}^\dagger \equiv \frac{1}{\sqrt{2}}(\xi_{\mathbf{p}} - i\eta_{\mathbf{p}}). \quad (3.374)$$

Using Eq. (3.28), we can express $\xi_{\mathbf{p}}$ and $\eta_{\mathbf{p}}$ in terms of the quasiparticle operators $\alpha_{\mathbf{p}}$ and $\alpha_{\mathbf{p}}^\dagger$ as follows:

$$\xi_{\mathbf{p}} = \frac{u_{\mathbf{p}} + v_{\mathbf{p}}}{\sqrt{2}}(\alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^\dagger), \quad \eta_{\mathbf{p}} = \frac{u_{\mathbf{p}} - v_{\mathbf{p}}}{\sqrt{2}}(\alpha_{\mathbf{p}} - \alpha_{-\mathbf{p}}^\dagger). \quad (3.375)$$

Using the hyperbolic angles (3.38) for the Bogoliubov coefficients, this becomes

$$\xi_{\mathbf{p}} = \frac{e^{\theta_{\mathbf{p}}}}{\sqrt{2}}(\alpha_{\mathbf{p}} + \alpha_{-\mathbf{p}}^\dagger), \quad \eta_{\mathbf{p}} = \frac{e^{-\theta_{\mathbf{p}}}}{\sqrt{2}}(\alpha_{\mathbf{p}} - \alpha_{-\mathbf{p}}^\dagger). \quad (3.376)$$

Transforming these to arbitrary times via (3.373), we find

$$\xi_{\mathbf{p}}(t) = \frac{e^{\theta_{\mathbf{p}}}}{\sqrt{2}}(\alpha_{\mathbf{p}} e^{-i\mathcal{E}_{\mathbf{p}}t/\hbar} + \alpha_{-\mathbf{p}}^\dagger e^{i\mathcal{E}_{\mathbf{p}}t/\hbar}), \quad \eta_{\mathbf{p}}(t) = \frac{e^{-\theta_{\mathbf{p}}}}{\sqrt{2}i}(\alpha_{\mathbf{p}} e^{-i\mathcal{E}_{\mathbf{p}}t/\hbar} - \alpha_{-\mathbf{p}}^\dagger e^{i\mathcal{E}_{\mathbf{p}}t/\hbar}), \quad (3.377)$$

where $\mathcal{E}(\mathbf{q})$ are the quasiparticle energies (3.291). These operators have the time-ordered correlation functions

$$\begin{aligned} \langle \xi_{\mathbf{p}}(t) \xi_{-\mathbf{p}}(t') \rangle &= e^{2\theta_{\mathbf{p}}} \frac{e^{-i\mathcal{E}_{\mathbf{p}}|t-t'|/\hbar}}{2}, & \langle \eta_{\mathbf{p}}(t) \eta_{-\mathbf{p}}(t') \rangle &= e^{-2\theta_{\mathbf{p}}} \frac{e^{-i\mathcal{E}_{\mathbf{p}}|t-t'|/\hbar}}{2}, \\ \langle \xi_{\mathbf{p}}(t) \eta_{-\mathbf{p}}(t') \rangle &= i \frac{e^{-i\mathcal{E}_{\mathbf{p}}|t-t'|/\hbar}}{2}, & \langle \eta_{\mathbf{p}}(t) \xi_{-\mathbf{p}}(t') \rangle &= -i \frac{e^{-i\mathcal{E}_{\mathbf{p}}|t-t'|/\hbar}}{2}. \end{aligned} \quad (3.378)$$

We now express the hyperbolic angles, remembering Eqs. (3.36) and (3.268), as

$$\cos 2\theta_{\mathbf{p}} = u_{\mathbf{p}}^2 + v_{\mathbf{p}}^2 = \frac{\varepsilon_{\mathbf{p}} + \bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}}, \quad \sin 2\theta_{\mathbf{p}} = -2u_{\mathbf{p}}v_{\mathbf{p}} = -\frac{\bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}}, \quad (3.379)$$

so that

$$e^{2\theta_{\mathbf{p}}} = \frac{\varepsilon_{\mathbf{p}}}{\mathcal{E}_{\mathbf{p}}} = \sqrt{\frac{\varepsilon_{\mathbf{p}}}{\varepsilon_{\mathbf{p}} + 2\bar{\Sigma}}}, \quad e^{-2\theta_{\mathbf{p}}} = \frac{\varepsilon_{\mathbf{p}} + 2\bar{\Sigma}}{\mathcal{E}_{\mathbf{p}}} = \sqrt{\frac{\varepsilon_{\mathbf{p}} + 2\bar{\Sigma}}{\varepsilon_{\mathbf{p}}}}. \quad (3.380)$$

Now we transform the interaction H''_{int} of Eq. (3.16) into the time-dependent operator

$$H''_{\text{int}}(t) = \frac{gA_0}{V\sqrt{2}} \sum_{\mathbf{p}, \mathbf{p}'} \xi_{\mathbf{p}'}(t) [\xi_{-\mathbf{p}-\mathbf{p}'}(t) \xi_{\mathbf{p}}(t) + \eta_{-\mathbf{p}-\mathbf{p}'}(t) \eta_{\mathbf{p}}(t)], \quad (3.381)$$

and use Wick's theorem¹⁴ to expand the correlation function into two-point correlation functions:

$$\begin{aligned} \langle \hat{T} \xi(t) [\xi^2(t) + \eta^2(t)] \xi(t') [\xi^2(t') + \eta^2(t')] \rangle &= 6 \langle \hat{T} \xi(t) \xi(t') \rangle^3 + 12 \langle \hat{T} \xi(t) \xi(t') \rangle \langle \hat{T} \xi(t) \eta(t') \rangle^2 \\ &\quad + 2 \langle \hat{T} \xi(t) \xi(t') \rangle \langle \hat{T} \eta(t) \eta(t') \rangle^2 + 4 \langle \hat{T} \eta(t) \eta(t') \rangle \langle \hat{T} \xi(t) \eta(t') \rangle^2 \\ &= 6I_{1,1,1} - 12I_{1,0,0} + 2I_{1,-1,-1} + 4I_{-1,0,0}. \end{aligned} \quad (3.382)$$

The associated diagrams are pictured in Fig. 3.15.

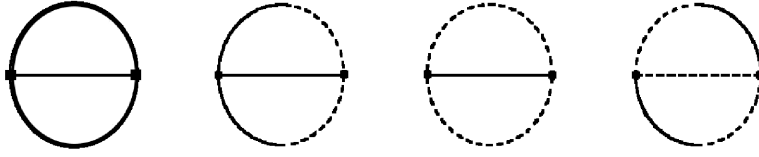


FIGURE 3.15 Diagrams picturing the Wick contractions in Eq. (3.382). A solid line represents a contraction $\langle \hat{T} \xi(t) \xi(t') \rangle$, a dashed line $\langle \hat{T} \eta(t) \eta(t') \rangle$, and a mixed line $\langle \hat{T} \xi(t) \eta(t') \rangle$ or $\langle \hat{T} \eta(t) \xi(t') \rangle$.

Inserting the above expansion into (3.372), and allowing for all intermediate three-quasiparticle states, we find the extra energy

$$\Delta_2 E = -\frac{g^2 A_0^2}{4} M (3I_{1,1,1} - 6I_{1,0,0} + I_{1,-1,-1} + 2I_{-1,0,0}) = -\frac{g^2 A_0^2}{4} M I, \quad (3.383)$$

where $I_{l,m,n}$ denotes the momentum integrals

$$I_{l,m,n} \equiv \int \frac{d^3 q_1 d^3 q_2}{(2\pi\hbar)^6} \left(\frac{\varepsilon_{\mathbf{p}_1}}{\mathcal{E}_{\mathbf{q}_1}} \right)^l \left(\frac{\varepsilon_{\mathbf{p}_2}}{\mathcal{E}_{\mathbf{q}_2}} \right)^m \left(\frac{\varepsilon_{\mathbf{p}_{12}}}{\mathcal{E}_{\mathbf{q}_{12}}} \right)^n \frac{1}{2M(\mathcal{E}_{\mathbf{q}_1} + \mathcal{E}_{\mathbf{q}_2} + \mathcal{E}_{\mathbf{q}_{12}})}, \quad (3.384)$$

and $\mathbf{q}_{12} \equiv \mathbf{q}_1 + \mathbf{q}_2$. They are simplified by a vector version of the substitution (3.50) to dimensionless wave vectors:

$$\mathbf{p} \equiv \hbar k_{\Sigma} \boldsymbol{\kappa}, \quad (3.385)$$

so that they become

$$I_{l,m,n} \equiv \hbar^{-2} k_{\Sigma}^4 \int \frac{d^3 \kappa_1 d^3 \kappa_2}{(2\pi)^6} \frac{\left(\frac{\kappa_1^2}{\kappa_1^2 + 2s} \right)^{l/2} \left(\frac{\kappa_2^2}{\kappa_2^2 + 2s} \right)^{m/2} \left(\frac{\kappa_{12}^2}{\kappa_{12}^2 + 2s} \right)^{n/2}}{A(\kappa_1) + A(\kappa_2) + A(\kappa_{12})}, \quad (3.386)$$

with the dimensionless quasiparticle energies

$$A(\kappa) \equiv 2M\mathcal{E}_{\mathbf{p}}/\hbar^2 k_{\Sigma}^2 = \sqrt{\kappa^2(\kappa^2 + 2s)}. \quad (3.387)$$

The integrals have a quadratic divergence that vanishes in dimensional regularization. There is, further, a logarithmic divergence which, in dimensional regularization, appears as a pole term proportional to $1/(D-3)$. This is omitted if we treat

¹⁴See to be derived in Section 7.17.1.

the cubic interaction term with the help of minimal subtraction. The remaining finite contribution was calculated in Ref. [31], yielding¹⁵

$$I = 3I_{1,1,1} - 6I_{1,0,0} + I_{1,-1,-1} + 2I_{-1,0,0} = -(4M\bar{\Sigma})^2\tilde{c}_3 = -16V\bar{\Sigma}^2M^3\tilde{c}_3. \quad (3.388)$$

The constant $\tilde{c}_3$ is calculated below in Eq. (3A.12). We insert this into (3.383) and replace A_0^2 by $V\Sigma_0/g$ according to Eq. (3.253). We further add $\Delta_2 E$ to the previous energy W_1 in Eq. (3.298), which changes it by $\Delta_2 W_1 = 4VgM^3\Sigma_0\bar{\Sigma}^2\tilde{c}_3$. Then we minimize $W_1 + \Delta_2 W_1$ with respect to $\bar{\Sigma}$, and obtain instead of (3.303) the following equation

$$\frac{\bar{\Sigma}}{g} \left[1 - 8g^2M^3\left(\frac{1}{2} + \tilde{c}_3\right) \frac{\rho_0}{\rho'_u + \delta'} \right] = \rho_0 - \delta \frac{\rho'_u - \delta'}{\rho'_u + \delta'}. \quad (3.389)$$

Inserting here the relation $\delta = 3\rho'_u$, we obtain

$$\frac{\bar{\Sigma}}{g} \left[1 - 8g^2M^3\left(\frac{1}{2} + \tilde{c}_3\right) \frac{\rho_0}{4\rho'_u} \right] = \rho_0 + \frac{3}{2}\rho_u = \rho + \frac{1}{2}\rho_u. \quad (3.390)$$

Going to reduced variables, the correspondingly modified relation (3.305) becomes

$$\frac{s}{\hat{a}_s} \left[1 - 8\hat{a}_s^2\left(\frac{1}{2} + \tilde{c}_3\right) \frac{1 - \hat{\rho}_u}{4\hat{\rho}'_u} \right] = \left(1 + \frac{1}{2}\hat{\rho}_u \right), \quad (3.391)$$

or

$$\frac{s}{\hat{a}_s} = 1 + \frac{1}{2}\hat{\rho}_u + 2\hat{a}_s\left(\frac{1}{2} + \tilde{c}_3\right) (1 - \hat{\rho}_u) \frac{s}{\hat{\rho}'_u}. \quad (3.392)$$

From this we find the equation

$$s = \hat{a}_s \left(1 + \frac{\sqrt{2}s^{3/2}}{24\pi^2} \right) + \hat{a}_s^2 \left(\frac{1}{2} + \tilde{c}_3 + \log s \right) \left(1 - \frac{\sqrt{2}s^{3/2}}{12\pi^2} \right) 6\pi^2\sqrt{2}s. \quad (3.393)$$

It is interesting to observe that the extra contribution vanishes on the transition line where $(\rho_u/\rho)_{\text{cr}} = 1$, i.e., at $s = s_{\text{cr}} = (12\pi^2/\sqrt{2})^{2/3} \approx 19.14$.

Appendix 3A Two-Loop Momentum Integrals

Here we calculate the integrals appearing in Eq. (3.383) following Ref. [31]. Let us first define the integrals in (3.386) as $I_{n,l,m} = \hbar^{-2}k_{\bar{\Sigma}}^4 J_{n,l,m}$ and study the integral $J_{n,l,m}$ which are all proportional to s^2 . Abbreviating $\int d^3\kappa/(2\pi)^3$ by $\int_{\kappa}$, we must evaluate

$$J_{l,m,n} = \int_{\kappa_1} \int_{\kappa_2} \frac{(\kappa_1/\sqrt{\kappa_1^2 + 2s})^l (\kappa_2/\sqrt{\kappa_2^2 + 2s})^m (r/\sqrt{r^2 + 2s})^n}{\kappa_1\sqrt{\kappa_1^2 + 2s} + \kappa_2\sqrt{\kappa_2^2 + 2s} + \kappa_{12}\sqrt{r^2 + 2s}}, \quad (3A.1)$$

where $\kappa_{12} = |\kappa_1 + \kappa_2| = \kappa_1^2 + \kappa_2^2 + 2\kappa_1 \cdot \kappa_2$. In $D = 3$, these integrals have quartic and quadratic ultraviolet divergences that cancel in the combination of integrals:

$$J = 6J_{0,0,1} - J_{-1,-1,1} - 3J_{1,1,1} - 2J_{-1,0,0} \quad (3A.2)$$

¹⁵See Ref. [31], Eq. (A.21).

needed in Eq. (3.388). The expression for J can be written as

$$J = \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{\kappa_1 \sqrt{\kappa_1^2 + s} + \kappa_2 \sqrt{\kappa_2^2 + s} + \kappa_{12} \sqrt{\kappa_{12}^2 + s}} \left[\frac{6\kappa_1}{\sqrt{\kappa_1^2 + s}} - \frac{2\sqrt{\kappa_1^2 + s}}{\kappa_1} \right. \\ \left. - \frac{3\kappa_1 \kappa_2 \kappa_{12}}{\sqrt{\kappa_1^2 + s} \sqrt{\kappa_2^2 + s} \sqrt{\kappa_{12}^2 + s}} - \frac{\kappa_1 \sqrt{\kappa_2^2 + s} \sqrt{\kappa_{12}^2 + s}}{\kappa_2 \kappa_{12} \sqrt{\kappa_2^2 + s}} \right]. \quad (3A.3)$$

This integral still has linear and logarithmic ultraviolet divergences. By subtracting and adding appropriate terms in the integrand of J , we can isolate the linear and logarithmic divergences into separate terms:

$$J = J_{\text{lin}} + J_{\text{log}} + J_{\text{num}}. \quad (3A.4)$$

The term containing the linear ultraviolet divergence is

$$J_{\text{lin}} = 2 \int_{\mathbf{\kappa}_1} \left[2 - \frac{\kappa_1}{\sqrt{\kappa_1^2 + 2s}} - \frac{\sqrt{\kappa_1^2 + 2s}}{\kappa_1} \right] \int_{\mathbf{\kappa}_2} \frac{1}{\kappa_2^2}. \quad (3A.5)$$

The term in (3A.4) containing the logarithmic ultraviolet divergence is

$$J_{\text{log}} = -s^2 \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \left\{ \frac{2}{(\kappa_1^2 + 4s)(\kappa_2^2 + 2s)(\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 2s)} \right. \\ \left. + \left[\frac{1}{\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 2s} - \frac{1}{2(\kappa_2^2 + 2s)} \right] \frac{1}{(\kappa_1^2 + 2s)^2} \right\}. \quad (3A.6)$$

The integral J_{num} obtained by subtracting (3A.5) and (3A.6) from (3A.3) is convergent in $D = 3$ dimensions and can be evaluated numerically. It is convenient to symmetrize the integrand over the six permutations of κ_1 , κ_2 , and κ_{12} , in order to avoid cancellations between different regions of momentum space. The resulting expression is

$$J_{\text{num}} = \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{6} \sum_{(\mathbf{\kappa}_1, \mathbf{\kappa}_2, \mathbf{\kappa}_{12})} \left\{ \frac{1}{\kappa_1 \sqrt{\kappa_1^2 + 2s} + \kappa_2 \sqrt{\kappa_2^2 + 2s} + \kappa_{12} \sqrt{\kappa_{12}^2 + 2s}} \times \right. \\ \times \left[\frac{6\kappa_1}{\sqrt{\kappa_1^2 + 2s}} - \frac{2\sqrt{\kappa_1^2 + 2s}}{\kappa_1} - \frac{3\kappa_1 \kappa_2 \kappa_{12}}{\sqrt{\kappa_1^2 + 2s} \sqrt{\kappa_2^2 + 2s} \sqrt{\kappa_{12}^2 + 2s}} - \frac{p \sqrt{\kappa_2^2 + 2s} \sqrt{r^2 + s}}{\kappa_2 \kappa_{12} \sqrt{\kappa_1^2 + 2s}} \right] \\ + \frac{2}{\kappa_2^2} \left[2 - \frac{\kappa_1}{\sqrt{\kappa_1^2 + 2s}} - \frac{\sqrt{\kappa_1^2 + 2s}}{\kappa_1} \right] + \frac{8s^2}{(\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 4s)(p^2 + s)(\kappa_2^2 + 2s)} \\ \left. + \left[\frac{1}{\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 4s} - \frac{1}{2(\kappa_2^2 + 2s)} \right] \frac{4s^2}{(\kappa_1^2 + 2s)^2} \right\}. \quad (3A.7)$$

Since s is the only scale in the integrand, dimensional analysis implies that the integral is proportional to s^2 . Evaluating the coefficient of s^2 numerically, Braaten and Nieto obtained

$$J_{\text{num}} = 2.10 \times 10^{-3} s^2. \quad (3A.8)$$

Because of the severe cancellations between the various terms in the integral, they were only able to calculate it to three significant figures.

The ultraviolet divergent integrals J_{lin} in (3A.5) and J_{log} in (3A.6) are evaluated using dimensional regularization. The integral over $\mathbf{\kappa}_2$ in (3A.5) vanishes since there is no scale in the integrand, and therefore $J_{\text{lin}} = 0$. The integral (3A.6) is evaluated in the limit $D \rightarrow 3$, and the result is

$$J_{\text{log}} = \frac{4\pi - 3\sqrt{3}}{192\pi^3} \left(\frac{1}{D-3} - 1.13459 \right) (2s)^{D-1}. \quad (3A.9)$$

Adding (3A.8) and (3A.9), we obtain the complete result for J using dimensional regularization:

$$J = \frac{4\pi - 3\sqrt{3}}{192\pi^3} \left(\frac{1}{D-3} \right) (2s)^{D-1} + c_3(2s)^{D-1} = J_1 + c_3(2s)^{D-1}, \quad (3A.10)$$

with $c_3 = 0.57(4\pi - 3\sqrt{3}/192\pi^3) \approx 0.001411$. The first term still has logarithmic divergence, and J may be rewritten as

$$J = \frac{4\pi - 3\sqrt{3}}{192\pi^3} \frac{(2s)^2}{D-3} e^{(D-3)\log(2s)^{D-3}} \approx \frac{4\pi - 3\sqrt{3}}{192\pi^3} (2s)^2 \left[\frac{1}{D-3} + \log(2s) + \dots \right]. \quad (3A.11)$$

The pole term is removed by a counter term in the total energy. The remainder modifies c_3 to

$$c_3(s) = c_3 + \log 2 + \log s \equiv \bar{c}_3 + \log s, \quad \bar{c}_3 \approx 0.695. \quad (3A.12)$$

Let us finally evaluate the logarithmically divergent term (3A.6). It can be written as

$$J_{\log} = -s^2 (2K_1 + K_2), \quad (3A.13)$$

where K_1 and K_2 are the following integrals:

$$K_1 = \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{(\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 4s)(\kappa_1^2 + 2s)(\kappa_2^2 + 2s)}, \quad (3A.14)$$

$$K_2 = \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \left[\frac{1}{\kappa_1^2 + \kappa_2^2 + \kappa_{12}^2 + 4s} - \frac{1}{2(\kappa_2^2 + 2s)} \right] \frac{1}{(\kappa_1^2 + 2s)^2}. \quad (3A.15)$$

We first consider the integral K_1 . Setting $\mathbf{\kappa}_{12} = \mathbf{\kappa}_1^2 + \mathbf{\kappa}_2^2 + 2\mathbf{\kappa}_1 \cdot \mathbf{\kappa}_2$ and introducing Feynman parameters, the integral becomes

$$K_1 = \int_0^1 dx \int_0^{1-x} dy \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{[(1-y)\kappa_1^2 + (1-x)\kappa_2^2 + z\mathbf{\kappa}_1 \cdot \mathbf{\kappa}_2 + s]^3}, \quad (3A.16)$$

where $z = 1 - x - y$. Dimensional regularization allows us to shift and rescale the momentum variables. We eliminate the scalar product in the denominator by performing the shift $\mathbf{\kappa}_1 \rightarrow \mathbf{\kappa}_1 - \mathbf{\kappa}_2 z/[2(1-y)]$. After rescaling $\mathbf{\kappa}_1$ by $(1-y)^{-1/2}$ and $\mathbf{\kappa}_2$ by $\{[(1-x)(1-y) - z^2/4]/(1-y)\}^{-1/2}$, and factorizing the integral into a Feynman parameter integral and an integral over the momenta, we obtain

$$K_1 = \int_0^1 dx \int_0^{1-x} dy [(1-x)(1-y) - z^2/4]^{-D/2} \int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{(\kappa_1^2 + \kappa_2^2 + 2s)^3}. \quad (3A.17)$$

The integral over the momenta can be done analytically:

$$\int_{\mathbf{\kappa}_1} \int_{\mathbf{\kappa}_2} \frac{1}{(\kappa_1^2 + \kappa_2^2 + 2s)^3} = \frac{\Gamma(3-D)}{2(4\pi)^D} (2s)^{D-3}, \quad (3A.18)$$

with a pole at $D = 3$ from the gamma function. To obtain K_1 for $D \approx 3$, we expand the Feynman parameter integral in powers of $D - 3$:

$$K_1 = \frac{\Gamma(3-D)}{2(4\pi)^D} (2s)^{D-3} \left\{ \int_0^1 dx \int_0^{1-x} dy \left[(1-x)(1-y) - \frac{z^2}{4} \right]^{-3/2} - \frac{D-3}{2} \int_0^1 dx \int_0^{1-x} dy \left[(1-x)(1-y) - \frac{z^2}{4} \right]^{-3/2} \ln \left[(1-x)(1-y) - \frac{z^2}{4} \right] \right\} + \dots, \quad (3A.19)$$

where $z = 1 - x - y$. The first integral in (3A.19) is equal to $4\pi/3$. The second integral has to be computed numerically. It has the value -9.43698 . Extracting the pole in $D - 3$ from the gamma function in (3A.19) and keeping all terms that survive in the limit $D \rightarrow 3$, we obtain

$$K_1 = -\frac{1}{96\pi^2}(2s)^{D-3} \left[\frac{1}{D-3} + 1.12646 + \gamma - \ln(4\pi) \right], \quad (3A.20)$$

where γ is Euler's constant. We next consider the integral K_2 in (3A.15). By introducing a Feynman parameter, it can be written as

$$K_2 = \int_0^1 dx (1-x) \int_{\kappa_1} \int_{\kappa_2} \left(\frac{1}{[\kappa_1^2 + x\kappa_2^2 + x\kappa_1 \cdot \kappa_2 + 2s]^3} - \frac{1}{[(1-x)\kappa_1^2 + x\kappa_2^2 + 2s]^3} \right). \quad (3A.21)$$

By shifting and rescaling the momentum variables, we can reduce the integral over the momenta to (3A.18). In the first term of (3A.21), we shift $\kappa_1 \rightarrow \kappa_1 - x\kappa_2/2$ and then rescale κ_2 by $(x(4-x)/4)^{-1/2}$. In the second term, we rescale κ_1 by $(1-x)^{-1/2}$ and κ_2 by $x^{-1/2}$. After integrating over κ_1 and κ_2 , we obtain

$$K_2 = \frac{\Gamma(3-D)}{2(4\pi)^D} (2s)^{D-3} \int_0^1 dx (1-x) x^{-D/2} \left[(1-x/4)^{-D/2} - (1-x)^{-D/2} \right]. \quad (3A.22)$$

To obtain K_2 in the limit $D \rightarrow 3$, we need to expand the integrand in (3A.22) in powers of $D - 3$:

$$K_2 = \frac{\Gamma(3-D)}{2(4\pi)^D} (2s)^{D-3} \left\{ \int_0^1 dx \left(\frac{8(1-x)}{\sqrt{x^3(4-x)^3}} - \frac{1}{\sqrt{x^3(1-x)}} \right) - \frac{D-3}{2} \int_0^1 dx \left(\frac{8(1-x)}{\sqrt{x^3(4-x)^3}} \ln \frac{x(4-x)}{4} - \frac{1}{\sqrt{x^3(1-x)}} \ln[x(1-x)] \right) \right\}. \quad (3A.23)$$

The integrals can be evaluated analytically. Extracting the pole in $D - 3$ from the gamma function and keeping all terms that survive in the limit $D \rightarrow 3$, we obtain

$$K_2 = \frac{\sqrt{3}}{64\pi^3} (2s)^{D-3} \left[\frac{1}{D-3} + \frac{4\pi}{3\sqrt{3}} - \frac{1}{2} \ln \frac{3}{4} - 1 + \gamma - \ln(4\pi) \right]. \quad (3A.24)$$

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4

Free Relativistic Particles and Fields

Having learned how the many-particle Schrödinger theory can be reformulated as a quantum field theory, we shall now try to find possible field theories for the description of relativistic many-particle systems. This will first be done classically. The fields will be quantized in Chapter 7.

4.1 Relativistic Particles

The nonrelativistic energy-momentum relation used in the Schrödinger theory

$$\varepsilon(\mathbf{p}) = \frac{\mathbf{p}^2}{2M} \quad (4.1)$$

is valid only for massive particles which move much slower than the velocity of light [2]

$$c = 2.99792458 \times 10^{10} \text{ cm/sec.} \quad (4.2)$$

If particles are accelerated to large velocities close to c this condition is no longer fulfilled. Instead of (14.275), the energy follows the relativistic law

$$\varepsilon(\mathbf{p}) = \sqrt{c^2 \mathbf{p}^2 + c^4 M^2}. \quad (4.3)$$

In particular, the light particles themselves, the photons, follow this law with the mass $M = 0$. It will be convenient to replace the energy by the new variable

$$p^0 \equiv \varepsilon(\mathbf{p})/c. \quad (4.4)$$

Then the relation (29.15) can be expressed as

$$p^{02} - \mathbf{p}^2 = M^2 c^2. \quad (4.5)$$

Thus, energy and momentum of a particle of mass are always such that the *four-vector*

$$p^\mu = (p^0, p^i) \quad (4.6)$$

is situated on the upper hyperboloid with $p^0 > 0$ in a four-dimensional energy-momentum space. This is called the *mass shell* of the particle of mass M . If the

particles are massless, the hyperboloid degenerates into a cone, the so-called *light cone*.

Since a free particle remains free when seen from any rotated, or uniformly moving, coordinate frame, energy and momentum transform in a way that keeps them always on the same mass shell. For a simple rotation of the frame this is obvious. The energy remains the same while the momentum $\mathbf{p}$ changes only its direction. For example, $\mathbf{p}$ may appear rotated around the z -axis by a transformation

$$p'^i = R_3(\varphi)^i_j p^j, \quad (4.7)$$

where $R_3(\varphi)$ is the matrix

$$R_3(\varphi) \equiv \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (4.8)$$

The angle φ is defined in such a way that, in the rotated frame, the momenta of the same particles appear rotated in the anticlockwise direction in the xy -plane, i.e., the coordinate axes are rotated clockwise with respect to the original frame. We speak of a *passive* rotation of the system. The effect is the same as if the observer had remained in the same frame but the experimental apparatus had been rotated in the anticlockwise sense, and with it all particle orbits. The transformations defined in this way are called *active* transformations. There are two equivalent ways of formulating all invariance principles, one based on the active and one on the passive way. In this text we shall use the passive way. The reader should be aware that different texts use different conventions and the formulas calculated in one cannot always be compared directly with those in the other, but may require changes which fortunately are rather straightforward.

For a general rotation by an angle φ with an axis pointing in the direction of the unit vector¹ $\hat{\varphi}$, the transformation has the matrix form

$$p'^i = R_{\hat{\varphi}}(\varphi)^i_j p^j. \quad (4.9)$$

We shall also write, with a slightly shorter notation for the rotation matrix,

$$p'^i = R^i_j(\varphi) p^j. \quad (4.10)$$

Explicitly, this transformation reads

$$\mathbf{p}' = \cos \varphi \mathbf{p}_{\perp} + \sin \varphi (\hat{\varphi} \times \mathbf{p}) + \mathbf{p}_{\parallel}. \quad (4.11)$$

Here $\mathbf{p}_{\parallel}$, $\mathbf{p}_{\perp}$ are the projections parallel and orthogonal to the rotation axis $\hat{\varphi}$:

$$\mathbf{p}_{\parallel} \equiv (\mathbf{p} \cdot \hat{\varphi}) \hat{\varphi}, \quad \mathbf{p}_{\perp} \equiv \mathbf{p} - \mathbf{p}_{\parallel}, \quad (4.12)$$

¹Hats on vectors in this section denote unit vectors, not Schrödinger operators.

respectively. The set of all rotations form a group called the *rotation group*.

Consider now another set of transformations in which the second frame moves with velocity v into the $-z$ -direction of the first. In the new frame, the z momentum of the particle will appear increased. The particle appears *boosted* in the z -direction with respect to the original observer. The momenta in x - and y -directions are unaffected. Since the total four-momentum still satisfies the mass shell condition (29.15), the combination $p^{02} - p^{32}$ has to remain invariant. This implies that there must be a hyperbolic transformation mixing p^0 and p^3 which may be parametrized by a hyperbolic angle ζ , called *rapidity*:

$$\begin{aligned} p'^0 &= \cosh \zeta p^0 + \sinh \zeta p^3, \\ p'^3 &= \sinh \zeta p^0 + \cosh \zeta p^3. \end{aligned} \quad (4.13)$$

This is called a pure Lorentz transformation. We may write this transformation in a 4×4 -matrix form as

$$p'^\mu = \begin{pmatrix} \cosh \zeta & 0 & 0 & \sinh \zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh \zeta & 0 & 0 & \cosh \zeta \end{pmatrix}^\mu_\nu p^\nu \equiv B_3(\zeta)^\mu_\nu p^\nu. \quad (4.14)$$

The subscript 3 of B_3 indicates that the particle is boosted into the z -direction. A similar matrix can be written down for x and y -directions. In an arbitrary direction $\hat{\zeta}$, the matrix elements are

$$B_{\hat{\zeta}}(\zeta) \equiv B(\zeta) = \left(\begin{array}{c|c} \cosh \zeta & \hat{\zeta}^i \sinh \zeta \\ \hline \hat{\zeta}^i \sinh \zeta & \delta^{ij} + \hat{\zeta}^i \hat{\zeta}^j (\cosh \zeta - 1) \end{array} \right). \quad (4.15)$$

The spatial velocity of a particle is given by

$$\mathbf{v} \equiv \partial \varepsilon(\mathbf{p}) / \partial \mathbf{p}. \quad (4.16)$$

In Schrödinger theory this is the velocity of a wave packet. In terms of $v \equiv |\mathbf{v}|$, one defines the *Einstein parameter*

$$\gamma \equiv \frac{1}{\sqrt{1 - v^2/c^2}} = \cosh \zeta. \quad (4.17)$$

With these quantities, we can rewrite (14.286) as

$$B(\zeta) = \left(\begin{array}{c|c} \gamma & \gamma v^i / c \\ \hline \gamma v^i / c & \delta^{ij} + (\gamma - 1) v^i v^j / v^2 \end{array} \right), \quad (4.18)$$

where $(\gamma - 1) v^i v^j / v^2$ is equal to $\gamma^2 v^i v^j / c^2 (\gamma - 1)$.

By combining rotations and boosts, one obtains a 6-parameter manifold of matrices

$$\Lambda(\zeta, \varphi) = B(\zeta)R(\varphi). \quad (4.19)$$

These are called *proper Lorentz transformations*. For all these, the combination

$$p'^{02} - \mathbf{p}'^2 = p^{02} - \mathbf{p}^2 = M^2 c^2 \quad (4.20)$$

is invariant. These matrices form a group, the *proper Lorentz group*. We can easily see that the Lorentz group allows reaching *every* momentum p^μ on the mass shell by applying an appropriate group element to some *fixed* reference momentum p_R^μ . For example, if the particle has a mass M we may choose for p_R^μ the so-called *rest momentum*

$$p_R^\mu = (Mc, 0, 0, 0), \quad (4.21)$$

and apply the boost in the $\hat{\mathbf{p}}$ -direction

$$\Lambda(\zeta) = B(\zeta), \quad (4.22)$$

with the rapidity given by

$$\cosh \zeta = \frac{p^0}{Mc}, \quad \sinh \zeta = \frac{|\mathbf{p}|}{Mc}. \quad (4.23)$$

With this, we can rewrite the general boost matrix (14.286) in the pure momentum form

$$B(\zeta) = \left(\begin{array}{c|c} p^0/M & |\mathbf{p}|p^i/M^2c^2 \\ \hline p^i|\mathbf{p}|/M^2c^2 & \delta^{ij} + \hat{p}^i\hat{p}^j (p^0/M - 1) \end{array} \right). \quad (4.24)$$

Instead of (14.294), we may use as a boost in the $\hat{\mathbf{p}}$ -direction the more general expressions

$$\Lambda(p) = B(\zeta)R(\varphi), \quad (4.25)$$

where $R(\varphi)$ is an arbitrary rotation. Also these leave the rest momentum p_R^μ invariant. In fact, the rotations form the largest subgroup of all proper Lorentz transformations which leaves the rest momentum p_R^μ invariant. It is referred to as the *little group* or *Wigner group* of a massive particle. It has an important physical significance since it serves to specify the intrinsic rotational degrees of freedom of the particle. If the particle is at rest it carries no orbital angular momentum. If it happens that its quantum mechanical state remains completely invariant under the little group R , the particle must also have zero intrinsic angular momentum or zero *spin*. Besides this trivial representation, the little group being a rotation group can have representations of any angular momentum $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$. In these cases, the state at rest has $2s + 1$ components which are linearly recombined with each other upon rotations.

The situation is quite different in the case of massless particles. They move with the speed of light and p^μ cannot be brought to rest by a Lorentz transformation from the light cone. There is, however, another standard reference momentum from which one can generate all other momenta on the light cone. It is given by

$$p_R^\mu = (1, 0, 0, 1)|\mathbf{p}|, \quad (4.26)$$

with an arbitrary size of the spatial momentum $|\mathbf{p}|$. It remains invariant under a different little group, which is again a three-parameter subgroup of the Lorentz group. The little groups will be discussed in detail in Section 4.15.3.

It is useful to write the invariant expression (4.20) as a square of a four-vector p^μ formed with the metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \quad (4.27)$$

namely

$$p^2 = g_{\mu\nu} p^\mu p^\nu. \quad (4.28)$$

In general, we define a scalar product between any two vectors as

$$pp' \equiv g_{\mu\nu} p^\mu p'^\nu = p^0 p'^0 - \mathbf{p} \mathbf{p}'. \quad (4.29)$$

Following Einstein's summation convention, repeated greek indices are summed from zero to 3 [recall (2.101)]. A space with this scalar product is called *Minkowski space*. It is useful to introduce the covariant components of any vector v^μ as

$$v_\mu \equiv g_{\mu\nu} v^\nu. \quad (4.30)$$

Then the scalar product can also be written as

$$pp' = p_\mu p'^\mu. \quad (4.31)$$

With this notation, the mass shell properties (4.20) for a particle before and after a Lorentz transformation simply reads

$$p'^2 = p^2 = M^2 c^2. \quad (4.32)$$

Note that, apart from the minus signs in the metric (4.296), the mass shell condition $p^2 = p^{02} - p^{12} - p^{22} - p^{32} = M^2 c^2$ which is invariant under Lorentz transformations, is completely analogous to the spherical condition $p^{42} + p^{12} + p^{22} + p^{32} = M^2 c^2$ which is invariant under rotations in a four-dimensional euclidean space. Both groups are parametrized by six parameters associated with linear transformations in the six planes: the six Lorentz transformations in the planes 12, 23, 31; 10, 20, 30, and the six rotation angles in the planes 12, 23, 31; 14, 24, 34. In the case of the four-dimensional euclidean space these are all rotations forming the group of *special*

orthogonal matrices called $SO(4)$. The first letter S indicates the property “*special*”. A group of matrices is called *special* if all matrices have a unit determinant. By analogy, the proper Lorentz group is denoted by $SO(1,3)$. The numbers in (1,3) indicate that, in the Minkowski metric (14.296), one diagonal element is equal to +1 and three are equal to -1.

The fact that all group elements are *special* follows from a direct calculation of the determinant of the matrices in (4.9) and (4.14).

How do we have to describe the quantum mechanics of a free relativistic particle in Minkowski space? Energy and momenta p^0 and p^i must be related to the time and space derivatives of particle waves in the usual way

$$\hat{p}^0 = i\hbar \frac{\partial}{\partial ct} \equiv i\hbar \frac{\partial}{\partial x^0}, \quad \hat{p}^i = -i\hbar \frac{\partial}{\partial x^i}. \quad (4.33)$$

In relativistic notation these read

$$\hat{p}_\mu = i\hbar \frac{\partial}{\partial x^\mu}. \quad (4.34)$$

Together with the coordinates, they satisfy the canonical commutation rules

$$\begin{aligned} [\hat{p}^\mu, \hat{p}^\nu] &= 0, \\ [x^\mu, x^\nu] &= 0, \\ [\hat{p}^\mu, x^\nu] &= i\hbar g^{\mu\nu}. \end{aligned} \quad (4.35)$$

We expect a spinless free particle with momenta p^i to be described by a field $\phi(x)$ of the plane-wave type that is, analogous to a nonrelativistic wave (2.212):

$$\phi_{\mathbf{p}}(x) = \mathcal{N} e^{-i(p^0 x^0 - p^i x^i)/\hbar} = \mathcal{N} e^{-ipx/\hbar}, \quad (4.36)$$

where $\mathcal{N}$ is some normalization factor. Since the zeroth component p^0 is fixed by the mass shell condition (14.279), only the spatial momentum needs to be specified, just as in the nonrelativistic plane wave solutions (2.212). However, in contrast to those, there are now two solutions for each momentum $\mathbf{p}$, one with energy $p^0 = \varepsilon(\mathbf{p}) = \sqrt{c^2 \mathbf{p}^2 + c^4 M^2}$, and one with $p^0 = -\varepsilon(\mathbf{p}) = -\sqrt{c^2 \mathbf{p}^2 + c^4 M^2}$. Thus we have two plane-wave solutions

$$\begin{aligned} \phi_{\mathbf{p}}^{(+)}(x) &= \mathcal{N} e^{-i(\varepsilon(\mathbf{p})x^0 - p^i x^i)/\hbar} = \mathcal{N} e^{-ipx/\hbar} \equiv \mathcal{N} f_{\mathbf{p}}(x), \\ \phi_{\mathbf{p}}^{(-)}(x) &= \mathcal{N} e^{i(\varepsilon(\mathbf{p})x^0 + p^i x^i)/\hbar} = \mathcal{N} f_{-\mathbf{p}}^*(x), \end{aligned} \quad (4.37)$$

of positive and negative energy, respectively. For later convenience, we have introduced the notation $f_{\mathbf{p}}(x)$ for the positive-energy solution $\phi_{\mathbf{p}}^{(+)}(x)$, so that $\phi_{\mathbf{p}}^{(-)}(x) = f_{-\mathbf{p}}^*(x)$.

The energies of $f_{\mathbf{p}}(x)$ and $f_{-\mathbf{p}}^*(x)$ are seen by applying $\hat{p}^0$ to these wave functions:

$$i\partial_0 f_{\mathbf{p}}(x) = \varepsilon(\mathbf{p}) f_{\mathbf{p}}(x), \quad i\partial_0 f_{-\mathbf{p}}^*(x) = -\varepsilon(\mathbf{p}) f_{-\mathbf{p}}^*(x). \quad (4.38)$$

The latter equation holds, of course, also for $f_{\mathbf{p}}^*(x)$. The solutions $f_{\mathbf{p}}(x)$ and $f_{\mathbf{p}}^*(x)$ will also be called positive- and negative-frequency wave functions, respectively. If not stated differently, the zeroth component p^0 will, from now on, always be identified with the *positive* energy $\varepsilon(\mathbf{p})$.

At this point we do not yet normalize the wave functions since we must first find a proper scalar product for calculating physical observables from these wave functions. This scalar product will be given in (4.177).

We have stated previously that permissible energy-momentum states of a free particle can be realized by considering *one and the same* particle in different co-ordinate frames connected by a transformation Λ . Suppose that we change the coordinates of the same spacetime point as follows:

$$x \rightarrow x' = \Lambda x. \quad (4.39)$$

Under this transformation the scalar product of any two vectors remains invariant:

$$x'y' = xy. \quad (4.40)$$

For rotations, this is obvious since $xy = x^0y^0 - \mathbf{x} \cdot \mathbf{y}$. For Lorentz transformations the invariance is a direct consequence of the fact that the boost matrix (14.285) satisfies the relation

$$g_{\mu\mu'} B_3(\zeta)^\mu{}_\nu B_3(\zeta)^{\mu'}{}_\lambda = g_{\mu\lambda}, \quad (4.41)$$

or in matrix notation

$$B_3^T(\zeta) g B_3(\zeta) = g. \quad (4.42)$$

The same relation holds obviously for the arbitrary boost matrix (14.286), and after a combination with all rotations for the general Lorentz transformation (14.290):

$$\Lambda^T g \Lambda = g, \quad (4.43)$$

or

$$g_{\mu\nu} \Lambda^\mu{}_\lambda \Lambda^\nu{}_\kappa = g_{\lambda\kappa}. \quad (4.44)$$

The invariance (14.305) of the scalar product is then verified in matrix notation as follows:

$$x'y' \equiv x'^T g y' = (\Lambda x)^T g (\Lambda y) = x^T \Lambda^T g \Lambda y = x^T g y = xy. \quad (4.45)$$

This holds also for scalar products between momentum and coordinate vectors

$$p'x' = px. \quad (4.46)$$

If the metric were euclidean, this would be the definition of orthogonal matrices. In fact, in the notation (4.45) of scalar products in which the metric is suppressed, we may write

$$(\Lambda p)(\Lambda x) = p \Lambda^{-1} \Lambda x = px, \quad (4.47)$$

so that there is no difference between the manipulation of orthogonal and Lorentz matrices.

When changing spacetime coordinates from x to $x' = \Lambda x$, the plane wave function of a particle behaves like

$$\phi_{\mathbf{p}}(x) = \mathcal{N} e^{-ip\Lambda^{-1}x'/\hbar} = \mathcal{N} e^{-i(\Lambda p)x'/\hbar} = \phi_{\mathbf{p}'}(x'). \quad (4.48)$$

This shows that in the new coordinates the same particle appears with a different momentum and energy:

$$p' = \Lambda p. \quad (4.49)$$

Consider now an observable field $\phi(x)$ describing a particle which does not possess any intrinsic orientational degree of freedom, i.e., no spin. The field can be an arbitrary superposition of different plane wave functions. After a coordinate transformation it will still have the same value at the same spacetime point. Thus $\phi'(x')$, as seen in the new frame, must be equal to $\phi(x)$ in the old frame:

$$\phi'(x') = \phi(x). \quad (4.50)$$

A field with this property is called a *scalar field* or, for historical reasons, a *Klein-Gordon field* [4].

4.2 Differential Operators for Lorentz Transformations

Equation (14.308) contains the same point of the physical system on both sides, labeled by different coordinates x and x' . For the derivation of consequences of symmetries (see Chapter 8), it is preferable to formulate the property (14.308) in the form of a transformation law at the same spacetime coordinates x (corresponding to different points of the physical system). Thus we shall express the transformation property (14.308) of a scalar field in the following form:

$$\phi(x) \xrightarrow{\Lambda} \phi'_{\Lambda}(x) = \phi(\Lambda^{-1}x). \quad (4.51)$$

For clarity, we have marked by a subscript Λ the transformation producing $\phi'(x)$. It is useful to realize that the inverse Lorentz transformation of the coordinates inside the field argument can also be achieved with the help of a differential operator. To find it we observe that the finite transformation matrices (4.9) and (4.18) can all be written in a convenient exponential form. We begin with the rotations. Consider the four-dimensional expression for the rotation (14.283) of the coordinate frame by an angle φ clockwise around the z -axis. It moves a point with the coordinates x to a point with the new coordinates $x'^{\mu} = R_3(\varphi)^{\mu}_{\nu} x^{\nu}$, where $R_3(\varphi)$ denotes the 4×4 -matrix

$$R_3(\varphi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \varphi & -\sin \varphi & 0 \\ 0 & \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (4.52)$$

This can be written in the exponential form

$$R_3(\varphi) = \exp \left\{ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \varphi \right\} \equiv e^{-iL_3\varphi}. \quad (4.53)$$

The matrix

$$L_3 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.54)$$

is called the *generator* of this rotation within the Lorentz group. There are similar generators for rotations around x - and y -directions:

$$L_1 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad (4.55)$$

$$L_2 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (4.56)$$

For all three cases we may write the generators as

$$L_i \equiv -i \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \epsilon_{ijk} \end{array} \right), \quad (4.57)$$

where ϵ_{ijk} is the completely antisymmetric *Levi-Civita tensor* with $\epsilon_{123} = 1$ (see [12]). The pure rotation matrix (4.9) is given by the exponential

$$\Lambda = e^{-i\varphi \mathbf{L}}, \quad (4.58)$$

as can also be verified by expanding the exponential in a power series.

Let us now find the generators of the pure Lorentz transformations: First in the z -direction where we see, from (14.285), that the boost matrix is

$$\begin{aligned} B_3(\zeta) &= \exp \left\{ \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \zeta \right\} \\ &= e^{-iM_3\zeta}, \end{aligned} \quad (4.59)$$

with the generator

$$M_3 = i \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (4.60)$$

Similarly we have in the other directions

$$M_1 = i \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (4.61)$$

$$M_2 = i \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (4.62)$$

The general Lorentz transformation matrix (14.286) is given by the exponential

$$\Lambda = e^{-i\boldsymbol{\zeta} \cdot \mathbf{M}}, \quad (4.63)$$

as can be verified by expanding the exponential in a power series.

The full Lorentz group is therefore generated by the six matrices L_i, M_i , to be collectively denoted by $G_a (a = 1, \dots, 6)$. Every element of the group can be written as

$$\Lambda = e^{-i(\boldsymbol{\varphi} \cdot \mathbf{L} + \boldsymbol{\zeta} \cdot \mathbf{M})} \equiv e^{-i\alpha_a G_a}. \quad (4.64)$$

If the exponential is expanded in a power series, one reobtains for $\boldsymbol{\zeta} = \mathbf{0}$ or $\boldsymbol{\varphi} = \mathbf{0}$ the general transformation matrices (4.9) or (14.286), respectively.

There exists a Lorentz-covariant way of specifying the generators of the Lorentz group. We introduce the 4×4 -matrices

$$(L^{\mu\nu})^{\lambda\kappa} = i(g^{\mu\lambda}g^{\nu\kappa} - g^{\mu\kappa}g^{\nu\lambda}), \quad (4.65)$$

labeled by the antisymmetric pair of indices $\mu\nu$, i.e.,

$$L^{\mu\nu} = -L^{\nu\mu}. \quad (4.66)$$

There are 6 independent matrices which coincide with the generators of rotations and boosts as follows:

$$L_i = \frac{1}{2}\epsilon_{ijk}L^{jk}, \quad (4.67)$$

$$M_i = L^{0i}. \quad (4.68)$$

With the generators (4.65), we can write every element (4.459) of the Lorentz group as follows:

$$\Lambda = e^{-i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}}, \quad (4.69)$$

where the antisymmetric angular matrix $\omega_{\mu\nu} = -\omega_{\nu\mu}$ collects both, rotation angles and rapidities:

$$\omega_{ij} = \epsilon_{ijk}\varphi^k, \quad (4.70)$$

$$\omega_{0i} = \zeta^i. \quad (4.71)$$

Summarizing the notation we have set

$$\Lambda = e^{-i(\varphi \cdot \mathbf{L} + \zeta \cdot \mathbf{M})} = e^{-i(\frac{1}{2}\varphi^i \epsilon_{ijk} L^{jk} + \zeta^i L^{0i})} = e^{-i(\frac{1}{2}\omega_{ij} L^{ij} + \omega_{0i} L^{0i})} = e^{-i\frac{1}{2}\omega_{\mu\nu} L^{\mu\nu}}. \quad (4.72)$$

Note that if the metric is euclidean, in which case it has the form

$$g_{\mu\nu} = \delta_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}_{\mu\nu}, \quad (4.73)$$

the situation is well familiar from basic matrix theorems in 4 dimensions. Then Λ would comprise all real orthogonal 4×4 -matrices which could be written as an exponential of all real antisymmetric 4×4 -matrices. In our case only the iL s are antisymmetric while the iM s are symmetric, a consequence of the minus signs in the Minkowski metric (14.296).

The reason for writing the group elements in this exponential form in terms of six generators is that thereby the multiplication rules of infinitely many group elements can be completely reduced to the knowledge of the commutation rules among the six generators $G_a = (L_i, M_i)$ of rotations and boosts. This is a consequence of the *Baker-Campbell-Hausdorff formula* written in the form (see Appendix 4A)

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A-B,[A,B]]+\dots}. \quad (4.74)$$

From this formula we find the multiplication rule

$$\begin{aligned} \Lambda_1 \Lambda_2 &= e^{-i\alpha_a^1 G_a} e^{-i\alpha_b^2 G_b} \\ &= \exp \left\{ -i\alpha_a^1 G_a - i\alpha_b^2 G_b + \frac{1}{2}[-i\alpha_a^1 G_a, -i\alpha_b^2 G_b] \right. \\ &\quad \left. + \frac{1}{12}[-i(\alpha_c^1 - \alpha_c^2)G_c, [-i\alpha_a^1 G_a, -i\alpha_b^2 G_b]] + \dots \right\}. \end{aligned} \quad (4.75)$$

The exponent involves only commutators among G_a 's. For the Lorentz group these can be calculated from the explicit 4×4 -matrices (4.54)–(4.56) and (4.60)–(4.62). The result is

$$[L_i, L_j] = i\epsilon_{ijk} L_k, \quad (4.76)$$

$$[L_i, M_j] = i\epsilon_{ijk} M_k, \quad (4.77)$$

$$[M_i, M_j] = -i\epsilon_{ijk} L_k. \quad (4.78)$$

This algebra of generators is called the *Lie algebra* of the group. The number of linearly independent matrices G_a (here 6) is called the *rank* r (here $r = 6$) of the Lie algebra. In the notation with the generators G_a , the algebra reads

$$[G_a, G_b] = if_{abc} G_c. \quad (4.79)$$

The commutator of two generators is a linear combination of generators. The coefficients f_{abc} are called *structure constants*. They are completely antisymmetric in a, b, c , and satisfy the relation

$$f_{abd}f_{dcf} + f_{bcd}f_{daf} + f_{cad}f_{dbf} = 0. \quad (4.80)$$

This guarantees that the generators obey the *Jacobi identity*

$$[[G_a, G_b], G_c] + [[G_b, G_c], G_a] + [[G_c, G_a], G_b] = 0, \quad (4.81)$$

which is the law of associativity for Lie Algebras. The relation (4.80) can easily be verified for the structure constants (4.76)–(4.78) using the identity for the ϵ -tensor

$$\epsilon_{ijl}\epsilon_{lkm} + \epsilon_{jkl}\epsilon_{lim} + \epsilon_{kil}\epsilon_{ljm} = 0. \quad (4.82)$$

The Jacobi identity implies that the r matrices with $r \times r$ elements

$$(F_c)_{ab} \equiv -if_{cab} \quad (4.83)$$

satisfy the commutation rules (4.79). They form the so-called *adjoint representation* of the Lie algebra. The matrix (4.57) for L_i is precisely of this type.

In terms of the matrices F_a of the adjoint representation, the commutation rules can also be written as

$$[G_a, G_b] = -(F_c)_{ab}G_c. \quad (4.84)$$

Continuing the expansion in terms of commutators in the exponent of (4.75), the commutators can be executed successively, and one remains at the end with an expression

$$\Lambda_{12} = e^{-i\alpha_a^{12}(\alpha^1, \alpha^2)G_a}, \quad (4.85)$$

with the parameters of the product α_a^{12} being completely determined by α_a^1 and α_a^2 for any given structure constants f_{abc} .

In the tensor notation $L^{\mu\nu}$ for L_i, M_i of Eqs. (4.67), (4.68), and with multiplication performed covariantly, so that products $L^{\mu\nu}L^{\lambda\kappa}$ have the matrix elements $(L^{\mu\nu})_{\sigma\tau}(L^{\lambda\kappa})^{\tau\delta}$, the commutators read

$$[L^{\mu\nu}, L^{\lambda\kappa}] = -i(g^{\mu\lambda}L^{\nu\kappa} - g^{\mu\kappa}L^{\nu\lambda} + g^{\nu\kappa}L^{\mu\lambda} - g^{\nu\lambda}L^{\mu\kappa}). \quad (4.86)$$

Due to the antisymmetry in $\mu \leftrightarrow \nu$ and $\lambda \leftrightarrow \kappa$ it is sufficient to specify only the simpler commutators

$$[L^{\mu\nu}, L^{\mu\lambda}] = -ig^{\mu\mu}L^{\nu\lambda}, \quad \text{no sum over } \mu, \quad (4.87)$$

thereby omitting vanishing components in (4.86) in which none of the indices $\mu\nu$ is equal to one of the indices $\lambda\kappa$.

After these preparations we are ready to derive a differential operator which achieves the transformation of the spacetime argument in (4.51). First we consider infinitesimal Lorentz matrices

$$\Lambda \equiv 1 - i \frac{1}{2} \omega_{\mu\nu} L^{\mu\nu}. \quad (4.88)$$

The transformation

$$x \xrightarrow{\Lambda} x' = \Lambda x \quad (4.89)$$

can be written as an infinitesimal symmetry transformation

$$\delta_s x = x' - x = -i \frac{1}{2} \omega_{\mu\nu} L^{\mu\nu} x. \quad (4.90)$$

Another way of expressing this coordinate transformation is

$$\delta_s x = x' - x = -i \frac{1}{2} \omega_{\mu\nu} \hat{L}^{\mu\nu} x, \quad (4.91)$$

where $\hat{L}^{\mu\nu}$ are the differential operators

$$\hat{L}^{\mu\nu} \equiv i(x^\mu \partial^\nu - x^\nu \partial^\mu). \quad (4.92)$$

Inserting the 4×4 matrix generators (4.65) into (4.90), or the corresponding differential operators (4.92) into (4.91), the infinitesimal coordinate transformations are explicitly

$$\delta_s x^\mu = \omega^\mu{}_\nu x^\nu. \quad (4.93)$$

The associated general field transformation law (4.51) takes the infinitesimal form

$$\phi(x) \xrightarrow{\Lambda} \phi(x) + \delta_s \phi(x), \quad \text{with} \quad \delta_s \phi(x) = -\omega^\mu{}_\nu x^\nu \partial_\mu \phi(x). \quad (4.94)$$

By analogy with Eq. (4.91), we can rewrite $\delta_s \phi(x)$ as

$$\delta_s \phi(x) = -i \frac{1}{2} \omega_{\mu\nu} \hat{L}^{\mu\nu} \phi(x), \quad (4.95)$$

where $\hat{L}^{\mu\nu}$ are the differential operators

$$\hat{L}^{\mu\nu} \equiv i(x^\mu \partial^\nu - x^\nu \partial^\mu). \quad (4.96)$$

In terms of the quantum mechanical momentum operators (4.34), these are equal to $1/\hbar$ times the operators of the four-dimensional angular momentum:

$$\hat{L}^{\mu\nu} \equiv \frac{1}{\hbar} (x^\mu \hat{p}^\nu - x^\nu \hat{p}^\mu). \quad (4.97)$$

They satisfy the same commutation relations (4.86) as the 4×4 -matrix generators $L^{\mu\nu}$ of the Lorentz group. They form a representation of the Lie algebra in terms of differential operators generating the Lorentz transformations.

In working out the commutation rules among the differential operators $\hat{L}^{\mu\nu}$, one conveniently uses the commutation rules between $\hat{L}^{\mu\nu}$ and x^λ as well as $\hat{p}^\lambda$:

$$[\hat{L}^{\mu\nu}, x^\lambda] = -i(g^{\mu\lambda} x^\nu - g^{\nu\lambda} x^\mu) = -(L^{\mu\nu})^\lambda{}_\kappa x^\kappa, \quad (4.98)$$

$$[\hat{L}^{\mu\nu}, \hat{p}^\lambda] = -i(g^{\mu\lambda} \hat{p}^\nu - g^{\nu\lambda} \hat{p}^\mu) = -(L^{\mu\nu})^\lambda{}_\kappa \hat{p}^\kappa. \quad (4.99)$$

These commutation rules identify x^λ and $\hat{p}^\lambda$ as vector operators [recall the definition in (2.113)]. In general, an operator $t^{\lambda_1, \dots, \lambda_n}$ is said to be a tensor operator of rank n if it is transformed by $L^{\mu\nu}$ like x^μ or $\hat{p}^\mu$ in each tensor index:

$$\begin{aligned} [\hat{L}^{\mu\nu}, \hat{t}^{\lambda_1, \dots, \lambda_n}] &= -i[(g^{\mu\lambda_1} \hat{t}^{\nu, \dots, \lambda_n} - g^{\nu\lambda_1} \hat{t}^{\mu, \dots, \lambda_n}) + \dots + (g^{\mu\lambda_n} \hat{t}^{\lambda_1, \dots, \nu} - g^{\nu\lambda_n} \hat{t}^{\lambda_1, \dots, \mu})] \\ &= -(L^{\mu\nu})^{\lambda_1}_{\kappa} \hat{t}^{\kappa\lambda_2, \dots, \lambda_n} - (L^{\mu\nu})^{\lambda_2}_{\kappa} \hat{t}^{\lambda_1\kappa, \dots, \lambda_n} - (L^{\mu\nu})^{\lambda_n}_{\kappa} \hat{t}^{\lambda_1\lambda_2, \dots, \kappa}. \end{aligned} \quad (4.100)$$

The simplest examples for such tensor operators are $\hat{t}^{\lambda_1, \dots, \lambda_n} = x^{\lambda_1} \dots x^{\lambda_n}$ or $\hat{t}^{\lambda_1, \dots, \lambda_n} = \hat{p}^{\lambda_1} \dots \hat{p}^{\lambda_n}$.

Note that the commutators (4.86) of the generators among each other imply that they, themselves, are tensor operators of rank 2.

It is worth observing that the differential operators $\hat{L}^{\mu\nu}$ can also be expressed in terms of the 4×4 matrix generators (4.65) as

$$\hat{L}^{\mu\nu} = \frac{i}{\hbar} (L^{\mu\nu})_{\lambda\kappa} x^\lambda \hat{p}^\kappa = \frac{i}{\hbar} x^T L^{\mu\nu} \hat{p} = -i \hat{p}^T L^{\mu\nu} x. \quad (4.101)$$

In this form, the operators $\hat{L}^{\mu\nu}$ follow the same algebraic construction rules as the operators $\hat{a}^\dagger M_i \hat{a}$ in Section 2.5. There we showed that sandwich constructions between creation and annihilation operators $\hat{a}^\dagger L^{\mu\nu} \hat{a}$ carry the commutation rules between the matrices $L^{\mu\nu}$ into a larger Hilbert space without changing their algebra. Since $-i\hat{p}_\mu$ and x^μ commute in the same way as $\hat{a}^\dagger$ and $\hat{a}$, the same argument applies to the sandwich construction (4.101), where the matrix generators $L^{\mu\nu}$ of Eq. (4.65) between $-i\hat{p}^\mu$ and x^ν produces an infinite-dimensional representation in terms of differential operators acting on the Hilbert space of square-integrable functions.

The commutation relations between the group generators (4.97) on the one side and vector and tensor operators on the other side can be used to calculate the effect of finite group transformations upon these operators. They can also be used to express the transformation property (14.308) in another way. A finite Lorentz transformation of a scalar field is obtained by exponentiating the generators just as in the 4×4 -representations (4.69) and (4.72). Thus we define the differential operator representation of finite group elements (4.69) as

$$\hat{D}(\Lambda) \equiv e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}. \quad (4.102)$$

Since the generators $\hat{L}^{\mu\nu}$ commute in the same way among each other as the 4×4 -matrix generators (4.65), the operators $\hat{D}(\Lambda)$ obey the same group multiplication rules as the 4×4 -matrices Λ . This follows directly from the expansion (4.75) of the product in terms of commutators.

Let us apply such a finite transformation to the vector x^μ and form

$$\hat{D}(\Lambda) x^\lambda \hat{D}^{-1}(\Lambda). \quad (4.103)$$

We do this separately for rotations and Lorentz transformations, first for rotations.

An arbitrary three-vector (x^1, x^2, x^3) is rotated around the 3-axis by the operator $\hat{D}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}$ with $\hat{L}_3 = -i(x^1\partial_2 - x^2\partial_1)$ by the operation

$$\hat{D}(R_3(\varphi)) x^i \hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3} x^i e^{i\varphi\hat{L}_3}. \quad (4.104)$$

The right-hand side is evaluated with the help of *Lie's expansion formula*:

$$e^{-i\hat{A}} \hat{B} e^{iA} = 1 - i[\hat{A}, \hat{B}] + \frac{i^2}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \dots \quad (4.105)$$

Since $\hat{L}_3$ commutes with x^3 , this component is unchanged by the operation (4.113):

$$\hat{D}(R_3(\varphi))x^3\hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}x^3e^{i\varphi\hat{L}_3} = x^3. \quad (4.106)$$

For x^1 and x^2 , the Lie expansion of (4.103) contains the commutators

$$-i[L_3, x^1] = x^2, \quad -i[L_3, x^2] = -x^1. \quad (4.107)$$

Thus, the first-order expansion term transforms the two-dimensional vector (x^1, x^2) into $(x^2, -x^1)$. The second-order terms are obtained by commuting the operator $-i\hat{L}_3$ with these components, yielding $-(x^1, x^2)$. To third-order, this is again transformed into $-(x^2, -x^1)$, and so on. Obviously, all even orders reproduce the initial two-dimensional vector (x^1, x^2) with an alternating sign, while all odd powers are proportional to $(x^2, -x^1)$:

$$\begin{aligned} e^{-i\varphi\hat{L}_3}(x^1, x^2)e^{i\varphi\hat{L}_3} &= \left(1 - \frac{1}{2!}\varphi^2 + \frac{1}{4!}\varphi^4 + \dots\right)(x^1, x^2) \\ &+ \left(\varphi - \frac{1}{3!}\varphi^3 + \frac{1}{5!}\varphi^5 + \dots\right)(x^2, -x^1). \end{aligned} \quad (4.108)$$

The even and odd powers can be summed up, and we obtain

$$e^{-i\varphi\hat{L}_3}(x^1, x^2)e^{i\varphi\hat{L}_3} = \cos \varphi (x^1, x^2) + \sin \varphi (x^2, -x^1). \quad (4.109)$$

Together with (4.106), the right-hand side corresponds precisely to the *inverse* of the rotation (4.52). Thus

$$\hat{D}(R_3(\varphi))x^i\hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}x^ie^{i\varphi\hat{L}_3} = \left(e^{i\varphi L_3}\right)^i_j x^j = R_3^{-1}(\varphi)^i_j x^j. \quad (4.110)$$

By performing successively rotations around the three axes we can generate, in this way, any rotation:

$$\hat{D}(R_\varphi(\varphi))x^i\hat{D}^{-1}(R_\varphi(\varphi)) = e^{-i\varphi\cdot\hat{\mathbf{L}}}x^ie^{i\varphi\cdot\hat{\mathbf{L}}} = \left(e^{i\varphi\cdot\mathbf{L}}\right)^i_j x^j = R_\varphi^{-1}(\varphi)^i_j x^j, \quad (4.111)$$

this being the finite rotation form of the commutation relation for the vector operator x^i :

$$[\hat{L}_i, x_k] = x_j(L_i)_{jk}. \quad (4.112)$$

This holds for any vector operator $\hat{v}^i$ instead of x^i [recall again the definition in (2.113)].

The time component x^0 is obviously unchanged by a rotation since $\hat{L}_3$ commutes with x^0 .

A similar calculation may be done for pure Lorentz transformations. Here we first consider a boost in the 3-direction $B_3(\zeta) = e^{-i\zeta\hat{M}_3}$ generated by $\hat{M}_3 = \hat{L}^{03} = -i(x^0\partial_3 + x^3\partial_0)$ [recall (4.68), (4.72), and (4.92)]. Note the positive relative sign of the two terms in the generator $\hat{L}^{03}$ that are caused by the fact that $\partial_i = -\partial^i$, in contrast to $\partial_0 = \partial^0$. Thus we form

$$\hat{D}(B_3(\zeta))x^i\hat{D}^{-1}(B_3(\zeta)) = e^{-i\zeta\hat{M}_3}x^ie^{i\zeta\hat{M}_3}. \quad (4.113)$$

The Lie expansion of the right-hand side involves the commutators

$$-i[M_3, x^0] = -x^3, \quad -i[M_3, x^3] = -x^0, \quad -i[M_3, x^1] = 0, \quad -i[M_3, x^2] = 0. \quad (4.114)$$

Thus the two-vector (x^1, x^2) is unchanged, while the two-vector (x^0, x^3) is transformed into $-(x^3, x^0)$. In the second expansion term, the latter becomes (x^0, x^3) , and so on, yielding

$$\begin{aligned} e^{-i\zeta\hat{M}_3}(x^0, x^3)e^{i\zeta\hat{M}_3} &= \left(1 + \frac{1}{2!}\zeta^2 + \frac{1}{4!}\zeta^4 + \dots\right)(x^0, x^3) \\ &\quad - \left(\zeta + \frac{1}{3!}\zeta^3 + \frac{1}{5!}\zeta^5 + \dots\right)(x^3, x^0), \end{aligned} \quad (4.115)$$

which can be summed up as

$$e^{-i\zeta\hat{M}_3}(x^0, x^3)e^{i\zeta\hat{M}_3} = \cosh \zeta (x^0, x^3) - \sinh \zeta (x^3, x^0). \quad (4.116)$$

Together with the invariance of (x^1, x^2) , this corresponds precisely to the inverse of the boost transformation (14.285). Hence we have

$$\hat{D}(B_3(\zeta))x^\lambda\hat{D}^{-1}(B_3(\zeta)) = e^{-i\zeta\hat{M}_3}x^\lambda e^{i\zeta\hat{M}_3} = (e^{i\zeta M_3})^\lambda{}_\kappa x^\kappa = B_3^{-1}(\zeta)^\lambda{}_\kappa x^\kappa. \quad (4.117)$$

By performing successively rotations and boosts in all directions, we find for the entire Lorentz group:

$$\hat{D}(\Lambda)x^\lambda\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}x^\lambda e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} = (e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^\lambda{}_{\lambda'}x^{\lambda'} = (\Lambda^{-1})^\lambda{}_{\lambda'}x^{\lambda'}, \quad (4.118)$$

where $\omega_{\mu\nu}$ are the parameters (4.70) and (4.71). In the last term on the right-hand side we have expressed the 4×4 -matrix Λ as an exponential of its generators as well, to emphasize the one-to-one correspondence between the generators $L^{\mu\nu}$ and their differential-operator representation $\hat{L}^{\mu\nu}$.

At first it may seem surprising that the group transformations appearing as a left-hand factor of the two sides of these equations are *inverse* to each other. However, we may easily convince ourselves that this is necessary to guarantee the correct group multiplication law. Indeed, if we perform two transformations after each other they appear in opposite order on the right- and left-hand sides:

$$\begin{aligned} \hat{D}(\Lambda_2\Lambda_1)x^\lambda\hat{D}^{-1}(\Lambda_2\Lambda_1) &= \hat{D}(\Lambda_2)\hat{D}(\Lambda_1)x^\lambda\hat{D}^{-1}(\Lambda_1)\hat{D}^{-1}(\Lambda_2) \\ &= (\Lambda_1^{-1})^\lambda{}_{\lambda'}\hat{D}(\Lambda_2)x^{\lambda'}\hat{D}^{-1}(\Lambda_2) = (\Lambda_1^{-1})^\lambda{}_{\lambda'}(\Lambda_2^{-1})^{\lambda'}{}_{\lambda''}x^{\lambda''} = [(\Lambda_2\Lambda_1)^{-1}]^\lambda{}_{\lambda'}x^{\lambda'}. \end{aligned} \quad (4.119)$$

If the right-hand side of (4.118) would contain Λ instead of Λ^{-1} , the order of the factors in $\Lambda_2\Lambda_1$ on the right-hand side of (4.119) would be opposite to the order in $\hat{D}(\Lambda_2\Lambda_1)$ on the left-hand side.

A straightforward extension of the operation (4.118) yields the transformation law for a tensor $\hat{t}^{\lambda_1, \dots, \lambda_n} = x^{\lambda_1} \dots x^{\lambda_n}$:

$$\begin{aligned} \hat{D}(\Lambda)\hat{t}^{\lambda_1, \dots, \lambda_n}\hat{D}^{-1}(\Lambda) &= e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\hat{t}^{\lambda_1, \dots, \lambda_n}e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} \\ &= (\Lambda^{-1})^{\lambda_1}_{\lambda'_1} \dots (\Lambda^{-1})^{\lambda_n}_{\lambda'_n} \hat{t}^{\lambda'_1, \dots, \lambda'_n} \\ &= (e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^{\lambda_1}_{\lambda'_1} \dots (e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^{\lambda_n}_{\lambda'_n} \hat{t}^{\lambda'_1, \dots, \lambda'_n}. \end{aligned} \quad (4.120)$$

This follows directly by inserting an auxiliary unit factor $1 = \hat{D}(\Lambda)\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}$ between each pair of neighboring coordinates x^{λ_i} in the product $\hat{t}^{\lambda_1, \dots, \lambda_n} = x^{\lambda_1} \dots x^{\lambda_n}$, and by performing the operation (4.120) on each of them. The last term in (4.120) can also be written as

$$\left[e^{i\frac{1}{2}\omega_{\mu\nu}(L^{\mu\nu} \times 1 \times 1 \dots \times 1 + \dots + 1 \times L^{\mu\nu} \times 1 \dots \times 1)} \right]^{\lambda_1 \dots \lambda_n}_{\lambda'_1 \dots \lambda'_n} \hat{t}^{\lambda'_1 \dots \lambda'_n}.$$

Since the commutation relations (4.100) determine the result completely, the transformation formula (4.120) is true for any tensor operator $\hat{t}^{\lambda_1, \dots, \lambda_n}$, and not only for those composed from a product of vectors x^{λ_i} .

For a field $\phi(x)$ which can be expanded into a power series, the transformation law (4.120) generalizes immediately to

$$\hat{D}(\Lambda)\phi(x)\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x)e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} = \phi(\Lambda^{-1}x) = \phi(e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}}x). \quad (4.121)$$

The finite transformation law (4.51) of a scalar field can therefore be expressed with the help of the differential operator $\hat{D}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}$ as

$$\phi(x) \xrightarrow{\Lambda} \phi'_\Lambda(x) = \phi(\Lambda^{-1}x) = \hat{D}(\Lambda)\phi(x)\hat{D}^{-1}(\Lambda) \equiv e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x)e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}. \quad (4.122)$$

The last factor on the right-hand side can, of course, be omitted if there are no x -dependent functions behind it.

If a particle has spin degrees of freedom, its field transforms differently from (4.122). Then the wave function has several components to account for the spin orientations. The transformation law must be such that the spin orientation in space remains the same at the same space point. This implies that the field components, which specify the size and orientation with respect to the different coordinate axes, will have to be transformed by certain matrices. How this is done for relativistic fields has first been understood for electromagnetic and gravitational fields which exhibit vector and tensor transformation properties, respectively. These will be recalled in Sections 4.6 and 4.9, before generalizing them in Sections 4.10 and 4.13 to spin 1/2, and in Section 4.18 to spins of arbitrary magnitude.

4.3 Space Inversion and Time Reversal

In addition to the continuous Lorentz transformations, there are also two important discrete transformations which leave scalar products $p_\mu x^\mu$ invariant. First there is the *space inversion*, also called *space reflection* or *parity transformation*,

$$P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \quad (4.123)$$

which reverses the direction of the spatial vectors, $\mathbf{x} \rightarrow -\mathbf{x}$. Note that a space inversion differs from a mirror reflection by a rotation. The space inversion maps the generators L_i, M_i of the Lorentz group into parity transformed generators

$$L_i \xrightarrow{P} L_i^P \equiv PL_iP^{-1} = L_i, \quad M_i \xrightarrow{P} M_i^P \equiv PM_iP^{-1} = -M_i. \quad (4.124)$$

This behavior is obvious in the tensor form of the generators $(L_i, M_i) = (\frac{1}{2}\epsilon_{ijk}L^{jk}, L^{0i})$. Each spacelike index gives rise to a factor -1 . The transformation preserves the commutation rules (4.77)–(4.78):

$$[L_i^P, L_j^P] = i\epsilon_{ijk}L_k^P, \quad (4.125)$$

$$[L_i^P, M_j^P] = i\epsilon_{ijk}M_k^P, \quad (4.126)$$

$$[M_i^P, M_j^P] = -i\epsilon_{ijk}L_k^P. \quad (4.127)$$

In general, a mapping of the generators into linear combinations of generators that have the same commutation rules is called an *automorphism* of the Lie algebra.

Second, there is the *time inversion* or *time reversal* transformation

$$T = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad (4.128)$$

which changes the sign of x^0 . When applied to the generators of the defining representation (L_i, M_i) , the time reversal transformation produces the same automorphism of the Lie algebra as the parity transformation (4.124). This, however, is a special feature of the reality of the Lorentz transformation matrices Λ which makes the 4×4 -matrices of the generators (4.54)–(4.56) and (4.60)–(4.62) purely imaginary.

Physically, a process is invariant under time reversal if we are unable to judge whether a movie of the process runs forward or backward. Running it backwards amounts to changing momentum and angular momentum L_i . Since momentum is generated by boost transformations, time reversal must change the direction of the generators M_i . For Hermitian matrices it is only necessary to change the eigenvalues,

such that we can also require that L_i goes into $-L_i^*$. In fact, there is a natural automorphism of the Lie algebra (4.77)–(4.78) in which we simply take the complex conjugate of the commutation rules, bringing them to

$$[-L_i^*, -L_j^*] = i\epsilon_{ijk}(-L_k^*), \quad (4.129)$$

$$[-L_i^*, -M_j^*] = i\epsilon_{ijk}(-M_k^*), \quad (4.130)$$

$$[-M_i^*, -M_j^*] = -i\epsilon_{ijk}(-L_k^*). \quad (4.131)$$

As we shall see in detail when discussing the time reversal properties of the various fields, this automorphism has precisely the desired observational consequences which we would like to associate with a time reversal transformation. Explicitly, time reversal transforms the generators as follows:

$$L_i \xrightarrow{T} L_i^T \equiv T L_i T^{-1} = -L_i^*, \quad M_i \xrightarrow{T} M_i^T \equiv T M_i T^{-1} = -M_i^*. \quad (4.132)$$

When the operations P and T are incorporated into the special Lorentz group $SO(1,3)$, one speaks of the *full Lorentz group*.

Note that the determinant of (14.315) and (14.310) is negative, so that the special Lorentz group $SO(1,3)$ no longer deserves the letter S in its name, and is called $O(1,3)$.

4.4 Free Relativistic Scalar Fields

The question now arises as to how the nonrelativistic free-field action

$$\mathcal{A} = \int dt d^3x \psi^*(\mathbf{x}, t) \left[i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right] \psi(\mathbf{x}, t), \quad (4.133)$$

introduced in (2.202), has to be modified in order to permit a quantum mechanical description of arbitrary relativistic n -particle states. According to the definition in (2.161), this is a local action. A field theory based on a local action is called *local field theory*. All field theories which explain successfully the properties of elementary particles have so far turned out to be local. The locality property seems to be extremely fundamental. Many fundamental forces have historically been discovered as *action-at-a-distance forces*. In the total field action, these correspond to nonlocal terms. Eventually, however, they have been shown to be the result of local actions that involve extra fields mediating the interaction. The initial idea for doing this came from Maxwell in the context of electromagnetism. Remember that the original Coulomb interaction was described by an action-at-a-distance which corresponds to a bilocal term in the action (see Section 2.8). Maxwell discovered that it can be reexpressed in terms of a local interaction by introducing an extra field called a *potential field*. In the relativistic generalization of the theory, this can further be viewed as a zeroth component of a four-dimensional *vector potential*. In the quantized version of the theory, the vector potential is associated with particles of light called *photons* (see Chapter 12). The same holds for gravitational forces

and their quanta, which represent particles called *gravitons*. In the description of nuclear forces, the same locality principle has led Yukawa to the discovery of the fundamental particle called π -meson (see Section 24.3, in particular Eqs. (24.31) and (24.32) for the two-body potential $V_2(\mathbf{x} - \mathbf{x}') \propto e^{-\mu|\mathbf{x} - \mathbf{x}'|}/|\mathbf{x} - \mathbf{x}'|$, and the associated wave equation obeyed by the π -field).

In order to accommodate the kinematic features discussed in the last section we shall require the action to be invariant under Lorentz transformations of coordinates (14.304) and fields [for example (14.308)]. Hence, space and time derivatives have to appear on equal footing, i.e., both must appear linearly or quadratically if we want to maintain the usual principle of classical mechanics in which all differential equations are of second order in time. Depending on the possible internal spin degrees of freedom there are different ways of making the action relativistic. These will now be discussed separately.

Consider first a field associated with a relativistic point particle which carries no spin degree of freedom, thus avoiding a nontrivial behavior under space rotations. Such a field was introduced in Eq. (14.308) as a *scalar field* and denoted by $\phi(x)$. As in the nonrelativistic case, the action of this field must contain the square of the spatial derivatives ∂_i^2 to guarantee rotational invariance. Since there must be Lorentz symmetry between space and time derivatives, we are led to a classical local action

$$\begin{aligned} \mathcal{A} = \int dx^0 L &= \int dx^0 d^3x \phi^*(\mathbf{x}, t) \left[-c_1 \hbar^2 (\partial_0^2 - \partial_{\mathbf{x}}^2) - c_2 \right] \phi(\mathbf{x}, t) \\ &= \int d^4x \phi^*(x) \left[-c_1 \hbar^2 \partial^\mu \partial_\mu - c_2 \right] \phi(x), \end{aligned} \quad (4.134)$$

where $c_1 \hbar^2, c_2$ are two arbitrary real constants.

It is easy to see that this action is indeed Lorentz invariant: Under the transformation (14.304), the four-volume element does not change:

$$dx^0 d^3x \equiv d^4x \rightarrow d^4x' = d^4x. \quad (4.135)$$

This follows directly from Eq. (4.43) which implies that the determinant of the matrices Λ has the values $\det \Lambda = \pm 1$. If we therefore take the action in the new frame

$$\mathcal{A} = \int d^4x' \phi^{*'}(x') \left[-c_1 \hbar^2 \partial'^\mu \partial'_\mu - c_2 \right] \phi'(x'), \quad (4.136)$$

we can use (14.308) and (14.319) to rewrite

$$\mathcal{A} = \int d^4x \phi^*(x) \left[-c_1 \hbar^2 \partial'^\mu \partial'_\mu - c_2 \right] \phi(x). \quad (4.137)$$

But since

$$\partial'_\mu = \Lambda_\mu{}^\nu \partial_\nu, \quad \partial'^\mu = \Lambda^\mu{}_\nu \partial^\nu \quad (4.138)$$

with

$$\Lambda_\mu{}^\nu \equiv g_{\mu\lambda} g^{\nu\kappa} \Lambda^\lambda{}_\kappa, \quad (4.139)$$

we see that

$$\partial'^2 = \partial^2, \quad (4.140)$$

and the transformed action coincides with the original action (14.319).

As in (2.161), we call the integrand of the action a *Lagrangian density*:

$$\mathcal{L}(x) = \phi^*(x) \left[-c_1 \hbar^2 \partial^\mu \partial_\mu - c_2 \right] \phi(x). \quad (4.141)$$

Then the invariance of the action under Lorentz transformations is a direct consequence of the Lagrangian density being a scalar field satisfying the transformation law (14.308):

$$\mathcal{L}'(x') = \mathcal{L}(x). \quad (4.142)$$

This follows directly from the invariance (4.140) and $\phi'(x') = \phi(x)$.

The free-field equation of motion is derived by varying the action (14.319) with respect to the fields $\phi(x)$, $\phi^*(x)$ independently. The independence of these variables is expressed by the functional differentiation rules

$$\frac{\delta \phi(x)}{\delta \phi(x')} = \delta^{(4)}(x - x'), \quad \frac{\delta \phi^*(x)}{\delta \phi^*(x')} = \delta^{(4)}(x - x') \quad (4.143)$$

$$\frac{\delta \phi(x)}{\delta \phi^*(x')} = 0, \quad \frac{\delta \phi^*(x)}{\delta \phi(x')} = 0. \quad (4.144)$$

Applying these rules to (14.319) we obtain directly

$$\begin{aligned} \frac{\delta \mathcal{A}}{\delta \phi^*(x)} &= \int d^4 x' \delta^{(4)}(x' - x) (-c_1 \hbar^2 \partial'^2 + c_2) \phi(x') \\ &= (-c_1 \hbar^2 \partial^2 + c_2) \phi(x) = 0. \end{aligned} \quad (4.145)$$

Similarly,

$$\begin{aligned} \frac{\delta \mathcal{A}}{\delta \phi(x)} &= \int d^4 x' \phi^*(x') (-c_1 \hbar^2 \partial'^2 + c_2) \delta^{(4)}(x' - x) \\ &= \phi^*(x) (-c_1 \hbar^2 \overset{\leftarrow}{\partial}^2 + c_2) = 0, \end{aligned} \quad (4.146)$$

where the arrow on top of the last derivative indicates that it acts on the field to the left. The second equation is just the complex conjugate of the previous one.

The field equations (4.145) and (4.146) can be derived directly from the Lagrangian density (4.141) by forming ordinary partial derivatives of $\mathcal{L}$ with respect to all fields and their derivatives. Indeed, a functional derivative of a local action can be expanded in terms of derivatives of the Lagrangian density according to the general rule

$$\frac{\delta \mathcal{A}}{\delta \phi(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial [\partial_\mu \phi(x)]} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial [\partial_\mu \partial_\nu \phi(x)]} + \dots, \quad (4.147)$$

and a similar expansion holds for the derivative with respect to $\phi^*(x)$. These expansions follow directly from the defining relations (4.143). Applying them to the Lagrangian density (4.141), the field equation for $\phi(x)$ is particularly simple:

$$\frac{\delta \mathcal{A}}{\delta \phi^*(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi^*(x)} = (-c_1 \hbar^2 \partial^2 + c_2) \phi(x) = 0. \quad (4.148)$$

For $\phi^*(x)$, on the other hand, all derivatives written out in (4.147) have to be evaluated to obtain

$$\frac{\delta \mathcal{A}}{\delta \phi(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial [\partial_\mu \phi(x)]} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial [\partial_\mu \partial_\nu \phi(x)]} = (-c_1 \hbar^2 \partial^2 + c_2) \phi^*(x) = 0. \quad (4.149)$$

The equation

$$\frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \partial_\mu \phi(x)} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial \partial_\mu \partial_\nu \phi(x)} + \dots = 0 \quad (4.150)$$

is the Euler-Lagrange equation of a general local field theory. This expression is invariant under partial integrations within the local action $\mathcal{A} = \int d^4x \mathcal{L}(x)$. Take for example a Lagrangian density which is equivalent to (4.141) by a partial integration in the action (4.137):

$$\mathcal{L} = c_1 \hbar^2 \partial \phi^*(x) \partial \phi(x) - c_2 \phi^*(x) \phi(x). \quad (4.151)$$

If this is inserted into (4.150), it produces once more the same field equations.

The field equations (4.148) and (4.149) are solved by the quantum mechanical plane waves (4.303) and (4.37) of positive and negative energies, respectively:

$$f_{\mathbf{p}}(x) = \mathcal{N} e^{-ipx/\hbar}, \quad f_{\mathbf{p}}^*(x) = \mathcal{N} e^{ipx/\hbar}. \quad (4.152)$$

These form a complete set of plane-wave solutions.

The field equations (4.148) and (4.149) require the four-momenta to satisfy the condition

$$c_1 p^\mu p_\mu - c_2 = 0. \quad (4.153)$$

This has precisely the form of the mass shell relation (29.25) if we choose

$$\frac{c_2}{c_1} = M^2 c^2. \quad (4.154)$$

A positive sign of c_1 is necessary for the field fluctuations to be stable. The size can be brought to unity by a multiplicative renormalization of the field. This makes the field normalization different from the nonrelativistic one in the action (4.317).

After this, the mass shell condition fixes the free-field action to the standard form

$$\mathcal{A} = \int d^4x \phi^*(x) [-\hbar^2 \partial^\mu \partial_\mu - M^2 c^2] \phi(x). \quad (4.155)$$

The nonrelativistic limit of the action (4.155) is obtained by removing, from the positive frequency part of the field $\phi(x)$, a fast trivial oscillating factor corresponding to the rest energy Mc^2 , replacing

$$\phi(x) \rightarrow e^{-iMc^2 t/\hbar} \frac{1}{\sqrt{2M}} \psi(\mathbf{x}, t). \quad (4.156)$$

For a plane wave $f_{\mathbf{p}}(x)$ of Eq. (4.152), the field $\psi(\mathbf{x}, t)$ becomes $\psi_{\mathbf{p}}(\mathbf{x}, t) = \sqrt{2M} \mathcal{N} e^{-i(p^0 c - Mc^2)t/\hbar} e^{i\mathbf{p}\mathbf{x}/\hbar}$. In the limit of large c , the first exponential becomes $e^{-i\mathbf{p}^2 t/2M}$, such that the field $\psi_{\mathbf{p}}(\mathbf{x}, t)$ coincides with the nonrelativistic plane wave (2.212) which extremizes the nonrelativistic action (14.317). The negative-frequency plane wave $f_{\mathbf{p}}^*(x)$ in (4.152), on the other hand, does not contribute in this limit since it is equal to $\sqrt{2M} \mathcal{N} e^{i(p^0 c + Mc^2)t/\hbar} e^{i\mathbf{p}\mathbf{x}/\hbar}$. This contains a temporal prefactor $e^{2iMc^2 t/\hbar}$ that oscillates with infinite frequency for $c \rightarrow \infty$, and is therefore equivalent to zero by the *Riemann-Lebesgue Lemma* [13].

The appearance of the constants $\hbar$ and c in all future formulas can be avoided if we work from now on with new fundamental units l_0, m_0, t_0 , and E_0 different from the ordinary CGS units. They are chosen to give $\hbar$ and c the value 1. Expressed in terms of the conventional length, time, mass, and energy, these new *natural units* are given by

$$l_0 = \frac{\hbar}{Mc}, \quad t_0 = \frac{\hbar}{Mc^2}, \quad (4.157)$$

$$m_0 = M, \quad E_0 = Mc^2. \quad (4.158)$$

If, for example, the particle is a proton with mass m_p , these units are

$$l_0 = 2.103138 \times 10^{-11} \text{cm} \quad (4.159)$$

= Compton wavelength of proton,

$$t_0 = l_0/c = 7.0153141 \times 10^{-22} \text{sec} \quad (4.160)$$

= time it takes light to cross the Compton wavelength,

$$m_0 = m_p = 1.6726141 \times 10^{-24} \text{g}, \quad (4.161)$$

$$E_0 = 938.2592 \text{MeV}. \quad (4.162)$$

For any other mass, they can easily be rescaled.

With these natural units we can drop c and $\hbar$ in all formulas and write the action simply as

$$\mathcal{A} = \int d^4x \phi^*(x) (-\partial^2 - M^2) \phi(x). \quad (4.163)$$

The Lagrange density of the complex scalar field may be taken either as

$$\mathcal{L}(x) = \phi^*(x) (-\partial^2 - M^2) \phi(x), \quad (4.164)$$

or

$$\mathcal{L}(x) = \partial_\mu \phi^*(x) \partial^\mu \phi(x) - M^2 \phi^*(x) \phi(x), \quad (4.165)$$

with an obvious modification for real fields $\phi(x)$. The surface term, by which the associated actions differ from each other after a partial integration, does not change the Euler-Lagrange equation (4.150).

Actually, since we are dealing with relativistic particles there is no fundamental reason to assume $\phi(x)$ to be a complex field. In the nonrelativistic theory this was necessary in order to construct a term linear in the time derivative:

$$\int dt \phi^* i \partial_t \phi. \quad (4.166)$$

For a real field $\phi(x)$ this would have been a pure surface term, that does not influence the dynamics of the system. For second-order time derivatives, as in (4.163), this is no longer necessary.

Thus we shall also study the real scalar field with an action

$$\mathcal{A} = \frac{1}{2} \int d^4x \phi(x) (-\partial^2 - M^2) \phi(x). \quad (4.167)$$

In this case it is customary to use a prefactor $1/2$ to normalize the field. Here the Lagrange density may be taken either as

$$\mathcal{L}(x) = \frac{1}{2} \phi^*(x) (-\partial^2 - M^2) \phi(x), \quad (4.168)$$

or as

$$\mathcal{L}(x) = \frac{1}{2} \{ [\partial \phi(x)]^2 - M^2 \phi^2(x) \}. \quad (4.169)$$

For either field we obtain the *Klein-Gordon equation*

$$(-\partial^2 - M^2) \phi(x) = 0. \quad (4.170)$$

For a complex field, there exists an important local conservation law, which generalizes Eq. (1.109) of the Schrödinger theory to relativistic fields. We define the four-vector of the probability current density:

$$j_\mu(x) = i \phi^* \overleftrightarrow{\partial}_\mu \phi, \quad (4.171)$$

which describes the probability flow of the Klein-Gordon particle. It is easy to verify that, due to (4.170), this satisfies the *current conservation law*

$$\partial_\mu j^\mu(x) = 0. \quad (4.172)$$

This conservation law will permit us, in Chapter 17, to couple electromagnetism to the field and identify $j^\mu(x)$ as the electromagnetic current (if we choose natural units in which the electric charge e is equal to unity).

The deeper reason for the existence of a conserved current will be understood in Subsection 8.11.1, where we shall see that it is intimately connected with an

invariance of the action (4.163) of a free complex scalar field under arbitrary changes of the phase of the field

$$\phi(x) \rightarrow e^{-i\alpha} \phi(x). \quad (4.173)$$

It is this invariance which gives rise to a conserved current density [see (8.270), also (17.68)].

The zeroth component of $j^\mu(x)$,

$$j^0(x) = c\rho(x) \quad (4.174)$$

describes the particle density $\rho(x)$. The spatial integral over $\rho(x)$:

$$Q(t) = \frac{1}{c} \int d^3x j^0(x). \quad (4.175)$$

is the total charge in natural units: Because of the local conservation law (4.172), the charge does not depend on time. This is seen by rewriting

$$\dot{Q}(t) = \int d^3x \partial_0 j^0(x) = \int d^3x \partial_\mu j^\mu(x) - \int d^3x \partial_i j^i(x) = - \int d^3x \partial_i j^i(x) \quad (4.176)$$

and applying, to the right-hand side, Gauss's theorem as in (1.110), assuming that currents vanish at spatial infinity.

By removing, from the positive-frequency solutions of the Klein-Gordon field $\phi(x)$, the fast oscillation as in (4.156), we can take the nonrelativistic limit and find that the nonrelativistic limit of the spatial part of the current density (4.171) satisfies the local conservation law (1.109) of the Schrödinger theory.

Since the current conservation law (4.172) is the direct relativistic generalization of the nonrelativistic probability conservation law (1.109), it is suggestive to define the matrix elements of the charge $Q(t)$ as the scalar product between relativistic wave functions such as the plane waves (4.152). For states of momenta $\mathbf{p}$ and $\mathbf{p}'$ we define the scalar product

$$(f_{\mathbf{p}'}, f_{\mathbf{p}})_t \equiv \int d^3x f_{\mathbf{p}'}^*(\mathbf{x}, t) i \overleftrightarrow{\partial}_0 f_{\mathbf{p}}(\mathbf{x}, t). \quad (4.177)$$

It is formed as a spatial integral at any fixed time, that actually does not need to be recorded in the notation, since the result does not depend on t due to charge conservation.

Analogous scalar products exist between positive- and negative-frequency solutions $f_{\mathbf{p}}(x)$ and $f_{\mathbf{p}}^*(x)$, and between two negative-frequency solutions $f_{\mathbf{p}}^*(x)$ of different momenta. Both sets of wave functions $f_{\mathbf{p}}(x)$ and $f_{\mathbf{p}}^*(x)$ are needed to span the space of all solutions of the Klein-Gordon equation. Within the scalar product (4.177), we choose to normalize the plane wave functions so that they satisfy the orthogonality relations

$$(f_{\mathbf{p}'}, f_{\mathbf{p}})_t = \delta_{\mathbf{p}', \mathbf{p}}, \quad (f_{\mathbf{p}'}, f_{\mathbf{p}}^*)_t = -\delta_{\mathbf{p}', \mathbf{p}}, \quad (f_{\mathbf{p}}^*, f_{\mathbf{p}})_t = 0. \quad (4.178)$$

The spatial integrals ensure that the spatial momenta are equal or opposite to each other. Then the energies p^0 are equal to each other, so that the time derivative in the scalar products produces either zero [between $f_{\mathbf{p}}(t)$ and $f_{-\mathbf{p}}^*(t)$], or a positive value between equal wave functions. In a finite volume V , these are the norms of the wave functions $f_{\mathbf{p}}(\mathbf{x}, t)$ or $f_{\mathbf{p}}^*(\mathbf{x}, t)$. They coincide with the matrix elements of the charge (4.175), if the appropriate plane wave is inserted for the field $\phi(x)$ in (4.171).

The charge of the plane waves with negative frequency $f_{\mathbf{p}}^*(x)$ is negative:

$$(f_{\mathbf{p}}^*, f_{\mathbf{p}}^*)_t \equiv \int d^3x f_{\mathbf{p}'}(\mathbf{x}, t) i \overleftrightarrow{\partial}_0 f_{\mathbf{p}}^*(\mathbf{x}, t) < 0, \quad (4.179)$$

so that the set of all scalar products is not positive-definite. Historically, this was an obstacle for the Klein-Gordon theory to represent a direct generalization of the Schrödinger theory to relativistic particles; rightfully so, as we shall see in Chapter 7.

In a finite total spatial volume V , the properly normalized wave functions (4.152) are explicitly

$$f_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{2Vp^0}} e^{-ipx}, \quad f_{\mathbf{p}}^*(\mathbf{x}, t) = \frac{1}{\sqrt{2Vp^0}} e^{ipx}, \quad (4.180)$$

where p^0 is the particle energy $p^0 = \omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$. The norms are ± 1 .

In an infinite volume, a convenient normalization is

$$f_{\mathbf{p}}(\mathbf{x}, t) = e^{-ipx}, \quad f_{\mathbf{p}}^*(\mathbf{x}, t) = e^{ipx}, \quad (4.181)$$

and the orthonormality relations become

$$\begin{aligned} (f_{\mathbf{p}'}, f_{\mathbf{p}})_t &= 2p^0 \delta^{(3)}(\mathbf{p}' - \mathbf{p}), \\ (f_{\mathbf{p}'}^*, f_{\mathbf{p}}^*)_t &= -2p^0 \delta^{(3)}(\mathbf{p}' - \mathbf{p}), \\ (f_{\mathbf{p}'}^*, f_{\mathbf{p}})_t &= 0, \end{aligned} \quad (4.182)$$

where $\delta^{(3)}(\mathbf{p}' - \mathbf{p}) = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p})$, as defined in Eq. (1.196). The convenience in having a factor $2p^0$ accompany the δ -function is that this combination has pleasant transformation properties under the Lorentz group. It yields unity when integrated over the Lorentz-invariant volume element in momentum space:

$$\int \frac{d^3p}{(2\pi)^3 2p^0}. \quad (4.183)$$

The Lorentz invariance is obvious by rewriting this as

$$\int \frac{d^4p}{(2\pi)^3} \Theta(p^0) \delta(p^2 - M^2). \quad (4.184)$$

4.5 Other Symmetries of Scalar Action

The actions (4.163) and (4.167) of a real or complex scalar field are invariant under more than just the Lorentz group.

4.5.1 Translations of Scalar Field

First, the actions are invariant under space as well as time translations of the coordinate system:

$$x'^{\mu} = x^{\mu} + a^{\mu}. \quad (4.185)$$

Recall that under Lorentz transformations, a scalar field at the same spacetime point remains unchanged by the change of coordinates:

$$\phi(x) \xrightarrow{\Lambda} \phi'_{\Lambda}(x) = \phi(\Lambda^{-1}x). \quad (4.186)$$

The same is true for translations:

$$\phi(x) \xrightarrow{a} \phi'_a(x) = \phi(x - a). \quad (4.187)$$

Inserting this into the Lagrangian density (4.164), we see that it transforms like a scalar field:

$$\mathcal{L}'(x) = \mathcal{L}(x - a). \quad (4.188)$$

Together with the trivial translational invariance of the volume integral, the action is indeed invariant.

The combinations of Lorentz transformations and translations,

$$x'^{\mu} = \Lambda^{\mu}_{\nu} x^{\nu} + a^{\mu}, \quad (4.189)$$

form a group called the *inhomogeneous Lorentz group* or *Poincaré group*. Under it, the scalar field transforms as

$$\phi(x) \longrightarrow \phi'(x) = \phi(\Lambda^{-1}(x - a)). \quad (4.190)$$

Thus, a free scalar field theory is not only Lorentz-invariant but also Poincaré-invariant. This holds also for real and complex scalar fields $\phi(x)$.

Translations can be generated by a differential operator in just the same way as Lorentz transformations in Eq. (4.122). Obviously we can write the translation (4.187) as

$$\phi(x) \longrightarrow \phi'_a(x) = \phi(x - a) = \hat{D}(a)\phi(x) \equiv e^{ia^{\mu}\hat{p}_{\mu}/\hbar}\phi(x), \quad (4.191)$$

where $\hat{p}_{\mu} = i\hbar\partial_{\mu}$ is the differential operator of momentum (4.34). This is proved by applying Lie's expansion formula (4.105) to the coordinates x^{μ} :

$$e^{ia^{\mu}\hat{p}_{\mu}/\hbar}x^{\lambda}e^{-ia^{\mu}\hat{p}_{\mu}/\hbar} = e^{-a^{\mu}\partial_{\mu}}x^{\lambda}e^{a^{\mu}\partial_{\mu}} = x^{\lambda} - a^{\lambda}, \quad (4.192)$$

Poincaré transformations are then obtained from operations

$$\phi(x) \longrightarrow \phi'_a(x) = \phi(\Lambda^{-1}(x - a)) = \hat{D}(a)\hat{D}(\Lambda)\phi(x) \equiv e^{ia^{\mu}\hat{p}_{\mu}/\hbar}e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x), \quad (4.193)$$

with the parameters $\omega_{\mu\nu}$ specified in (4.70) and (4.71). This follows from the behavior of the coordinate vector:

$$e^{ia^{\mu}\hat{p}_{\mu}/\hbar}e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}x^{\lambda}e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}e^{-ia^{\mu}\hat{p}_{\mu}/\hbar}x^{\lambda} = (\Lambda^{-1})^{\mu}_{\nu}(x - a)^{\nu}, \quad (4.194)$$

thus extending (4.118) to the Poincaré group. The last equation states in a global way the vector properties of x^{μ} under Poincaré transformations.

4.5.2 Space Inversion of Scalar Field

Second, the scalar actions (4.163) and (4.167) are invariant under the operation of *space inversion* [see (14.315)], under which the coordinates go into

$$x \xrightarrow{P} x'_P = \tilde{x} \equiv (x^0, -x^i), \quad (4.195)$$

whereas the scalar field is transformed as follows:

$$\phi(x) \xrightarrow{P} \phi'_P(x) = \phi(\tilde{x}). \quad (4.196)$$

Note that this transformation behavior is not the only possible one. Since the parity operation is not related continuously to the identity, there is no reason why the field $\phi(x)$ should transform into itself as it does for the continuous group of Lorentz transformations. The parity operation forms, together with the unit element, a group called the *group of space reflections*. The group multiplication table reads as follows:

$$\begin{array}{c|cc} & 1 & P \\ \hline 1 & 1 & P \\ P & P & 1 \end{array}. \quad (4.197)$$

The only requirement to be satisfied by the field is to be consistent with the group multiplication law in the table. This is assured if the successive application of two parity operations, which result in the identity operation, leads back to the original field (*cyclicity* of order 2). It is therefore possible to choose any transformation law

$$\phi(x) \xrightarrow{P} \phi'_P(x) = \eta_P \phi(\tilde{x}), \quad (4.198)$$

as long as η_P satisfies $\eta_P^2 = 1$. This allows for two solutions, the above trivial one in (4.198) with $\eta_P = 1$, and the alternating one with $\eta_P = -1$, i.e.,

$$\eta_P = \pm 1. \quad (4.199)$$

Thus the scalar field could also pick up a negative sign upon space reflection.

If the interactions to which a particle is subjected are invariant under the parity operation, the value of η_P is a characteristic property of the particle. It is called the *intrinsic parity* of the particle. States with positive or negative intrinsic parities are familiar in quantum mechanics where they appear as bound states with even or odd orbital angular momentum, respectively. Only a particle with $\eta_P = 1$ is called a proper *scalar particle*, while $\eta_P = -1$ is called a *pseudoscalar particle*.

The most important fundamental particles of odd parity are the π -mesons which are the source of the long-range part of nuclear interactions. The pseudoscalar nature is most simply seen in the decay of π^0 into two photons, which is the main reason for the finite lifetime $\tau = (8.4 \pm 0.6) \times 10^{-17}$ sec of this particle (branching ratio of two-photon with respect to all decay channels is 98.798%). In the rest frame of the pion, the two final photons emerge in opposite directions and are polarized

parallel to each other. Under a space inversion, the two-photon state is transformed into itself, but with reversed polarization directions. This corresponds to a negative parity.

The negative parity of a charged pion π^- , whose lifetime is much longer [$\tau = (2.6030 \pm 0.0024) \times 10^{-8} \text{sec}$], can be deduced from the existence of the absorption of a π^- -meson at rest by a deuteron. The deuteron is a bound state of a neutron and a proton in an s -wave with parallel spins, so that the total angular momentum of a deuteron at rest is $J = 1$. For an s -wave, the parity of the orbital wave function is positive. An additional pion at rest does not change J . The final state consists of two neutrons flying apart in opposite directions. By the Pauli principle, their wave function has to be antisymmetric. Thus it can only be in spin-singlet states for even orbital angular momenta l , or in spin-triplet states for odd l . Since the final total angular momentum must be $J = 1$, only the spin-triplet $l = 1$ state is allowed. This, however, has a negative parity, which can only be caused by the additional π^- -meson being a pseudoscalar particle. Note that the intrinsic parities of proton and neutron do not matter in this argument since these particles are present before and after the absorption process.

If particles with definite intrinsic parity interact with each other and the interactions are invariant under space reflection, the intrinsic parity supplies characteristic selection rules in scattering and decay processes. In quantum mechanics, for example, decays of atomic states in the dipole approximation have to change the parity of the state since the dipole operator itself has a negative parity.

4.5.3 Time Reversal of Scalar Field

As a second extension of the Lorentz invariance of the scalar actions (4.163) or (4.167) we can reverse the sign of the time axis via the time reversal transformation

$$x \xrightarrow{T} x'_T = -\tilde{x}, \quad (4.200)$$

which has the same multiplication table as the parity transformation:

$$\begin{array}{|c|c|c|} \hline & 1 & T \\ \hline 1 & 1 & T \\ T & T & 1 \\ \hline \end{array} . \quad (4.201)$$

The field transforms like

$$\phi(x) \xrightarrow{T} \phi'_T(x) = \eta_T \phi(x_T), \quad (4.202)$$

where again

$$\eta_T = \pm 1. \quad (4.203)$$

Note that this transformation law holds for both real and complex fields. The field transformation law (4.202) should not be confused with the corresponding

transformation law of wave functions. In order to clarify this point consider non-relativistic Schrödinger theory. There, given a solution $\psi(\mathbf{x}, t)$ of the free-particle Schrödinger equation

$$\left(i\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)\psi(\mathbf{x}, t) = 0, \quad (4.204)$$

the wave function $\psi^*(\mathbf{x}, -t)$ represents also a solution with the same energy. The presence of only a single time derivative necessitates the complex conjugation. A plane-wave solution of momentum $\mathbf{p}$

$$\psi_{\mathbf{p}}(\mathbf{x}, t) = e^{-iEt/\hbar + i\mathbf{p}\mathbf{x}/\hbar}, \quad (4.205)$$

transforms like

$$\psi_{\mathbf{p}}(\mathbf{x}, t) \xrightarrow{T} \psi'_{\mathbf{p}T}(\mathbf{x}, t) = \eta_T \psi_{\mathbf{p}}^*(\mathbf{x}, -t). \quad (4.206)$$

This satisfies the Schrödinger equation

$$\left(i\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)\psi'_{\mathbf{p}T}(\mathbf{x}, t) = 0. \quad (4.207)$$

From (4.205) we see that the right-hand side of (4.206) is equal to

$$\eta_T \psi_{-\mathbf{p}}(\mathbf{x}, t). \quad (4.208)$$

The particle momentum in the transformed wave function is reversed, so that the particle appears to run *backwards in time*.

Since the transformation law (4.206) involves complex conjugation, scalar products between two arbitrary wave functions $\langle\psi_2(t)|\psi_1(t)\rangle = \int d^3x \psi_2^*(\mathbf{x}, t)\psi_1(\mathbf{x}, t)$ go over into their complex conjugates at the negative time:

$$\langle\psi_2(t)|\psi_1(t)\rangle \xrightarrow{T} {}_T\langle\psi'_2(t)|\psi'_1(t)\rangle_T = \langle\psi_2(-t)|\psi_1(-t)\rangle^* = \langle\psi_1(-t)|\psi_2(-t)\rangle. \quad (4.209)$$

This property guarantees the preservation of probabilities under this transformation. In general, any transformation which carries all scalar products into their Hermitian conjugates is referred to as *antiunitary*. Antiunitarity implies that the time reversal operation is necessarily *antilinear*. A transformation is antilinear if the coefficients of a linear combination of wave functions go over into their complex conjugates.

At the level of Schrödinger differential operators, antiunitarity produces a sign reversal in the transformation properties of energy and momentum. The defining representation

$$T^{-1}tT = -t, \quad T^{-1}\mathbf{x}T = \mathbf{x} \quad (4.210)$$

implies that

$$T^{-1}i\partial_tT = -i\partial_t, \quad T^{-1}i\partial_{\mathbf{x}}T = i\partial_{\mathbf{x}}. \quad (4.211)$$

The antiunitary representation of this operation is

$$\mathcal{T}^{-1}i\partial_t\mathcal{T} = i\partial_t, \quad \mathcal{T}^{-1}i\partial_{\mathbf{x}}\mathcal{T} = -i\partial_{\mathbf{x}}. \quad (4.212)$$

It leaves the energy invariant, while reversing the direction of the momentum:

$$E \xrightarrow{T} E, \quad \mathbf{p} \xrightarrow{T} -\mathbf{p}. \quad (4.213)$$

Thus particles keep their positive energy but run backwards in time. A unitary representation would have the opposite effect and produce a state which cannot be found in nature.

In contrast to the wave functions, the *Schrödinger field operator*, which was the result of second quantization in Chapter 2, transforms under time reversal like

$$\hat{\psi}(\mathbf{x}, t) \xrightarrow{T} \hat{\psi}'_T(\mathbf{x}, t) = \eta_T \hat{\psi}(\mathbf{x}, -t). \quad (4.214)$$

At the operator level, the effects of complex conjugation are brought about by the antilinearity of the time reversal operator $\mathcal{T}$ in the second-quantized Hilbert space. In fact, the transformation law (4.206) for the wave functions can be derived from (4.214). In terms of $\mathcal{T}$, the transformation (4.214) reads

$$\hat{\psi}(\mathbf{x}, t) \xrightarrow{T} \mathcal{T}^{-1} \hat{\psi}(\mathbf{x}, t) \mathcal{T} = \eta_T \hat{\psi}(\mathbf{x}, -t). \quad (4.215)$$

Expanding the field operator terms of creation and annihilation operators as in Eq. (2.215),

$$\hat{\psi}(\mathbf{x}, t) = \int d^3p \psi_{\mathbf{p}}(\mathbf{x}, t) \hat{a}_{\mathbf{p}}, \quad (4.216)$$

and using the antilinearity of $\mathcal{T}$, we obtain

$$\mathcal{T}^{-1} \hat{\psi}(\mathbf{x}, t) \mathcal{T} = \int d^3p \psi_{\mathbf{p}}^*(\mathbf{x}, t) \mathcal{T}^{-1} \hat{a}_{\mathbf{p}} \mathcal{T} = \int d^3p e^{iEt/\hbar - i\mathbf{p}\mathbf{x}/\hbar} \mathcal{T}^{-1} \hat{a}_{\mathbf{p}} \mathcal{T}. \quad (4.217)$$

According to (4.215), the right-hand side has to be equal to

$$\eta_T \int d^3p e^{iEt/\hbar + i\mathbf{p}\mathbf{x}/\hbar} \hat{a}_{\mathbf{p}}, \quad (4.218)$$

which implies that the annihilation operators transform like

$$\mathcal{T}^{-1} \hat{a}_{\mathbf{p}} \mathcal{T} = \eta_T \hat{a}_{-\mathbf{p}}. \quad (4.219)$$

A particle of momentum $\mathbf{p}$ goes over into a particle of momentum $-\mathbf{p}$, which is the correct transformation law.

Thus, in spite of their contradictory appearance, the two transformation laws (4.206) for wave functions and (4.214) for Schrödinger fields, with their antiunitary operator implementation (4.215) after field quantization, are completely consistent with each other. Thus we need no longer to be astonished about the absence of a complex conjugation on the right-hand side of the field transformation law (4.202).

Another feature of antiunitarity, which has to be kept in mind, is that the time-reversed field operator does not satisfy the Schrödinger equation of the original field

$$\left(i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right) \hat{\psi}(\mathbf{x}, t) = 0, \quad (4.220)$$

but the transformed equation

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)^* \hat{\psi}'_T(\mathbf{x}, t) = 0. \quad (4.221)$$

This follows immediately by multiplying (4.220) with the operator $\mathcal{T}$ from the left and passing $\mathcal{T}$ on to the right-hand side of the differential operator. The antilinearity causes the complex conjugation of the differential operator in (4.222). This is necessary to produce the correct Schrödinger equation (4.207) for the time-reversed wave functions.

At first sight the field equation appears to be in contradiction with the correspondence principle from which one might expect equations for operators to go directly over into those for classical objects in the limit of small $\hbar$. Properly, however, this limit must be taken on equations for measurable *amplitudes*, not the operators themselves, and these *do* follow the Schrödinger equation.² Take for instance the single-particle amplitude of an arbitrary state $|\Psi\rangle$ in the Heisenberg picture $\langle 0|\hat{\psi}(\mathbf{x}, t)|\Psi\rangle$, which satisfies

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right) \langle 0|\hat{\psi}(\mathbf{x}, t)|\Psi\rangle = 0. \quad (4.222)$$

For the time-reversed field operator (4.214), the equation is

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)^* \langle 0|\hat{\psi}(\mathbf{x}, -t)|\Psi\rangle = 0. \quad (4.223)$$

The time-reversed amplitude on the right-hand side is the amplitude for the time reversed state $\mathcal{T}|\Psi\rangle$ (since $\langle 0|\mathcal{T}^{-1} = \langle 0|$):

$$\langle 0|\hat{\psi}(\mathbf{x}, -t)|\Psi\rangle = \langle 0|\mathcal{T}^{-1}\hat{\psi}(\mathbf{x}, t)\mathcal{T}|\Psi\rangle = \langle 0|\hat{\psi}(\mathbf{x}, t)\mathcal{T}|\Psi\rangle. \quad (4.224)$$

This obeys the Schrödinger equation

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right) \langle 0|\hat{\psi}(\mathbf{x}, -t)\mathcal{T}|\Psi\rangle, \quad (4.225)$$

as it should.

The operator implementation of the time reversal transformation will be discussed in detail in Chapter 7 for fields and particles of different spin (see Subsections 7.1.6, 7.4.4, 7.5.4, and 7.7.1). An important observation should, however, be made right here: As a consequence of antiunitarity, the phase factor η_T appearing in the time reversal transformation of a complex field is arbitrary. It cannot be fixed in the usual way by applying the transformations T twice. The antilinearity will change η_T , that arises in the first transformation, into η_T^* , so that the combined phase factor is $\eta_T\eta_T^* = 1$. This is fulfilled for *any* phase factor $\eta_T = e^{i\gamma}$, not just ± 1 .

Since the phase factor η_T is arbitrary, it may be chosen arbitrarily, for instance

$$\eta_T \equiv 1. \quad (4.226)$$

²This is a manifestation of *Ehrenfest's theorem* for the semiclassical limit of field equations.

4.5.4 Charge Conjugation of Scalar Field

At the level of a relativistic scalar field $\phi(x)$ there is one further discrete symmetry. We can change $\phi(x)$ into $\phi^*(x)$ without changing the action (4.163). This operation is called *charge conjugation* denoted by C . Since $C^2 = 1$, a complex field can transform in two possible ways

$$\phi(x) \xrightarrow{C} \phi'_C(x) = \eta_C \phi^*(x), \quad (4.227)$$

where the phase factor can take the values

$$\eta_C = \pm 1. \quad (4.228)$$

For a real field with the action (4.167), we may simply drop the complex conjugation on the right-hand side of (4.227).

An explanation is necessary for the name of this operation. In Eq. (4.171) we have seen that there exists a conserved current $j^\mu(x)$ which can be used to couple the complex scalar field to electromagnetism. If this is done, $j^\mu(x)$ becomes an electromagnetic current density, and the integral $Q(t) = \int d^3x j^0(x)$ is the charge of the field system. Now, under the transformation (4.227) this electromagnetic current density changes its sign:

$$j^\mu(x) \xrightarrow{C} j_C^{\mu'}(x) = -j^\mu(x). \quad (4.229)$$

Thus the transformation reverses the charge of the field, and this is why the discrete operation C is called charge conjugation.

As we shall discuss later in Chapter 24, electromagnetic and strong interactions are invariant under charge conjugation, implying that the phase factor η_C is a fixed measurable property of the particle, called *charge parity*.

Take for instance the field of the neutral meson π^0 . As mentioned above, the particle decays with a lifetime of $(8.4 \pm 0.6) \times 10^{-17}$ sec, mostly into two photons. Since these are neutral particles, they have a charge parity on their own. Whatever it is (we shall see in Subsection 4.7.2 that it is negative), the two-photon state must have a positive charge parity, and this must consequently be the charge parity of the π^0 -meson.

4.6 Electromagnetic Field

Electromagnetic fields propagate with light velocity, and their field equations have no mass term [3]. They exist with two polarization degrees of freedom (right and left linear or circular polarizations), and are described by the usual electromagnetic action. Historically, this was the very first example of a relativistic classical field theory, and it could also have served as a guideline for the previous construction of the action (4.167) of a real scalar field $\phi(\mathbf{x})$.

4.6.1 Action and Field Equations

The action may be given in terms of a real auxiliary four-vector potential $A_\mu(x)$ from which the physical electric and magnetic fields can be derived as follows:

$$E^i = -(\partial^0 A^i - \partial^i A^0) = -\partial_t A^i - \partial_i A^0, \quad (4.230)$$

$$B^i = -\frac{1}{2}\epsilon_{ijk}(\partial^j A^k - \partial^k A^j) = \frac{1}{2}\epsilon_{ijk}(\partial_j A^k - \partial_k A^j). \quad (4.231)$$

It is useful to introduce the so-called *four-curl* of the vector potential, the tensor

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \quad (4.232)$$

Its six components are directly the electric and magnetic field strengths

$$F_{0i} = -F^{0i} = -\partial^0 A^i + \partial^i A^0 = -\partial_0 A^i - \partial_i A^0 = E^i, \quad (4.233)$$

$$F_{ij} = F^{ij} = \partial^i A^j - \partial^j A^i = -\partial_i A^j + \partial_j A^i = -\epsilon_{ijk} B^k, \quad (4.234)$$

or, in a more conventional notation,

$$\mathbf{E}(x) = -\frac{1}{c}\dot{\mathbf{A}}(x) - \nabla A^0(x), \quad (4.235)$$

$$\mathbf{B}(x) = \nabla \times \mathbf{A}(x). \quad (4.236)$$

For this reason the tensor $F_{\mu\nu}$ is also called the *field tensor*. Note that $F^{\mu\nu}$ is related to the fields B_i and E_i in the same way as the generators $L_{\mu\nu}$ of the Lorentz group were related to L_i and M_i in Eq. (4.67).

The electromagnetic action reads

$$\mathcal{A} = \int d^4x \mathcal{L} = -\frac{1}{4} \int d^4x F_{\mu\nu} F^{\mu\nu} = \int d^4x \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2). \quad (4.237)$$

The four-curl $F_{\mu\nu}$ satisfies a so-called *Bianchi identity* for any smooth A_μ :

$$\partial_\mu \tilde{F}^{\mu\nu} = 0, \quad (4.238)$$

where

$$\tilde{F}^{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\lambda\kappa} F_{\lambda\kappa} \quad (4.239)$$

is the *dual field tensor*, with $\epsilon^{\mu\nu\lambda\kappa}$ being the four-dimensional Levi-Civita tensor with $\epsilon_{0123} = 1$. Note that

$$F_{\mu\nu} \tilde{F}^{\mu\nu} = 4\mathbf{E} \cdot \mathbf{B} \quad (4.240)$$

is a pseudoscalar.

Equation (4.238) can be rewritten as

$$\frac{1}{2}\epsilon^{\mu\nu\lambda\kappa} \partial_\mu F_{\lambda\kappa} = \frac{1}{2}\epsilon^{\mu\nu\lambda\kappa} (\partial_\mu \partial_\lambda - \partial_\lambda \partial_\mu) A_\kappa(x) = 0. \quad (4.241)$$

Multiplying this by another ϵ -tensor and using the tensor identity

$$\begin{aligned} \epsilon_{\mu\nu\lambda\kappa}\epsilon^{\mu\nu'\lambda'\kappa'} &= \delta_{\nu}^{\nu'}\delta_{\lambda}^{\lambda'}\delta_{\kappa}^{\kappa'} + \delta_{\nu}^{\lambda'}\delta_{\lambda}^{\kappa'}\delta_{\kappa}^{\nu'} + \delta_{\nu}^{\kappa'}\delta_{\lambda}^{\nu'}\delta_{\kappa}^{\lambda'} \\ &- \delta_{\nu}^{\lambda'}\delta_{\lambda}^{\nu'}\delta_{\kappa}^{\kappa'} - \delta_{\nu}^{\nu'}\delta_{\lambda}^{\kappa'}\delta_{\kappa}^{\lambda'} - \delta_{\nu}^{\kappa'}\delta_{\lambda}^{\lambda'}\delta_{\kappa}^{\nu'}, \end{aligned} \quad (4.242)$$

we obtain the integrability condition of a lemma attributed to H.A. Schwarz [11], according to which the derivatives of an integrable function will always commute:

$$(\partial_{\mu}\partial_{\nu} - \partial_{\nu}\partial_{\mu})A_{\lambda}(x) = 0. \quad (4.243)$$

The equations of motion which extremize the action are

$$\frac{\delta\mathcal{A}}{\delta A^{\mu}(x)} = -\partial_{\mu}\frac{\partial\mathcal{L}(x)}{\partial[\partial_{\mu}A_{\nu}(x)]} = \frac{1}{2}\partial_{\mu}F^{\mu\nu}(x) = 0, \quad (4.244)$$

or more explicitly

$$(g^{\mu\nu}\partial^2 - \partial^{\mu}\partial^{\nu})A_{\nu}(x) = 0. \quad (4.245)$$

Separating the equations (4.238) and (4.244) into space and time components they are seen to coincide with the four Maxwell's equations in empty space:

$$\partial_{\mu}\tilde{F}^{\mu\nu} = 0 : \quad \nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0, \quad (4.246)$$

$$\partial_{\mu}F^{\mu\nu} = 0 : \quad \nabla \cdot \mathbf{E} = 0, \quad \nabla \times \mathbf{B} - \partial_t \mathbf{E} = 0. \quad (4.247)$$

The first equation in (4.246) states that there can be no magnetic monopoles. The second equation is *Faraday's law* of induction. The first equation in (4.247) is *Coulomb's law* in the absence of charges, the second is *Ampère's law* in the absence of currents (including, however, Maxwell's displacement current caused by the time derivative of the electric field).

In terms of the vector field $A^{\mu}(x)$, the action reads explicitly

$$\begin{aligned} \mathcal{A} = \int d^4x \mathcal{L}(x) &= -\frac{1}{2} \int d^4x [\partial^{\mu}A^{\nu}(x)\partial_{\mu}A_{\nu}(x) - \partial^{\nu}A_{\nu}(x)\partial^{\mu}A_{\mu}(x)] \\ &= \frac{1}{2} \int d^4x A_{\mu}(x)(g^{\mu\nu}\partial^2 - \partial^{\mu}\partial^{\nu})A_{\nu}(x). \end{aligned} \quad (4.248)$$

The latter form is very similar to the scalar action (4.167). The first piece is the same as in (4.167) for each of the spatial components A^1, A^2, A^3 . The time component A^0 , however, appears with an opposite sign. A field with this property is called a *ghost field*. When trying to quantize such a field, the associated particle states turn out to have a negative norm. In a consistent physical theory, such states must never appear in any scattering process.

In comparison with the scalar field action (4.319), the second gradient term $\partial^{\nu}A_{\nu}\partial^{\mu}A_{\mu}$ in the action (4.248) is novel. It exists here as an additional possible Lorentz invariant since A_{μ} is a vector field under Lorentz transformations.

It is instructive to insert the individual components A^0 and $\mathbf{A} = (A^1, A^2, A^3)$ into the action and find

$$\mathcal{A} = \frac{1}{2} \int d^4x \left[A^0(x)(-\nabla^2)A^0(x) - 2A^0(x)\partial_0\nabla^i A^i(x) - \mathbf{A}(x)(\partial_0^2 - \nabla^2)\mathbf{A}(x) - A^i(x)\nabla^i\nabla^j A^j(x) \right]. \quad (4.249)$$

This shows that the field component A^0 appears without a time derivative. As a consequence, the component A^0 remains classical when going over to quantum field theory in Chapter 7. It will be fully determined by the classical field equation.

4.6.2 Gauge Invariance

The field tensor (4.232) is invariant under local gauge transformations

$$A_\mu(x) \longrightarrow A'_\mu(x) = A_\mu(x) + \partial_\mu\Lambda(x), \quad (4.250)$$

where $\Lambda(x)$ is any smooth field which satisfies the integrability condition

$$(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu)\Lambda(x) = 0. \quad (4.251)$$

Gauge invariance implies that one scalar field degree of freedom in $A^\mu(x)$ does not contribute to the physically observable electromagnetic fields $\mathbf{E}(x)$ and $\mathbf{B}(x)$. This degree of freedom can be removed by *fixing a gauge*. One way to do that is to require the vector potential to satisfy the *Lorenz gauge condition*, which means that the field A^μ has a vanishing four divergence [1]:

$$\partial_\mu A^\mu(x) = 0. \quad (4.252)$$

For a vector field satisfying this condition, the field equations (4.245) decouple and become simply four massless Klein-Gordon equations:

$$-\partial^2 A_\nu(x) = 0. \quad (4.253)$$

If a vector potential $A^\mu(x)$ does not satisfy this condition, one may always perform a gauge transformation (4.250) to a new field $A'^\mu(x)$ that has no four divergence. We merely have to choose a gauge function $\Lambda(x)$ solving the differential equation

$$-\partial^2\Lambda(x) = \partial_\mu A^\mu(x), \quad (4.254)$$

and $A'^\mu(x)$ will satisfy $\partial_\mu A'^\mu(x) = 0$.

There are infinitely many solutions to equation (4.254). Given one solution $\Lambda(x)$ which leads to the Lorenz gauge, one can add any solution of the homogeneous Klein-Gordon equation without changing the four-divergence of $A^\mu(x)$. The associated gauge transformation

$$A_\mu(x) \longrightarrow A_\mu(x) + \partial_\mu\Lambda'(x), \quad \partial^2\Lambda'(x) = 0, \quad (4.255)$$

are called *restricted gauge transformations* or *gauge transformations of the second kind*, or *on-shell gauge transformations*. If a vector potential $A^\mu(x)$ in the Lorenz gauge solves the field equations (4.245), the gauge transformations of the second kind can be used to remove the spatial divergence $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$. Under (4.255), the components $A^0(\mathbf{x}, t)$ and $\mathbf{A}(\mathbf{x}, t)$ go over into

$$\begin{aligned} A^0(x) &\rightarrow A'^0(\mathbf{x}, t) = A^0(\mathbf{x}, t) + \partial_0 \Lambda'(\mathbf{x}, t), \\ \mathbf{A}(x) &\rightarrow \mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) - \nabla \Lambda'(\mathbf{x}, t). \end{aligned} \quad (4.256)$$

Thus, if we choose the gauge function

$$\Lambda'(\mathbf{x}, t) = - \int d^3x' \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|} \nabla \cdot \mathbf{A}(\mathbf{x}', t), \quad (4.257)$$

then

$$\nabla^2 \Lambda'(\mathbf{x}, t) = \nabla \cdot \mathbf{A}(\mathbf{x}, t) \quad (4.258)$$

and the gauge-transformed field $\mathbf{A}'(\mathbf{x}, t)$ has no spatial divergence, being completely transverse:

$$\nabla \cdot \mathbf{A}'(\mathbf{x}, t) = \nabla \cdot [\mathbf{A}(\mathbf{x}, t) - \nabla \Lambda(\mathbf{x}, t)] = 0. \quad (4.259)$$

This condition

$$\nabla \cdot \mathbf{A}(\mathbf{x}, t) = 0 \quad (4.260)$$

is known as the *Coulomb gauge*- or *radiation gauge* of the vector potential $\mathbf{A}(\mathbf{x}, t)$.

The solution (4.257) to the differential equation (4.258) is undetermined up to an arbitrary solution $\Lambda'(x)$ of the homogeneous Poisson equation

$$\nabla^2 \Lambda'(\mathbf{x}, t) = 0. \quad (4.261)$$

Together with the property $\partial^2 \Lambda'(\mathbf{x}, t) = 0$ from (4.255), one also has

$$\partial_t^2 \Lambda'(\mathbf{x}, t) = 0. \quad (4.262)$$

This leaves only trivial linear functions $\Lambda'(\mathbf{x}, t)$ of $\mathbf{x}$ and t which do not describe propagating waves.

Another possible gauge is obtained by removing the zeroth component of the vector potential $A^\mu(x)$ to satisfy the field equations (4.245). We form again

$$A'^\mu(x) = A^\mu(x) + \partial^\mu \Lambda(x), \quad (4.263)$$

but now with a gauge function

$$\Lambda(\mathbf{x}, t) = - \int^t dt' A_0(\mathbf{x}, t'). \quad (4.264)$$

Then $A'^\mu(x)$ will indeed satisfy (4.245), while having the property

$$A'^0(x) = 0. \quad (4.265)$$

This is called the *axial gauge*. The solutions of Eqs. (4.264) are determined up to a trivial constant, leaving no more gauge freedom of the second kind, as in (4.255).

For free fields, the Coulomb gauge and the axial gauge coincide. This is a consequence of Coulomb's law $\nabla \cdot \mathbf{E} = 0$ in Eq. (4.247). By expressing $\mathbf{E}(x)$ explicitly in terms of the spatial and time-like components of the vector potential,

$$\mathbf{E}(x) = -\partial_0 \mathbf{A}(x) - \nabla A^0(x), \quad (4.266)$$

Coulomb's law reads

$$\nabla^2 A^0(\mathbf{x}, t) = -\nabla \cdot \dot{\mathbf{A}}(\mathbf{x}, t). \quad (4.267)$$

This shows that if $\nabla \cdot \mathbf{A}(x) = 0$, also $A^0(x) = 0$, and vice versa.

The differential equation (4.267) can be integrated to

$$A^0(\mathbf{x}, t) = \frac{1}{4\pi} \int d^3x' \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\nabla \cdot \dot{\mathbf{A}})(\mathbf{x}', t). \quad (4.268)$$

In an infinite volume with asymptotically vanishing fields there is no freedom of adding to the left-hand side a nontrivial solution of the homogeneous Poisson equation

$$\nabla^2 A^0(\mathbf{x}, t) = 0, \quad (4.269)$$

which in principle would be possible.

In the presence of charges, Coulomb's law will have a source term and read [see Eq. (12.52)]

$$\nabla \cdot \mathbf{E}(\mathbf{x}, t) = \rho(\mathbf{x}, t), \quad (4.270)$$

where $\rho(\mathbf{x}, t)$ is the electric charge density. Now the divergence of (4.266) yields the equation

$$\nabla^2 A^0(\mathbf{x}, t) = -\nabla \cdot \dot{\mathbf{A}}(\mathbf{x}, t) - \rho(\mathbf{x}, t), \quad (4.271)$$

which is solved by

$$A^0(\mathbf{x}, t) = \frac{1}{4\pi} \int d^3x' \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\rho + \nabla \cdot \dot{\mathbf{A}})(\mathbf{x}', t). \quad (4.272)$$

In contrast to the previous (4.268), the vanishing of $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$ no longer implies $A^0(\mathbf{x}, t) \equiv 0$, but determines it to be the instantaneous Coulomb potential around the charge distribution $\rho(\mathbf{x}', t)$:

$$A^0(\mathbf{x}, t) = \frac{1}{4\pi} \int d^3x' \frac{1}{|\mathbf{x}' - \mathbf{x}|} \rho(\mathbf{x}', t). \quad (4.273)$$

Remarkably, there is no retardation. This is an apparent violation of the relativity principle. The contradiction will be resolved due to gauge invariance in Chapters 7 and 12.

Note that the fields A^μ can still be modified by adding $\partial^\mu \Lambda$ and one has the possibility of choosing $\Lambda(\mathbf{x}, t)$ either to satisfy the Coulomb gauge

$$\nabla \cdot \mathbf{A}(\mathbf{x}, t) \equiv 0, \quad (4.274)$$

or any other gauge, such as the axial gauge

$$A^0(\mathbf{x}, t) \equiv 0. \quad (4.275)$$

Only for free fields the two gauges coincide.

The gauge properties of the free-field action (4.248) can be made more explicit with the help of the transverse projection operator [compare (4G.1)]

$$P_t^{\mu\nu} \equiv g^{\mu\nu} - \frac{\partial^\mu \partial^\nu}{\partial^2}, \quad (4.276)$$

which has the property

$$P_t^{\mu\nu} g_{\nu\lambda} P_t^{\lambda\kappa} = P_t^{\nu\kappa}. \quad (4.277)$$

Then the action (4.248) contains only the transverse part

$$A_t^\mu \equiv P_t^{\mu\nu} A_\nu. \quad (4.278)$$

of the vector potential:

$$\mathcal{A} = \frac{1}{2} \int d^4x A_\mu(x) P_t^{\mu\nu} \partial^2 A_\nu(x) = \frac{1}{2} \int d^4x g_{\mu\nu} A_t^\mu(x) \partial^2 A_t^\nu(x). \quad (4.279)$$

A gauge transformation (4.264) changes the field $A^\mu(x)$ only by a gradient of a scalar field $\Lambda(x)$, and this contributes only to the longitudinal part of the vector field

$$A_l^\mu \equiv P_l^{\mu\nu} A_\nu, \quad (4.280)$$

where [compare (4G.1)]

$$P_l^{\mu\nu} \equiv \frac{\partial^\mu \partial^\nu}{\partial^2} = g^{\mu\nu} - P_t^{\mu\nu}. \quad (4.281)$$

It therefore leaves the transverse part A_t^μ invariant due to the orthogonality relation

$$P_t^{\mu\nu} g_{\nu\lambda} P_l^{\lambda\kappa} = 0. \quad (4.282)$$

The completeness relation $P_l^{\mu\nu} + P_t^{\mu\nu} = 1$ ensures that any vector field $A^\mu(x)$ can be decomposed into a sum $A^\mu(x) = A_t^\mu(x) + A_l^\mu(x)$.

4.6.3 Lorentz Transformation Properties of Electromagnetic Fields

The Lorentz transformation properties of the electromagnetic fields were understood a long time ago within classical electrodynamics. They are the origin of the famous *Lorentz force* acting on charged particles in motion. The experimentally observed electric and magnetic forces can be derived by going from the laboratory frame with

fields $\mathbf{E}$, $\mathbf{B}$ to the reference frame of the moving particle with fields $\mathbf{E}'$, $\mathbf{B}'$, via the transformation

$$\mathbf{E}_{||}' = \mathbf{E}_{||}, \quad \mathbf{E}_{\perp}' = \gamma \left(\mathbf{E}_{\perp} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right), \quad (4.283)$$

$$\mathbf{B}_{||}' = \mathbf{B}_{||}, \quad \mathbf{B}_{\perp}' = \gamma \left(\mathbf{B}_{\perp} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right), \quad (4.284)$$

with $\mathbf{v}$ being the velocity of the particle and $\gamma \equiv 1/\sqrt{1 - v^2/c^2}$ the Einstein parameter (4.17). These equations can also be written without separating transverse and longitudinal components as

$$\mathbf{E}' = \gamma \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right) - \frac{\gamma^2}{\gamma + 1} \frac{\mathbf{v}}{c} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{E} \right), \quad (4.285)$$

$$\mathbf{B}' = \gamma \left(\mathbf{B} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right) - \frac{\gamma^2}{\gamma + 1} \frac{\mathbf{v}}{c} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{B} \right). \quad (4.286)$$

The transformed fields exert the observed electric and magnetic forces $e\mathbf{E}' + g\mathbf{B}'$. The subscripts $||$ and $\perp$ indicate projections of the fields parallel and orthogonal to $\mathbf{v}$. From this transformation one may *derive* the transformation law of the vector field A_μ under Lorentz transformations. Let the frame, in which the moving particle is at rest, be related to the laboratory frame by

$$x' = B(\zeta)x, \quad (4.287)$$

where $B(\zeta)$ is a boost into the $\mathbf{v}$ -direction with a rapidity ζ determined by the velocity v via the hyperbolic relations

$$\cosh \zeta = \gamma = 1/\sqrt{1 - v^2/c^2}, \quad \sinh \zeta = \gamma \frac{v}{c}, \quad \tanh \zeta = \frac{v}{c}. \quad (4.288)$$

Then the transformation law (4.284) is equivalent to

$$A'^\mu(x') = B^\mu{}_\nu(\zeta) A^\nu(x), \quad (4.289)$$

apart from an arbitrary gauge transformation. An analogous transformation law holds for rotations, so that the transformations (4.284) and their rotated forms correspond to the Lorentz transformations:

$$A'^\mu(x') = \Lambda^\mu{}_\nu A^\nu(x), \quad (4.290)$$

plus possible gauge transformations. In the notation (4.51), we write the transformation law as

$$A^\mu(x) \xrightarrow{\Lambda} A'^\mu(x) = \Lambda^\mu{}_\nu A^\nu(\Lambda^{-1}x). \quad (4.291)$$

By analogy with Eq. (4.122) for the scalar field, and recalling (4.69), this transformation can be generated as follows:

$$A^\mu(x) \xrightarrow{\Lambda} A'^\mu(x) = \hat{D}(\Lambda) \Lambda^\mu{}_\nu A^\nu(x) \equiv e^{-i\frac{1}{2}\omega_{\lambda\kappa} \hat{J}^{\lambda\kappa}} A^\mu(x), \quad (4.292)$$

with the parameters $\omega_{\mu\nu}$ specified in (4.70) and (4.71), and the combined operator being

$$\hat{J}^{\lambda\kappa} \equiv L^{\lambda\kappa} \times \hat{1} + 1 \times \hat{L}^{\lambda\kappa} \quad (4.293)$$

being the generators of Lorentz transformations of both spacetime vector indices and field arguments. The former are generated by the 4×4 matrices $L_{\mu\nu}$ of Eq. (4.65), the latter by the differential operators (4.92). The combined generators (4.293) are called the generators of the *total four-dimensional angular momentum*. The two generators on the right-hand side of Eq. (4.293) act upon different spaces, transforming once the vector index and once the spacetime coordinate x . Often one therefore writes, shorter and somewhat sloppily,

$$\hat{J}^{\mu\nu} \equiv L^{\mu\nu} + \hat{L}^{\mu\nu}, \quad (4.294)$$

with the tacit understanding that the right-hand side abbreviated the direct sum (4.293) of spin and orbital generators.

Since the two terms in (4.293) act independently on space and spin indices, the operators $\hat{J}^{\lambda\kappa}$ satisfy the same commutation rules as $L^{\lambda\kappa}$ and $\hat{L}^{\lambda\kappa}$:

$$[\hat{J}^{\mu\nu}, \hat{J}^{\lambda\kappa}] = -i(g^{\mu\lambda} \hat{J}^{\nu\kappa} - g^{\mu\kappa} \hat{J}^{\nu\lambda} + g^{\nu\kappa} \hat{J}^{\mu\lambda} - g^{\nu\lambda} \hat{J}^{\mu\kappa}). \quad (4.295)$$

The transformation laws (4.290) and (4.292) differ from those of a scalar field in Eqs. (14.308) and (4.122) in the way discussed above for particles with nonzero intrinsic angular momentum. The field has several components. It points in the same spatial direction before and after the change of coordinates. This is ensured by its components changing in the same way as the coordinates of the point x_μ .

Note that the four-divergence $\partial^\mu A_\mu(x)$ is a scalar field in the sense defined in (14.308). Indeed

$$\partial'^\mu A'_\mu(x') = (\Lambda^\mu{}_\nu \partial^\nu) \Lambda_\mu{}^\lambda A_\lambda(x) = \partial^\nu A_\nu(x). \quad (4.296)$$

For this reason the second term in the action (4.248) is Lorentz-invariant, just as the mass term in (4.167). The invariance of the first term is shown similarly:

$$A'^\nu(x') \partial'^2 A'_\nu(x') = \Lambda^\nu{}_\lambda A^\lambda(x) \partial'^2 \Lambda_\nu{}^\kappa A_\kappa(x') = A^\nu(x) \partial'^2 A_\nu(x) = A^\nu(x) \partial^2 A_\nu(x). \quad (4.297)$$

Hence the action (4.248) does not change under Lorentz transformations, as it should.

4.7 Other Symmetries of Electromagnetic Action

Just as the scalar action, also the electromagnetic action (4.237) is invariant under more symmetry transformations than those of the Lorentz group.

4.7.1 Translations of the Vector Field

Under spacetime translations (4.185) of the coordinates, the vector field transforms like

$$A'^\mu(x) = A^\mu(x - a). \quad (4.298)$$

The combination of these with Lorentz transformations forms the Poincaré group (4.189),

$$x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu, \quad (4.299)$$

under which the field $A^\mu(x)$ transforms like

$$A'^\mu(x) = \Lambda^\mu_\nu A^\nu(\Lambda^{-1}(x - a)), \quad (4.300)$$

leaving the action (4.248) invariant.

As in the scalar equation (4.193), we can generate all Poincaré transformations of the vector potential $A^\mu(x)$ with the help of differential operators such as

$$A^\mu(x) \longrightarrow A'^\mu(x) = \hat{D}(a)\hat{D}(\Lambda)\Lambda^\mu_\nu A^\nu(x) \equiv e^{ia^\mu \hat{p}_\mu/\hbar} e^{-i\frac{1}{2}\omega_{\lambda\kappa} \hat{J}^{\lambda\kappa}} A^\mu(x), \quad (4.301)$$

with the parameters $\omega_{\mu\nu}$ specified in (4.70), (4.71).

4.7.2 Space Inversion, Time Reversal, and Charge Conjugation of the Vector Field

Under space inversion, the four-vector $A^\mu(x)$ behaves as follows:

$$A^\mu(x) \xrightarrow{P} A'^\mu_P(x) = \tilde{A}^\mu(\tilde{x}). \quad (4.302)$$

Under time reversal one has

$$A^\mu(x) \xrightarrow{T} A'^\mu_T(x) = \tilde{A}^\mu(-\tilde{x}), \quad (4.303)$$

where

$$\tilde{A}^\mu = (A^0, -A^i). \quad (4.304)$$

In principle, there is the possibility of a vector field $V^\mu(x)$ transforming like

$$V^\mu(x) \xrightarrow{P} V'^\mu_P(x) = \eta_P \tilde{V}^\mu(\tilde{x}), \quad (4.305)$$

with $\eta_P = \pm 1$. For $\eta_P = -1$ the field $V^\mu(x)$ is called an *axial vector field*. The electromagnetic gauge field $A^\mu(x)$, however, is definitely a proper vector field. This follows from the vector nature of the electric field and the axial vector nature of the magnetic field, which are observed in the laboratory.

Similarly, the behavior of a physically observable vector field V^μ with respect to time reversal is given by

$$V^\mu(x) \xrightarrow{T} V'^\mu_T(x) = \eta_T \tilde{V}^{\mu*}(x_T), \quad (4.306)$$

with an arbitrary phase factor η_T . If the vector field is real and physically observable, then the only alternatives are $\eta_T = \pm 1$. For the electromagnetic vector potential $A^\mu(x)$, the phase factor η_T is as specified in (4.303). It reflects the fact that under time reversal, all spatial currents change their directions whereas the zeroth component stays the same. This reverses the direction of the $\mathbf{B}$ -field but has no influence on the $\mathbf{E}$ -field generated by flowing charges.

The complex conjugation on the right-hand side of (4.306) has the same origin as in the transformation law (4.227) of the complex scalar field. The operation of charge conjugation is performed by exchanging the sign of all charges without changing their direction of flow. Then both $\mathbf{E}$ and $\mathbf{B}$ change their directions. Hence

$$A^\mu(x) \xrightarrow{C} A'^\mu_C(x) = -A^\mu(x). \quad (4.307)$$

In general, the vector field could be transformed as

$$A^\mu(x) \xrightarrow{C} A'^\mu_C(x) = \eta_C A^\mu(x), \quad (4.308)$$

with $\eta_C = \pm 1$. The fact that the electromagnetic field has $\eta_C = -1$ means that it is odd under charge conjugation.

4.8 Plane-Wave Solutions of Maxwell's Equations

The plane-wave solutions of the field equations (4.245) are direct extensions of Eqs. (4.180) and (4.181):

$$f_{\mathbf{k}}^\mu(\mathbf{x}, t) = \frac{1}{\sqrt{2V k^0}} \epsilon^\mu(\mathbf{k}, \lambda) e^{-ikx}, \quad f_{\mathbf{k}}^{\mu*} = \frac{1}{\sqrt{2V k^0}} \epsilon^{\mu*}(\mathbf{k}, \lambda) e^{ikx}, \quad (4.309)$$

or

$$f_{\mathbf{k}}^\mu(\mathbf{x}, t) = \epsilon^\mu(\mathbf{k}, \lambda) e^{-ikx}, \quad f_{\mathbf{k}}^{\mu*} = \epsilon^{\mu*}(\mathbf{k}, \lambda) e^{ikx}, \quad (4.310)$$

with the momentum on the mass shell with $M = 0$, the so-called *light cone*. The momentum-dependent four-vectors $\epsilon^\mu(\mathbf{k}, \lambda)$ specify the polarization of the plane electromagnetic wave. The label λ counts the different polarization states. In the Lorenz gauge, the vector potential must have a vanishing four divergence (4.252), implying the condition

$$k_\mu \epsilon^\mu(\mathbf{k}, \lambda) = 0. \quad (4.311)$$

Being solutions of the wave equations, there is a further restricted gauge freedom (4.255). We may add to the solutions $f_{\mathbf{k}}^\mu(\mathbf{x}, t)$ or $f_{\mathbf{k}}^{\mu*}(\mathbf{x}, t)$ the total gradient of a function $\Lambda(x)$ which is itself a plane wave $\Lambda(x) = e^{-ikx}$ with $k^2=0$, thus solving also the Klein-Gordon equation. The total gradient adds to the polarization vector a term proportional to the four-momentum k^μ :

$$\epsilon^\mu(\mathbf{k}, \lambda) \rightarrow \epsilon'^\mu(\mathbf{k}, \lambda) = \epsilon^\mu(\mathbf{k}, \lambda) + k^\mu \Lambda(\mathbf{k}, \lambda). \quad (4.312)$$

By choosing

$$\Lambda(\mathbf{k}, \lambda) = -\frac{1}{\mathbf{k}^2} \mathbf{k} \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda), \quad (4.313)$$

the spatial part of the polarization vector $\epsilon'^\mu(\mathbf{k}, \lambda)$ acquires the property

$$\mathbf{k} \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda) = 0, \quad (4.314)$$

which is the Coulomb gauge (4.260) for the polarization vector.

We can also choose

$$\Lambda(\mathbf{k}, \lambda) = -\frac{1}{k^0} \epsilon^0(\mathbf{k}, \lambda), \quad (4.315)$$

and $\epsilon'^\mu(\mathbf{k}, \lambda)$ will satisfy

$$\epsilon^0(\mathbf{k}, \lambda) = 0, \quad (4.316)$$

which is the axial gauge (4.265) for the polarization vector. In Section 4.6.2 we showed that the two gauges coincide for free fields. Here we can see this once more explicitly. The Lorenz gauge (4.311) implies that spatial and time-like components of $\epsilon^\mu(\mathbf{k}, \lambda)$ are related by

$$k^0 \epsilon^0(\mathbf{k}, \lambda) = \mathbf{k} \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda), \quad (4.317)$$

so that the two conditions (4.314) and (4.316) are indeed the same, and

$$\epsilon^\mu(\mathbf{k}, \lambda) = \left(\frac{1}{k^0} \mathbf{k} \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda), \boldsymbol{\epsilon}(\mathbf{k}, \lambda) \right). \quad (4.318)$$

Since the four-component vectors $\epsilon^0(\mathbf{k}, \lambda)$ are restricted by two conditions, only two of them can be independent. These will be labeled by $\lambda = \pm 1$ and are constructed as follows:

In the axial gauge with (4.316), we set

$$\epsilon^\mu(\mathbf{k}, \lambda) \equiv (0, \boldsymbol{\epsilon}(\mathbf{k}, \lambda)), \quad (4.319)$$

and impose on the spatial part the Coulomb gauge property (4.314). This equation is solved by two polarization vectors orthogonal to the spatial momentum $\mathbf{k}$. These are defined uniquely by the following consideration: If $\mathbf{k}$ points in the z -direction, then the two vectors $\boldsymbol{\epsilon}(\mathbf{k}, \pm 1)$ coincide with the eigenvectors $\boldsymbol{\epsilon}(\pm 1)$ of the 3×3 - matrix L_3 of the rotation group in Eq. (4.54), with eigenvalues ± 1 . There are three eigenvectors $\boldsymbol{\epsilon}(\lambda)$ ($\lambda = 1, 0, -1$) which are determined by the equations

$$L_3 \boldsymbol{\epsilon}(\lambda) = \lambda \boldsymbol{\epsilon}(\lambda), \quad \lambda = 1, 0, -1. \quad (4.320)$$

The result is

$$\boldsymbol{\epsilon}(\pm 1) = \mp \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix}, \quad \boldsymbol{\epsilon}(0) = -\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (4.321)$$

The opposite signs of $\epsilon(\pm 1)$ are chosen to comply with the so-called *Condon-Shortley phase convention*³ to be discussed in detail in Subsection 4.18.3 (see p. 356 and Fig. 4.3). They ensure that the 3×3 raising and lowering matrices formed from the 3×3 spatial submatrices of the generators (4.55) and (4.56),

$$L_{\pm} = L_1 \pm iL_2 = \begin{pmatrix} 0 & 0 & \mp 1 \\ 0 & 0 & -i \\ \pm 1 & i & 0 \end{pmatrix}, \quad (4.322)$$

have the positive matrix elements

$$L_+ \epsilon(-1) = \sqrt{2} \epsilon(0), \quad L_+ \epsilon(0) = \sqrt{2} \epsilon(+1), \quad (4.323)$$

$$L_- \epsilon(+1) = \sqrt{2} \epsilon(0), \quad L_- \epsilon(0) = \sqrt{2} \epsilon(-1). \quad (4.324)$$

The vectors $\epsilon(\pm 1)$ and $\epsilon(0)$ are the so-called *spherical components* of the three-dimensional unit vectors:

$$\epsilon_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \epsilon_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \epsilon_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (4.325)$$

related by

$$\epsilon(\pm 1) \equiv \mp \frac{1}{\sqrt{2}} (\epsilon_1 \pm i\epsilon_2). \quad (4.326)$$

Together with the unit vector

$$\epsilon(0) = \epsilon_3, \quad (4.327)$$

they form a basis of the unitary spin-1 representation of the rotation group.

In order to obtain the polarization vectors $\epsilon(\mathbf{k}, \pm 1)$ for momenta in an arbitrary direction, we must rotate $\epsilon(\pm 1)$ into the direction $\hat{\mathbf{k}}$. We shall use the rotation matrix⁴

$$R(\theta, \phi) = e^{-i\phi L_3} e^{-i\theta L_2} = \begin{pmatrix} \cos \theta \cos \phi & -\sin \phi & \sin \theta \cos \phi \\ \cos \theta \sin \phi & \cos \phi & \sin \theta \sin \phi \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}, \quad (4.328)$$

with the spherical angles

$$\theta \in [0, \pi), \quad \phi \in [0, 2\pi), \quad (4.329)$$

to arrive at a momentum direction

$$\hat{\mathbf{k}} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}, \quad (4.330)$$

³E.U. Condon and G.H. Shortley, *Theory of Atomic Spectra*, Cambridge University Press, New York, 1935.

⁴Some authors prefer to use the rotation matrix $R(\theta, \phi) = e^{-i\phi L_3} e^{-i\theta L_2} e^{i\phi L_3}$.

with the polarization vectors

$$\boldsymbol{\epsilon}(\mathbf{k}, \pm 1) = \mp \frac{1}{\sqrt{2}} \begin{pmatrix} \cos \theta \cos \phi \mp i \sin \phi \\ \cos \theta \sin \phi \pm i \cos \phi \\ -\sin \theta \end{pmatrix}. \quad (4.331)$$

Together with the third vector

$$\boldsymbol{\epsilon}(\mathbf{k}, 0) \equiv \hat{\mathbf{k}}, \quad (4.332)$$

for which there is no electromagnetic plane wave, they form a representation of spin 1 that diagonalizes $\mathbf{L}^2$ and the *helicity matrix* $H = \hat{\mathbf{k}} \cdot \mathbf{L}$ formed from the matrices $\mathbf{L}$ of Eq. (4.57). The labels $\lambda = \pm 1$ specify the two helicities of a light wave running along $\hat{\mathbf{k}}$. They are observed in the form of right and left circularly polarized light.

Since the spatial polarization vectors (4.331) are orthogonal to the momentum vector $\mathbf{k}$, they are also referred to as *transverse polarization vectors*, and the Coulomb gauge condition (4.314) is also called *transverse gauge condition*.

The spatial polarization vectors $\boldsymbol{\epsilon}(\mathbf{k}, \lambda)$ are orthonormal:

$$\boldsymbol{\epsilon}(\mathbf{k}, \lambda) \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda')^* = \delta_{\lambda\lambda'}, \quad \lambda, \lambda' = 0, \pm 1, \quad (4.333)$$

and they are transversely complete:

$$\sum_{\lambda=-1,1} \epsilon^i(\mathbf{k}, \lambda) \epsilon^j(\mathbf{k}, \lambda)^* = P_T^{ij}(\mathbf{k}) \equiv \delta^{ij} - \frac{k^i k^j}{\mathbf{k}^2}. \quad (4.334)$$

The matrix $P_T^{ij}(\mathbf{k})$ is a projection into a direction transverse to $\mathbf{k}$. It satisfies the defining property of a projection matrix

$$P_T^{ij}(\mathbf{k}) P_T^{ik}(\mathbf{k}) = P_T^{jk}(\mathbf{k}). \quad (4.335)$$

The contribution of $\lambda = 0$ to the polarization sum (4.334) is the longitudinal projection

$$\sum_{\lambda=0} \epsilon^i(\mathbf{k}, \lambda) \epsilon^j(\mathbf{k}, \lambda)^* = P_L^{ij}(\mathbf{k}) \equiv \epsilon^i(\mathbf{k}, 0) \epsilon^j(\mathbf{k}, 0)^* = \frac{k^i k^j}{\mathbf{k}^2}. \quad (4.336)$$

The orthonormality (4.333) goes over to the four-dimensional polarization vectors in the axial gauge (4.319) as follows:

$$\epsilon_\mu(\mathbf{k}, \lambda) \epsilon^\mu(\mathbf{k}, \lambda')^* = -\delta_{\lambda\lambda'}, \quad \lambda, \lambda' = 0, \pm 1. \quad (4.337)$$

These vectors have the reflection property

$$\epsilon^\mu(\mathbf{k}, \lambda) = \epsilon^\mu(\mathbf{k}, -\lambda)^*, \quad (4.338)$$

which follows from the fact that $\mathbf{k} \rightarrow -\mathbf{k}$ corresponds to $\theta \rightarrow \pi - \theta$, $\phi \rightarrow \phi + \pi \pmod{2\pi}$.

In four dimensions, the polarization sum over the two helicities in (4.334) leads to the following 4×4 polarization tensor:

$$P_T^{\mu\nu}(\mathbf{k}) = \sum_{\lambda=\pm 1} \epsilon^\mu(\mathbf{k}, \lambda) \epsilon^\nu(\mathbf{k}, \lambda)^*. \quad (4.339)$$

In the axial gauge where the polarization vectors have the form (4.319), this reads

$$\begin{aligned} P_T^{\mu\nu}(\mathbf{k}) &= \sum_{\lambda=\pm 1} \epsilon^\mu(\mathbf{k}, \lambda) \epsilon^\nu(\mathbf{k}, \lambda)^* = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & P_T^{ij}(\mathbf{k}) \end{array} \right)^{\mu\nu} \\ &= \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \delta^{ij} - k^i k^j / \mathbf{k}^2 \end{array} \right)^{\mu\nu} = -g^{\mu\nu} + \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -k^i k^j / \mathbf{k}^2 \end{array} \right)^{\mu\nu}. \end{aligned} \quad (4.340)$$

This is a 4×4 -matrix projecting into a purely spatial two-dimensional subspace transverse to the vector $\mathbf{k}$. It contains only purely spatial nonzero components $P_T^{ij}(\mathbf{k})$. There is also an associate longitudinal projection tensor which reads in the Lorenz gauge (4.317)

$$P_L^{\mu\nu}(\mathbf{k}) = \epsilon^\mu(\mathbf{k}, 0) \epsilon^\nu(\mathbf{k}, 0)^* = \left(\begin{array}{c|c} 1 & 0 \\ \hline 1 & P_L^{ij}(\mathbf{k}) \end{array} \right)^{\mu\nu} = \left(\begin{array}{c|c} 1 & 0 \\ \hline 1 & k^i k^j / \mathbf{k}^2 \end{array} \right)^{\mu\nu}. \quad (4.341)$$

The projection is obviously noncovariant since it lends a special significance to the zeroth component of the electromagnetic vector field. To exhibit the noncovariance, it is useful to introduce a fixed timelike unit vector

$$\eta^\mu \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (4.342)$$

We also define a purely spacelike unit vector orthogonal to it, pointing along the direction of $\mathbf{k}$:

$$\bar{k}^\mu \equiv \begin{pmatrix} 0 \\ \hat{\mathbf{k}} \end{pmatrix}. \quad (4.343)$$

This can be expressed in terms of η^μ and the momentum vector k^μ as follows:

$$\bar{k}^\mu \equiv \frac{k^\mu - (k\eta)\eta^\mu}{\sqrt{(k\eta)^2 - k^2}}. \quad (4.344)$$

The fixed vector eliminates the zeroth component of k^μ , no matter whether it is on-shell or off-shell.

We readily show that the polarization sum (4.340) can be rewritten as

$$\begin{aligned} P_T^{\mu\nu}(k) &\equiv -g^{\mu\nu} + \eta^\mu \eta^\nu - \bar{k}^\mu \bar{k}^\nu = -g^{\mu\nu} + \eta^\mu \eta^\nu + P_L^{\mu\nu}(k) \\ &= -g^{\mu\nu} - \frac{k^\mu k^\nu}{(k\eta)^2 - k^2} + k\eta \frac{k^\mu \eta^\nu + k^\nu \eta^\mu}{(k\eta)^2 - k^2} - k^2 \frac{\eta^\mu \eta^\nu}{(k\eta)^2 - k^2}. \end{aligned} \quad (4.345)$$

In the Lorenz gauge it is useful to introduce, in addition to the three four-dimensional polarization vectors (4.318), also an extra fourth vector that points parallel to the four-momentum of the particle. It will be called *scalar polarization vector*, and denoted by

$$\epsilon^\mu(\mathbf{k}, s) \equiv k^\mu = (\omega_{\mathbf{k}}, \mathbf{k}). \quad (4.346)$$

The associated vector field corresponds to a pure gauge degree of freedom, since in x -space it has the form $\partial^\mu \Lambda$. As such, it transforms under an extra independent and irreducible representation of the Lorentz group describing a scalar particle degree of freedom. Thus, it certainly does not contribute to the gauge-invariant electromagnetic action and is no longer part of the vector particle.

One may define scalar products by complete analogy with those for scalar field in Eqs. (4.177), except that they contain an extra contraction of the polarization indices:

$$(f_{\mathbf{p}'}, f_{\mathbf{p}}) \equiv \int d^3x f_{\mathbf{p}'}^{\mu*}(\mathbf{x}, t) i \overleftrightarrow{\partial}_0 f_{\mu\mathbf{p}}(\mathbf{x}, t), \quad (4.347)$$

with obvious definitions between positive- and negative-frequency solutions, $f_{\mathbf{p}'}(t)$ and $f_{\mathbf{p}}^*(t)$, and between two negative-frequency solutions $f_{\mathbf{p}'}^*(t)$.

4.9 Gravitational Field

The gravitational field is carried by a varying metric $g_{\mu\nu}(x)$ in spacetime. Its presence manifests itself in a local dependence of the invariant distance between events:

$$(ds)^2 = g_{\mu\nu}(x) dx^\mu dx^\nu. \quad (4.348)$$

The distances in such a spacetime no longer satisfy the axioms of *Minkowski geometry* since the spacetime can have a local curvature. According to the *equivalence principle* of general relativity, the motion of point particles is independent of their mass. All point particles follow the lines of shortest distance in this geometry, the so-called *geodesics*.

The generation of the gravitational field is governed by a complicated nonlinear theory and deserves a detailed treatment on its own, not to be elaborated in this text. In the present context we merely state a few relevant facts about a very weak gravitational field running through empty spacetime. It may be described by a small deviation of the metric $g_{\mu\nu}(x)$ from the Minkowski metric (4.27), which in this context will be denoted by $\eta_{\mu\nu}$, for better distinction. The deviation is

$$h_{\mu\nu}(x) \equiv g_{\mu\nu}(x) - \eta_{\mu\nu}. \quad (4.349)$$

Note that, while the metric depends linearly on $h_{\mu\nu}(x)$,

$$g_{\mu\nu}(x) \equiv \eta_{\mu\nu}(x) + h_{\mu\nu}, \quad (4.350)$$

the tensor $g^{\mu\nu}$, being the inverse of $g_{\mu\nu}$, has a nonlinear expansion

$$g^{\mu\nu}(x) \equiv \eta^{\mu\nu}(x) - h^{\mu\nu} + h^\mu{}_\lambda h^{\lambda\nu} - h^\mu{}_\lambda h^\lambda{}_\kappa h^{\kappa\nu} + \mathcal{O}(h^3). \quad (4.351)$$

4.9.1 Action and Field Equations

The action of the field $h_{\mu\nu}(x)$ is obtained from the famous *Einstein-Hilbert action* of the gravitational field

$$\overset{\text{f}}{\mathcal{A}} = -\frac{1}{2\kappa} \int d^4x \sqrt{-g} R, \quad (4.352)$$

where R is the *curvature scalar* of spacetime, and κ is related to the famous Newton gravitational constant

$$G_N \approx 6.673 \cdot 10^{-8} \text{ cm}^3 \text{ g}^{-1} \text{ s}^{-2} \quad (4.353)$$

by

$$\frac{1}{\kappa} = \frac{c^3}{8\pi G_N}. \quad (4.354)$$

A natural length scale of gravitational physics is the *Planck length*, which can be formed from a combination of Newton's gravitational constant (4.353), the light velocity $c \approx 3 \times 10^{10} \text{ cm/s}$, and Planck's constant $\hbar \approx 1.05459 \times 10^{-27}$:

$$l_P = \left(\frac{c^3}{G_N \hbar} \right)^{-1/2} \approx 1.615 \times 10^{-33} \text{ cm}. \quad (4.355)$$

This is the Compton wavelength $l_P \equiv \hbar/m_P c$ associated with the Planck mass defined by

$$m_P = \left(\frac{c\hbar}{G_N} \right)^{1/2} \approx 2.177 \times 10^{-5} \text{ g} = 1.22 \times 10^{22} \text{ MeV}/c^2. \quad (4.356)$$

The constant $1/\kappa$ in the action (4.352) can be expressed in terms of the Planck length as

$$\frac{1}{\kappa} = \frac{\hbar}{8\pi l_P^2}. \quad (4.357)$$

The curvature scalar R is formed from the *Riemann curvature tensor* $R_{\mu\nu\lambda}{}^\kappa$ by the contraction $R = R_\mu{}^\mu \equiv g^{\mu\nu} R_{\mu\nu}$ with the *Ricci tensor* $R_{\nu\lambda} \equiv R_{\mu\nu\lambda}{}^\mu$. The symbol g denotes the determinant of the metric tensor $g_{\mu\nu}$ which makes the volume element $\sqrt{-g}d^4x$ invariant under coordinate transformations. The curvature tensor may be written as a covariant curl [10]

$$R_{\mu\nu\lambda}{}^\kappa \equiv (\partial_\mu \Gamma_\nu - \partial_\nu \Gamma_\mu)_\lambda{}^\kappa - [\Gamma_\mu, \Gamma_\nu]_\lambda{}^\kappa \quad (4.358)$$

of the matrices $(\Gamma_\mu)_\nu{}^\lambda$ formed from the *Christoffel connection*

$$(\Gamma_\mu)_\nu{}^\lambda \equiv \Gamma_{\mu\nu}{}^\lambda = \frac{1}{2} g^{\lambda\kappa} (\partial_\mu g_{\nu\kappa} + \partial_\nu g_{\mu\kappa} - \partial_\kappa g_{\mu\nu}), \quad (4.359)$$

in terms of which it reads

$$R_{\mu\nu\lambda}{}^\kappa \equiv \partial_\mu \Gamma_{\nu\lambda}{}^\kappa - \partial_\nu \Gamma_{\mu\lambda}{}^\kappa - \Gamma_{\mu\lambda}{}^\delta \Gamma_{\nu\delta}{}^\kappa + \Gamma_{\mu\lambda}{}^\delta \Gamma_{\nu\delta}{}^\kappa. \quad (4.360)$$

Using this the integrand in (4.352) can be replaced by

$$\sqrt{-g}R = \partial_\lambda \left[(g^{\mu\nu} \sqrt{-g}) (\Gamma_{\mu\nu}{}^\lambda - \delta_\mu{}^\lambda \Gamma_{\nu\kappa}{}^\kappa) \right] + \sqrt{-g} g^{\mu\nu} (\Gamma_{\mu\lambda}{}^\kappa \Gamma_{\nu\kappa}{}^\lambda - \Gamma_{\mu\nu}{}^\lambda \Gamma_{\lambda\kappa}{}^\kappa). \quad (4.361)$$

The first term is a pure divergence, and it may be omitted in the action (4.352), keeping only the second term. After setting $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$, and inserting $g^{\mu\nu}$ from (4.351), we calculate

$$\begin{aligned} \sqrt{-g} &= e^{(1/2)\text{tr} \log(-\eta_{\mu\nu} - h_{\mu\nu})} = e^{(1/2)\text{tr} \log(-\eta_{\mu\nu})} e^{(1/2)h_\mu{}^\mu - (1/4)h_\mu{}^\nu h_\nu{}^\mu + \dots} \\ &= 1 + \frac{1}{2}h_\mu{}^\mu - \frac{1}{4}h_\mu{}^\nu h_\nu{}^\mu + \frac{1}{8}(h_\mu{}^\mu)^2 + \dots \end{aligned} \quad (4.362)$$

We also expand the Christoffel symbols to linear order in $h_{\mu\nu}$,

$$\Gamma_{\mu\nu}{}^\lambda \approx \gamma_{\mu\nu}{}^\lambda \equiv \frac{1}{2} (\partial_\mu h_\nu{}^\lambda + \partial_\nu h_\mu{}^\lambda - \partial^\lambda h_{\mu\nu}). \quad (4.363)$$

Inserting this into (4.360), we find the linear contributions to the curvature tensor (4.360):

$$R_{\mu\nu\lambda\kappa} \approx \frac{1}{2} [\partial_\mu \partial_\lambda h_{\nu\kappa} - \partial_\nu \partial_\kappa h_{\mu\lambda} - (\mu \leftrightarrow \nu)] + \dots \quad (4.364)$$

For the *Ricci tensor* defined by the contraction

$$R_\mu{}^\kappa \equiv g^{\nu\lambda} R_{\mu\nu\lambda}{}^\kappa \quad (4.365)$$

this amounts to

$$R_{\mu\kappa} \approx -\frac{1}{2} (\partial^2 h_{\mu\kappa} - \partial_\mu \partial_\lambda h_{\lambda\kappa} - \partial_\kappa \partial_\lambda h_{\lambda\mu} + \partial_\mu \partial_\kappa h) + \dots \quad (4.366)$$

The ensuing *scalar curvature* $R \equiv R_\mu{}^\mu$ starts out like⁵

$$R \approx \partial^2 h - \partial_\mu \partial_\nu h^{\mu\nu} + \dots \equiv \partial^2 h^s + \dots, \quad (4.367)$$

where h^s is the result of applying the scalar projection operator $P_{\mu\nu,\lambda\kappa}^s$ of Eq. (4G.6) to $h^{\lambda\kappa}$ and taking the trace

$$h^s \equiv \partial^2 h - \partial_\mu \partial_\nu h^{\mu\nu} = \eta^{\mu\nu} P_{\mu\nu,\lambda\kappa}^s h^{\lambda\kappa}. \quad (4.368)$$

The quadratic part of the action is found by inserting (4.363) into Eq. (4.361), which contributes to R in (4.367) a quadratic term

$$\Delta^{(2)} R = -g^{\mu\nu} (\Gamma_{\mu\lambda}{}^\kappa \Gamma_{\nu\kappa}{}^\lambda - \Gamma_{\mu\nu}{}^\lambda \Gamma_{\lambda\kappa}{}^\kappa). \quad (4.369)$$

⁵The omitted quadratic parts in $h_{\mu\nu}$ have been given in Appendix B of Ref. [16].

The corresponding quadratic action governing free gravitational waves is

$$\mathcal{A}^{(2)} = -\frac{1}{2\kappa} \int d^4x \Delta^{(2)} R. \quad (4.370)$$

Explicitly this reads

$$\begin{aligned} \mathcal{A}^{(2)} \approx & -\frac{1}{8\kappa} \int d^4x \left\{ (\partial_\mu h_\nu{}^\lambda + \partial_\nu h_\mu{}^\lambda - \partial^\lambda h_{\mu\nu})(\partial^\nu h_\lambda{}^\mu + \partial_\lambda h^{\mu\nu} - \partial^\mu h^\nu{}_\lambda) \right. \\ & \left. - (\partial_\mu h^{\mu\lambda} + \partial_\mu h^{\mu\lambda} - \partial^\lambda h_\mu{}^\mu)(\partial_\nu h_\lambda{}^\nu + \partial_\lambda h_\nu{}^\nu - \partial^\nu h_{\nu\lambda}) \right\}. \end{aligned} \quad (4.371)$$

Using the symmetry of $h_{\mu\nu}$, the right-hand side can be rearranged to

$$\mathcal{A}^{(2)} = -\frac{1}{8\kappa} \int d^4x (h^{\nu\lambda} \partial^2 h_{\nu\lambda} + 2\partial^\mu h_{\mu\nu} \partial_\lambda h^{\nu\lambda} - 2h \partial_\mu \partial_\nu h^{\mu\nu} - h \partial^2 h), \quad (4.372)$$

where h is defined to be the trace of the tensor $h_{\mu\nu}$, i.e., $h \equiv h_\lambda{}^\lambda$. An alternative way of writing this is

$$\mathcal{A} = -\frac{1}{8\kappa} \int d^4x h_{\mu\nu} \epsilon^{\lambda\mu\kappa\sigma} \epsilon_\lambda{}^{\nu\tau\delta} \partial_\kappa \partial_\tau h_{\sigma\delta}. \quad (4.373)$$

The equivalence can be verified with the help of the identity

$$\epsilon^{\lambda\mu\kappa\sigma} \epsilon_\lambda{}^{\nu\tau\delta} = -\eta^{\mu\nu} \eta^{\kappa\tau} \eta^{\sigma\delta} - \eta^{\mu\tau} \eta^{\kappa\delta} \eta^{\sigma\nu} - \eta^{\mu\delta} \eta^{\kappa\nu} \eta^{\sigma\tau} + \eta^{\mu\nu} \eta^{\kappa\delta} \eta^{\sigma\tau} + \eta^{\mu\tau} \eta^{\kappa\nu} \eta^{\sigma\delta} + \eta^{\mu\delta} \eta^{\kappa\tau} \eta^{\sigma\nu}. \quad (4.374)$$

A further useful way of writing the field action (4.373) is obtained by using the *Einstein tensor*

$$G^{\mu\nu} \equiv R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R, \quad (4.375)$$

whose linear approximation reads

$$\begin{aligned} G^{\mu\kappa} &= R^{\mu\kappa} - \frac{1}{2} g^{\mu\kappa} R \\ &\approx -\frac{1}{2} (\partial^2 h^{\mu\kappa} - \partial^\mu \partial_\lambda h^{\lambda\kappa} - \partial^\kappa \partial_\lambda h^{\lambda\mu} + \partial^\mu \partial^\kappa h) + \frac{1}{2} \eta^{\mu\kappa} (\partial^2 h - \partial_\nu \partial_\lambda h^{\nu\lambda}), \end{aligned} \quad (4.376)$$

with a trace $G \equiv G_\mu{}^\mu = -R = -(\partial^2 h - \partial_\mu \partial_\nu h^{\mu\nu})$. This may be written as a four-dimensional double curl:

$$G^{\mu\nu} \approx -\frac{1}{4} \epsilon^{\lambda\mu\kappa\sigma} \epsilon_\lambda{}^{\nu\tau\delta} \partial_\kappa \partial_\tau h_{\sigma\delta}, \quad (4.377)$$

from which we see that the action (4.373) becomes simply

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \frac{1}{4\kappa} \int d^4x h_{\mu\nu} G^{\mu\nu}. \quad (4.378)$$

The Einstein tensor plays a similar role in gravity as the dual field tensor $\tilde{F}_{\mu\nu}$ does in electromagnetism [recall (4.238)]. First, being a double-curl (4.377), it trivially satisfies a Bianchi identity

$$\partial_\mu G^{\mu\nu} = 0 \quad (4.379)$$

for any smooth single-valued field $h_{\mu\nu}(x)$, i.e., any field $h_{\mu\nu}(x)$ which satisfies the integrability condition $(\partial_\lambda \partial_\kappa - \partial_\kappa \partial_\lambda)h_{\mu\nu}(x) = 0$. Second, it is invariant under local gauge transformations [just as (4.239) is under (4.250)]:

$$h_{\mu\nu}(x) \rightarrow h_{\mu\nu}(x) + \partial_\mu \Lambda_\nu(x) + \partial_\nu \Lambda_\mu(x). \quad (4.380)$$

These are the linearized versions of Einstein's *general coordinate transformations*:

$$x^\mu \rightarrow x^\mu + \Lambda^\mu(x). \quad (4.381)$$

As a consequence of this invariance, the symmetric tensor $h_{\mu\nu}(x)$ carries only 6 instead of 10 independent physical components.

The free-field equations are obtained by variation of $\mathcal{A}^f$ with respect to $h_{\mu\nu}(x)$:

$$\frac{\delta \mathcal{A}^f}{\delta h_{\mu\nu}(x)} = \frac{1}{2\kappa} G^{\mu\nu}(x) = 0. \quad (4.382)$$

Thus, for a free gravitational field, the Einstein tensor vanishes, and so does the Ricci tensor $R_{\mu\nu} = G_{\mu\nu} - \frac{1}{2}g_{\mu\nu}G$:

$$R_{\mu\nu}(x) = 0. \quad (4.383)$$

In the presence of masses, the field equation (4.382) will be modified. After adding an action $\mathcal{A}^m$ of the matter fields to the field action $\mathcal{A}^f$, the right-hand side will be shown in Eq. (5.71) to become equal to the tensor $\overset{m}{T}{}^{\mu\nu}(x) = -2\sqrt{-g}^{-1}\delta \mathcal{A}^m / \delta g_{\mu\nu}(x)$. This is the total symmetric energy-momentum tensor of the material particles to be derived in (5.66). The vanishing of the variation of the total action

$$\mathcal{A}^{\text{tot}} = \mathcal{A}^f + \mathcal{A}^m = 0 \quad (4.384)$$

extends therefore the field equation (4.382) by a source term due to matter:

$$G_{\mu\nu}(x) = \kappa \overset{m}{T}{}^{\mu\nu}(x) \quad (4.385)$$

4.9.2 Lorentz Transformation Properties of Gravitational Field

Under Lorentz transformations, $h_{\mu\nu}(x)$ behaves of course like a tensor. In a straightforward generalization of the transformation law (4.290) we may immediately write

$$h'^{\mu\nu}(x) = \Lambda^\mu{}_\lambda \Lambda^\nu{}_\kappa h^{\lambda\kappa}(\Lambda^{-1}x). \quad (4.386)$$

This transformation can be generated by analogy with (4.292) as follows:

$$h^{\mu\nu}(x) \xrightarrow{\Lambda} h'^{\mu\nu}(x) = \hat{D}(\Lambda) \Lambda^\mu_\lambda \Lambda^\nu_\kappa h^{\lambda\kappa}(x) \equiv e^{-i\frac{1}{2}\omega_{\lambda\kappa} \hat{J}^{\lambda\kappa}} h^{\mu\nu}(x), \quad (4.387)$$

with the parameters $\omega_{\mu\nu}$ specified in (4.70) and (4.71), and the operator

$$\hat{J}^{\lambda\kappa} \equiv L^{\lambda\kappa} \times 1 \times \hat{1} + 1 \times L^{\lambda\kappa} \times \hat{1} + 1 \times 1 \times \hat{L}^{\lambda\kappa}. \quad (4.388)$$

This is a direct generalization of the total angular momentum operator (4.293). The commutation rules between the generators $\hat{J}^{\mu\nu}$ are of course given by (4.295), as in the case of the vector potential.

4.9.3 Other Symmetries of Gravitational Action

Just as the scalar and electromagnetic actions, the gravitational action (4.378) is invariant under extensions of the Lorentz group.

4.9.4 Translations of Gravitational Field

Under spacetime translations (4.185), the gravitational field transforms like a scalar field in (4.187) and a vector field in (4.298):

$$h'^{\mu\nu}(x) = h^{\mu\nu}(x - a). \quad (4.389)$$

The combinations of translations and Lorentz transformations

$$x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu \quad (4.390)$$

form the Poincaré group (4.189). Under these the fields transform like

$$h'^{\mu\nu}(x) = \Lambda^\mu_\lambda \Lambda^\nu_\kappa h^{\lambda\kappa}(\Lambda^{-1}(x - a)), \quad (4.391)$$

leaving the action (4.378) invariant.

As in the scalar and vector cases (4.193) and (4.301), we can of course generate all Poincaré transformations on the field with the help of differential operators:

$$h^{\mu\nu}(x) \longrightarrow h'^{\mu\nu}(x) = \hat{D}(a) \hat{D}(\Lambda) \Lambda^\mu_\lambda \Lambda^\nu_\kappa h^{\lambda\kappa}(x) \equiv e^{ia^\mu \hat{P}_\mu / \hbar} e^{-i\frac{1}{2}\omega_{\lambda\kappa} \hat{J}^{\lambda\kappa}} h^{\mu\nu}(x), \quad (4.392)$$

with the parameters $\omega_{\mu\nu}$ specified in (4.70), (4.71).

4.9.5 Space Inversion, Time Reversal, and Charge Conjugation of Gravitational Field

Since $h_{\mu\nu}(x)$ determines the invariant distances in space via (4.348) and (4.350), it transforms like $dx_\mu dx_\nu$ under space inversion and time reversal. Under charge conjugation, it is invariant.

Thus we have, under space inversion,

$$h^{\mu\nu}(x) \xrightarrow{P} h'^{\mu\nu}_P(x) = \tilde{h}^{\mu\nu}(\tilde{x}), \quad (4.393)$$

where the tilde reverses the sign of $h^{\mu\nu}(x)$ for each spatial index, whereas under time reversal, the field $h^{\mu\nu}$ transforms like

$$h^{\mu\nu}(x) \xrightarrow{T} h'^{\mu\nu}_T(x) = \tilde{h}^{\mu\nu}(x_T). \quad (4.394)$$

In principle, an arbitrary tensor field $t_{\mu\nu}(x)$ has two possible transformation behaviors under space inversion:

$$t^{\mu\nu}(x) \xrightarrow{P} t'^{\mu\nu}_P(x) = \eta_P \tilde{t}^{\mu\nu}(\tilde{x}), \quad (4.395)$$

with $\eta_P = \pm 1$, where in the case $\eta_P = -1$ the field $t^{\mu\nu}(x)$ is called a *pseudotensor field*. The gravitational field $h^{\mu\nu}(x)$, however, is definitely a tensor field. This follows from its metric nature and the distance definition in (4.348), (4.350).

Similarly, the phase factor of a tensor field $t^{\mu\nu}(x)$ arising from time reversal could in principle be

$$t^{\mu\nu}(x) \xrightarrow{T} t'^{\mu\nu}_T(x) = \eta_T \tilde{t}^{\mu\nu}(x_T), \quad (4.396)$$

with an arbitrary phase factor η_T . For an observable real field, however, only $\eta_T = \pm 1$ are admissible. The gravitational field has $\eta_T = 1$ to preserve the definition of the distance in (4.348), (4.350) under space inversion.

Under charge conjugation, the gravitational interactions are invariant, so that

$$h^{\mu\nu}(x) \xrightarrow{C} h'^{\mu\nu}_C(x) = h^{\mu\nu}(x). \quad (4.397)$$

In general, a tensor field $t_{\mu\nu}(x)$ could transform like

$$t^{\mu\nu}(x) \xrightarrow{C} t'^{\mu\nu}_C(x) = \eta_C t^{\mu\nu}(x), \quad (4.398)$$

with $\eta_C = \pm 1$.

4.9.6 Gravitational Plane Waves

To discuss the properties of gravitational waves we remove the gauge freedom (4.380) by fixing a specific gauge, the so-called *Hilbert gauge*:

$$\partial_\mu h^{\mu\nu}(x) = \frac{1}{2} \partial^\nu h_\lambda{}^\lambda(x). \quad (4.399)$$

It corresponds to the Lorenz gauge of electromagnetism [recall (4.252)].

The Hilbert gauge can always be achieved by a gauge transformation. If $h_{\mu\nu}(x)$ is not in this gauge, we simply perform the transformation (4.380) and determine $\Lambda_\mu(x)$ from the differential equation

$$-\partial^2 \Lambda^\nu(x) = \partial_\mu h^{\mu\nu}(x) - \frac{1}{2} \partial^\nu h(x). \quad (4.400)$$

The gauge transformation (4.380) can be used to fix another property of $h_{\mu\nu}$. By applying it to the trace $h(x) \equiv h_\mu{}^\mu(x)$, using the special gauge function $\Lambda_\nu = \partial_\nu \Lambda$, we find

$$h(x) \rightarrow h'(x) = h(x) + 2\partial^2 \Lambda(x). \quad (4.401)$$

This can be used to arrive at a traceless field $h_{\mu\nu}(x)$. If $h(x)$ is nonzero, $h'(x)$ vanishes if we choose

$$\Lambda(x) = -(1/2\partial^2)h(x). \quad (4.402)$$

It is useful to introduce the field

$$\phi_{\mu\nu}(x) \equiv h_{\mu\nu}(x) - \frac{1}{2}\eta_{\mu\nu}h(x). \quad (4.403)$$

With this, the Einstein tensor (4.376) reads

$$G^{\mu\kappa} \approx -\frac{1}{2}(\partial^2 \phi^{\mu\kappa} - \partial^\mu \partial_\lambda \phi^{\lambda\kappa} - \partial^\kappa \partial_\lambda \phi^{\lambda\mu}) - \frac{1}{2}\eta^{\mu\nu} \partial_\lambda \partial_\kappa \phi^{\lambda\kappa} \quad (4.404)$$

with the trace $G = G_\mu{}^\mu = -\frac{1}{2}(\partial^2 \phi + 2\partial_\mu \partial_\nu \phi^{\mu\nu})$. Under the gauge transformations (4.380), the field $\phi_{\mu\nu}(x)$ changes like

$$\phi^{\mu\nu}(x) \rightarrow \phi^{\mu\nu}(x) + \partial^\mu \Lambda^\nu(x) + \partial^\nu \Lambda^\mu(x) - \eta^{\mu\nu} \partial_\kappa \Lambda^\kappa(x), \quad (4.405)$$

and the Einstein tensor is invariant.

Imposing now the Hilbert gauge condition (4.399), we see that

$$\partial^\nu \phi_{\mu\nu}(x) = 0, \quad (4.406)$$

and the Einstein tensor (4.404) reduces to

$$G_{\mu\nu} = -\frac{1}{2}\partial^2 \phi_{\mu\nu}. \quad (4.407)$$

The free-field equation of motion (4.382) implies a massless Klein-Gordon equation for each field component:⁶

$$-\partial^2 \phi_{\mu\nu}(x) = 0. \quad (4.408)$$

This must be solved in the Hilbert gauge (4.406).

Since the graviton field obeys the zero-mass Klein-Gordon equation (4.408), the plane waves in the field $\phi^{\mu\nu}(x)$ are proportional to e^{-ikx} and e^{ikx} , with k^0 lying on the light cone $k^0 = \omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2}$. These waves are accompanied by symmetric polarization tensors $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ [compare (4.309)]:

$$f_{\mathbf{k}}^{\mu\nu}(\mathbf{x}, t) = \frac{1}{\sqrt{2V k^0}} \epsilon^{\mu\nu}(\mathbf{k}, \lambda) e^{-ikx}, \quad f_{\mathbf{k}}^{\mu\nu*} = \frac{1}{\sqrt{2V k^0}} \epsilon^{\mu\nu*}(\mathbf{k}, \lambda) e^{ikx}. \quad (4.409)$$

⁶Compare Eq. (4.253) for the electromagnetic field in the Lorenz gauge.

In the Hilbert gauge, the polarization tensors $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ satisfy the transversality condition

$$k_\mu \epsilon^{\mu\nu}(\mathbf{k}, \lambda) = 0. \quad (4.410)$$

For a plane wave, we can further perform a gauge transformation (4.405) with functions $\Lambda_\mu(x)$ which satisfy the zero-mass Klein-Gordon equation $\partial^2 \Lambda_\mu(x) = 0$. These are the gauge transformations of the second type that are completely analogous to their electromagnetic versions (4.255). The functions $\Lambda_\mu(x)$ can be chosen to have the plane-wave form

$$\Lambda_\mu(x) = \Lambda_\mu e^{\pm i k x}, \quad \text{with } k^2 = 0. \quad (4.411)$$

The vector Λ_μ is a constant that makes the transformed polarization tensor $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ traceless:

$$\epsilon_\mu{}^\mu(\mathbf{k}, \lambda) = 0. \quad (4.412)$$

It is also chosen to make it axial in the sense analogous to (4.319):

$$\epsilon^{\mu 0}(\mathbf{k}, \lambda) = 0. \quad (4.413)$$

Under a gauge transformation of the second kind, the Fourier transforms $\phi^{\mu\nu}(k)$ of the field $\phi^{\mu\nu}(x)$ receive an additional term

$$\phi^{\mu\nu}(k) \rightarrow \phi^{\mu\nu}(k) + k^\mu \Lambda^\nu + k^\nu \Lambda^\mu - \eta^{\mu\nu} k_\kappa \Lambda^\kappa, \quad (4.414)$$

which does not contribute to any observable quantities.

In principle, there exists ten possibilities of forming symmetric transverse polarization tensors $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ from the transverse polarization vectors (4.318). For their construction we recall the extra vector (4.346). This is the *scalar polarization vector* that points parallel to the four-momentum:

$$\epsilon^\mu(\mathbf{k}, s) \equiv k^\mu. \quad (4.415)$$

This polarization is unphysical since it corresponds to a pure gauge transformation. The gauge condition (4.410) eliminates four of these combinations. The remaining six polarization tensors are constructed from symmetrized tensor products of the transverse polarization vectors (4.331) by forming the combinations:

$$\begin{aligned} \epsilon_H^{\mu\nu}(\mathbf{k}, 2) &\equiv \epsilon_H^\mu(\mathbf{k}, 1) \epsilon_H^\nu(\mathbf{k}, 1), \\ \epsilon_H^{\mu\nu}(\mathbf{k}, 1) &\equiv \frac{1}{\sqrt{2}} [\epsilon_H^\mu(\mathbf{k}, 1) \epsilon_H^\nu(\mathbf{k}, 0) + (\mu \leftrightarrow \nu)], \\ \epsilon_H^{\mu\nu}(\mathbf{k}, 0) &\equiv \frac{1}{\sqrt{6}} [\epsilon_H^\mu(\mathbf{k}, 1) \epsilon_H^\nu(\mathbf{k}, -1) + (\mu \leftrightarrow \nu)] + \frac{2}{\sqrt{6}} \epsilon_H^\mu(\mathbf{k}, 0) \epsilon_H^\nu(\mathbf{k}, 0), \\ \epsilon_H^{\mu\nu}(\mathbf{k}, -1) &\equiv \frac{1}{\sqrt{2}} [\epsilon_H^\mu(\mathbf{k}, -1) \epsilon_H^\nu(\mathbf{k}, 0) + (\mu \leftrightarrow \nu)], \\ \epsilon_H^{\mu\nu}(\mathbf{k}, -2) &\equiv \epsilon_H^\mu(\mathbf{k}, -1) \epsilon_H^\nu(\mathbf{k}, -1), \\ \epsilon_H^{\mu\nu}(\mathbf{k}, s) &\equiv \frac{1}{\sqrt{3}} [\epsilon_H^\mu(\mathbf{k}, 1) \epsilon_H^\nu(\mathbf{k}, -1) + (\mu \leftrightarrow \nu)] - \frac{1}{\sqrt{3}} \epsilon_H^\mu(\mathbf{k}, 0) \epsilon_H^\nu(\mathbf{k}, 0). \end{aligned} \quad (4.416)$$

These combinations are formed with the help of the Clebsch-Gordan coefficients calculated in Appendix 4E and listed in Table 4.2. They couple two spin-one objects symmetrically to five components of spin 2 and one component of spin zero.

$$\begin{aligned}
|2\ 2\rangle &= |1\ 1\rangle|1\ 1\rangle, \\
|2\ 1\rangle &= \frac{1}{\sqrt{2}}(|1\ 1\rangle|1\ 0\rangle + |1\ 0\rangle|1\ 1\rangle), \\
|2\ 0\rangle &= \frac{1}{\sqrt{6}}(|1\ 1\rangle|1\ -1\rangle + |1\ -1\rangle|1\ 1\rangle) + \frac{2}{\sqrt{6}}|1\ 0\rangle|1\ 0\rangle, \\
|2\ -1\rangle &= \frac{1}{\sqrt{2}}(|1\ -1\rangle|1\ 0\rangle + |1\ 0\rangle|1\ -1\rangle), \\
|2\ -2\rangle &= |1\ -1\rangle|1\ -1\rangle, \\
|0\ 0\rangle &= \frac{1}{\sqrt{3}}(|1\ 1\rangle|1\ -1\rangle + |1\ -1\rangle|1\ 1\rangle) - \frac{1}{\sqrt{3}}|1\ 0\rangle|1\ 0\rangle. \quad (4.417)
\end{aligned}$$

Since the polarization vectors of the three spin-one states satisfy $k_\mu \epsilon_H^\mu(\mathbf{k}, \lambda) = 0$, the resulting tensors satisfy automatically the Hilbert gauge condition (4.410). In addition, they are traceless by construction:

$$\epsilon_{H\mu}{}^\mu(\mathbf{k}, \lambda) = 0, \quad (4.418)$$

as follows directly from the explicit four-vectors in the Lorenz gauge (4.318):

$$\epsilon_H^\mu(\mathbf{k}, \pm 1) = \begin{pmatrix} 0 \\ \boldsymbol{\epsilon}(\mathbf{k}, \pm 1) \end{pmatrix}, \quad \epsilon_H^\mu(\mathbf{k}, 0) = \begin{pmatrix} 1 \\ \hat{\mathbf{k}} \end{pmatrix}. \quad (4.419)$$

They satisfy the orthogonality properties $\epsilon_H^\mu(\mathbf{k}, -1)\epsilon_{H\mu}(\mathbf{k}, +1) = 0$ and $\epsilon_H^\mu(\mathbf{k}, \pm 1)\epsilon_{H\mu}(\mathbf{k}, 0) = 0$. The tracelessness of the polarization tensors is, of course, a consequence of the invariance under the gauge transformation (4.401).

The gauge invariance of the second type (4.414) reduces the six degrees of freedom allowed by the gauge condition (4.410) to only two physical degrees.

Setting $\Lambda^\mu = \epsilon_H^\mu(\mathbf{k}, 1)$, $\epsilon_H^\mu(\mathbf{k}, -1)$, and $\epsilon_H^\mu(\mathbf{k}, s)$, and using (4.410), we see that the three combinations (4.414) become precisely the polarization tensors $\epsilon_H^\mu(\mathbf{k}, \pm 1)$ and $\epsilon_H^{\mu\nu}(\mathbf{k}, s)$, respectively.

Note that not only the scalar polarization vector $\epsilon_H^\mu(\mathbf{k}, s)$, but also the polarization vector $\epsilon_H^\mu(\mathbf{k}, 0)$ is unphysical. This is seen by introducing, in addition to the longitudinal polarization vector (4.346), a further linearly independent four-component object

$$\epsilon^\mu(\mathbf{k}, \bar{s}) = (k^0, -\mathbf{k}). \quad (4.420)$$

This four-component object is not a vector as can be seen by forming the product with the polarization vector $\epsilon_\mu(\mathbf{k}, s)$ yielding:

$$\epsilon_\mu(\mathbf{k}, s)\epsilon^\mu(\mathbf{k}, \bar{s}) = k^{02} + \mathbf{k}^2 = 2\mathbf{k}^2,$$

which is not Lorentz-invariant. We shall call the object $\epsilon^\mu(\mathbf{k}, \bar{s})$ an *antiscalar*. The four objects $\epsilon_H^\mu(\mathbf{k}, \pm 1)$, $\epsilon^\mu(\mathbf{k}, s)$, $\epsilon^\mu(\mathbf{k}, \bar{s})$ form a complete basis in the space of polarization vectors. This is expressed in the completeness relation

$$\epsilon_H^\mu(\mathbf{k}, 1)\epsilon_H^\nu(\mathbf{k}, -1) + \epsilon_H^\mu(\mathbf{k}, -1)\epsilon_H^\nu(\mathbf{k}, 1) + \frac{1}{2\mathbf{k}^2}[\epsilon^\mu(\mathbf{k}, s)\epsilon^\nu(\mathbf{k}, \bar{s}) + (\mu \leftrightarrow \nu)] = -\eta^{\mu\nu}. \quad (4.421)$$

Using (4.339), this can be rewritten as

$$P_T^{\mu\nu}(\mathbf{k}) + \frac{1}{2\mathbf{k}^2}[\epsilon^\mu(\mathbf{k}, s)\epsilon^\nu(\mathbf{k}, \bar{s}) + (\mu \leftrightarrow \nu)] = -\eta^{\mu\nu}. \quad (4.422)$$

The first two terms on the left-hand side can obviously be replaced by the polarization tensor $\epsilon_H^{\mu\nu}(\mathbf{k}, 0)$, so that (4.421) may be rewritten as

$$\epsilon_H^{\mu\nu}(\mathbf{k}, 0) = -\eta^{\mu\nu} - \frac{1}{2\mathbf{k}^2}[\epsilon^\mu(\mathbf{k}, s)\epsilon^\nu(\mathbf{k}, \bar{s}) + (\mu \leftrightarrow \nu)]. \quad (4.423)$$

Inserting on the right-hand side the explicit form $\epsilon_H^\mu(\mathbf{k}, s) = k^\mu$ for the scalar polarization vector (4.415), and setting $\epsilon_H^\mu(\mathbf{k}, \bar{s})/2\mathbf{k}^2 = \Lambda^\mu$, the right-hand side can be rewritten as $-k^\mu\Lambda^\nu - k^\nu\Lambda^\mu + \eta^{\mu\nu}k_\kappa\Lambda^\kappa$, thus demonstrating that the polarization tensor $\epsilon_H^{\mu\nu}(\mathbf{k}, 0)$ is of the pure gauge form (4.414), and thus unphysical.

Hence we remain with only two physical polarization tensors $\epsilon_H^{\mu\nu}(\mathbf{k}, \pm 2)$. These describe gravitational waves with helicities $\lambda = \pm 2$. An analysis of the temporal behavior of the fields shows that the tensors $\epsilon_H^{\mu\nu}(\mathbf{k}, \pm 2)$ give the gravitational waves a circular polarization, anticlockwise or clockwise around the momentum direction, respectively. These are analogs of the circularly polarized light waves whose polarization vectors $\epsilon_H^\mu(\mathbf{k}, \pm 1)$ were discussed in Section 4.8.

In electromagnetism, one often describes plane waves with the help of real polarization vectors

$$\epsilon_H^\mu(\mathbf{k}, 1) = -[\epsilon_H^\mu(\mathbf{k}, +1) + \epsilon_H^\mu(\mathbf{k}, -1)], \quad \epsilon_H^\mu(\mathbf{k}, 2) = i[\epsilon_H^\mu(\mathbf{k}, +1) - \epsilon_H^\mu(\mathbf{k}, -1)]. \quad (4.424)$$

These describe linearly polarized light waves whose field vectors oscillate along the directions orthogonal to the momentum $\mathbf{k}$. By analogy, we introduce the real combinations of the two physical polarization tensors

$$\epsilon_{H+}^{\mu\nu}(\mathbf{k}) \equiv \frac{1}{\sqrt{2}}[\epsilon_H^{\mu\nu}(\mathbf{k}, +2) + \epsilon_H^{\mu\nu}(\mathbf{k}, -2)], \quad (4.425)$$

$$\epsilon_{H\times}^{\mu\nu}(\mathbf{k}) = \frac{1}{\sqrt{2}i}[\epsilon_H^{\mu\nu}(\mathbf{k}, +2) - \epsilon_H^{\mu\nu}(\mathbf{k}, -2)]. \quad (4.426)$$

The motion of a circular ring of mass points in a plane gravitational wave $h_{\mu\nu}(x)$, with the polarization tensors (4.425) or (4.426), reveals the physical properties of the associated waves. They distort the circular ring periodically into an ellipsoidal one, in which the principal axes point in the directions 1 and 2. A wave carrying the polarization tensor $\epsilon_{H\times}^{\mu\nu}(\mathbf{k})$ has the same effect with the axes rotated by 45 degrees. For more details see Section 5.5.

The spatial components of the two polarization tensors satisfy the completeness relation

$$\begin{aligned}\epsilon_{H+}^{ij}(\mathbf{k})\epsilon_{H+}^{kl}(\mathbf{k}) + \epsilon_{H\times}^{ij}(\mathbf{k})\epsilon_{H\times}^{kl}(\mathbf{k}) &= \epsilon_H^{ij}(\mathbf{k}, 2)[\epsilon_{H+}^{kl}(\mathbf{k}, 2)]^* + \epsilon_H^{ij}(\mathbf{k}, -2)[\epsilon_{H\times}^{kl}(\mathbf{k}, -2)]^* \\ &= P_{TT}^{ij,kl}(\hat{\mathbf{k}}),\end{aligned}\quad (4.427)$$

where $P_{TT}^{ij,kl}(\hat{\mathbf{k}})$ is the projection matrix

$$P_{TT}^{ij,kl}(\hat{\mathbf{k}}) \equiv \frac{1}{2} \left[P_T^{ik}(\hat{\mathbf{k}})P_T^{jl}(\hat{\mathbf{k}}) + P_T^{il}(\hat{\mathbf{k}})P_T^{jk}(\hat{\mathbf{k}}) \right] - \frac{1}{2}P_T^{ij}(\hat{\mathbf{k}})P_T^{kl}(\hat{\mathbf{k}}), \quad (4.428)$$

formed from products of the transverse projection matrices (4.334) of the electromagnetic waves. It is easy to verify the projection property of (4.428):

$$P_{TT}^{ij}(\hat{\mathbf{k}})P_{TT}^{st,kl}(\hat{\mathbf{k}}) = P_{TT}^{ij,kl}(\hat{\mathbf{k}}). \quad (4.429)$$

Let us apply this projection to the purely spatial part of a gravitational plane wave $h^{\lambda\kappa}(x)$ in the Hilbert gauge (4.399), which by a further gauge transformation of the second kind (4.414) has been made traceless and axial. In this way, the field $\phi_\mu{}^\nu$ has been transformed to satisfy $\phi_\mu{}^\mu = 0$, $\phi_0{}^\mu = 0$. The result is a *transverse-traceless* field:

$$h_{TT}^{ij}(x) = P_{TT}^{ij,kl}h_{kl}(x). \quad (4.430)$$

Its modes briefly called *TT-waves*. The explicit form of the nonzero purely spatial components of $P_{TT}^{\mu\nu,\lambda\kappa}(\hat{\mathbf{k}})$ is

$$P_{TT}^{ij,lm}(\hat{\mathbf{k}}) = \delta^{il}\delta^{jm} - \frac{1}{2}\delta^{ij}\delta^{lm} - 2\delta^{il}\hat{k}^j\hat{k}^m + \frac{1}{2}\delta^{ij}\hat{k}^l\hat{k}^m + \frac{1}{2}\delta^{lm}\hat{k}^i\hat{k}^j + \frac{1}{2}\hat{k}^i\hat{k}^j\hat{k}^l\hat{k}^m. \quad (4.431)$$

If this is applied to any symmetric tensor $h_{lm}(x)$, the result is transverse

$$\partial^l h_{ml} = 0, \quad (4.432)$$

since $k_i P_{TT}^{ij,lm}(\hat{\mathbf{k}}) = 0$, and it is traceless since

$$P_{TT}^{ii,lm}(\hat{\mathbf{k}}) = 0, \quad P_{TT}^{ij,ll}(\hat{\mathbf{k}}) = 0. \quad (4.433)$$

The latter is a reflection of the gauge property (4.418) that was derived from the particular gauge invariance under (4.401). If $P_{TT}^{ij,lm}(\hat{\mathbf{k}})$ is applied to a symmetric traceless tensor, it can be simplified to

$$P_{TT}^{ij,lm}(\hat{\mathbf{k}}) = \delta^{il}\delta^{jm} - 2\delta^{il}\hat{k}^j\hat{k}^m + \frac{1}{2}\hat{k}^i\hat{k}^j\hat{k}^l\hat{k}^m. \quad (4.434)$$

After the on-shell gauge fixing of the second type of the fields $h_{\mu\nu}$ in the Hilbert gauge, the field components have the gauge properties $h_0{}^\mu = 0$, $h_\mu{}^\mu = 0$.

The full set of projection matrices in the space of symmetric tensor fields, which are not restricted by any gauge condition, is summarized in Appendix 4G. There we derive a completeness relation (4G.17) which permits decomposing any symmetric tensor field $h_{\mu\nu}$ into its irreducible components under transformations of the Lorentz group:

$$h_{\mu\nu} = h_{\mu\nu}^{(2)} + h_{\mu\nu}^l + h_{\mu\nu}^s, \quad (4.435)$$

where

$$h_{\mu\nu}^{(2)} \equiv P_{\mu\nu,\lambda\kappa}^{(2)}h^{\lambda\kappa}, \quad h_{\mu\nu}^l \equiv P_{\mu\nu,\lambda\kappa}^l h^{\lambda\kappa}, \quad h_{\mu\nu}^s \equiv P_{\mu\nu,\lambda\kappa}^s h^{\lambda\kappa}. \quad (4.436)$$

4.10 Free Relativistic Fermi Fields

For Fermi fields, the situation is technically more involved. Experimentally, fermions always have an even number of spin degrees of freedom. We shall denote the associated field by ψ_a , where the index a labels the different spin components. Under rotations, these spin components are transformed into each other, as observed experimentally in the *Stern-Gerlach experiment*. We shall see below that Lorentz transformations also lead to certain well-defined mixtures of different spin components.

The question arises as to whether we can construct a Lorentz-invariant action involving $(2s + 1)$ spinor field components. To see the basic construction principle we use as a guide the known transformation law (4.290) for the four-vector field A^μ . For an arbitrary *spinor field* we postulate the transformation law

$$\psi_a(x) \xrightarrow{\Lambda} \psi'_a(x') = D_{ab}(\Lambda) \psi_b(x), \quad (4.437)$$

with an appropriate $(2s + 1) \times (2s + 1)$ spinor transformation matrix $D_{ab}(\Lambda)$ which we have to construct. This can be done by purely mathematical arguments. The construction is the subject of the so-called *group representation theory*. First of all, we perform two successive Lorentz transformations,

$$x'' = \Lambda x = \Lambda_2 x' = \Lambda_2 \Lambda_1 x. \quad (4.438)$$

Since the Lorentz transformations Λ_1, Λ_2 are elements of a group, the product $\Lambda \equiv \Lambda_2 \Lambda_1$ is again a Lorentz transformation. Under the individual factors Λ_2 and Λ_1 , the field transforms as

$$\begin{aligned} \psi(x) &\xrightarrow{\Lambda_1} \psi'(x') = D(\Lambda_1) \psi(x), \\ \psi'(x') &\xrightarrow{\Lambda_2} \psi''(x'') = D(\Lambda_2) \psi'(x'), \end{aligned} \quad (4.439)$$

so that under $\Lambda = \Lambda_2 \Lambda_1$ the spinor goes over into

$$\psi(x) \xrightarrow{\Lambda_2 \Lambda_1} \psi''(x'') = D(\Lambda_2) D(\Lambda_1) \psi(x). \quad (4.440)$$

For the combined Λ , the transformation matrix is $D(\Lambda)$, so that

$$\psi''(x'') = D(\Lambda_2 \Lambda_1) \psi(x). \quad (4.441)$$

Comparing this with (4.440) shows that the matrices $D(\Lambda)$ mixing the spinor field components under the Lorentz group must follow a group multiplication law. Their products must be the same for the group elements itself. Thus the mapping

$$\Lambda \rightarrow D(\Lambda) \quad (4.442)$$

is a *homomorphism*, and the various $D(\Lambda)$'s form a *matrix representation* of the group.

Note that the transformation law (4.290) for the vector field $A^\mu(x)$ follows the same rule with

$$D(\Lambda) \equiv \Lambda = e^{-i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}} \quad (4.443)$$

being the defining 4×4 -representation of the Lorentz group. The parameters $\omega_{\mu\nu}$ are specified in (4.70) and (4.71).

The scalar field transformation law (14.308) follows trivially the same rule, where $D(\Lambda) \equiv 1$ is the identity representation.

The group laws for Λ and $D(\Lambda)$ are sufficiently stringent to allow only for a countable set of *fundamental*⁷ finite-dimensional transformation matrices $D(\Lambda)$. We shall see below that these are characterized by two quantum numbers, s_1 and s_2 , with either one of these taking all possible half-integer or integer values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$. The representation spaces associated with $D^{(s_1, s_2)}(\Lambda)$ will turn out to harbor particles of spins $|s_1 - s_2|$ to $s_1 + s_2$. Hence, particles with a single fixed spin s can only follow the $D^{(s, 0)}(\Lambda)$ or $D^{(0, s)}(\Lambda)$ transformation laws.

In Sections 4.18 and 4.19 we shall learn how the representation matrices $D^{(s_1, s_2)}(\Lambda)$ are most efficiently constructed. We have to determine all possible sets of six matrices which satisfy the commutation relations (4.86). Any set of such matrices forms a representation of the Lie algebra defined by (4.86).

In this general framework, the scalar particles studied so far transform with the trivial representation $D^{(0, 0)}(\Lambda) \equiv 1$ of the Lorentz group. They are said to have spin zero.

Let us now study the smallest nontrivial representation.

4.11 Spin-1/2 Fields

The smallest matrices satisfying the subalgebra (4.76) associated with the rotation subgroup of the Lorentz group are

$$L_i = \frac{\sigma^i}{2}, \quad (4.444)$$

where σ^i are the *Pauli matrices*

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.445)$$

The two-component basis on which $\mathbf{L}^2$ and L_3 are diagonal, with eigenvalues $3/4$ and $\pm 1/2$, respectively, are the Pauli spinors

$$\chi^{(\frac{1}{2})} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi^{(-\frac{1}{2})} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (4.446)$$

⁷Mathematically, *fundamental* means that the representation is irreducible. Any arbitrary representation is equivalent to a direct sum of irreducible ones.

The full Lie algebra (4.76)–(4.78) can be satisfied in two inequivalent ways, either by the choice

$$M_i = -i\sigma^i/2, \quad (4.447)$$

or by

$$M_i = i\sigma^i/2. \quad (4.448)$$

The first amounts to the representation

$$(L_i, M_i) = \left(\frac{\sigma^i}{2}, -i\frac{\sigma^i}{2} \right) \quad (4.449)$$

that is also denoted by $(\frac{1}{2}, 0)$, the second to

$$(L_i, M_i) = \left(\frac{\sigma^i}{2}, i\frac{\sigma^i}{2} \right) \quad (4.450)$$

denoted by $(0, \frac{1}{2})$. Exponentiating these generators we obtain the global representations of the Lorentz group:

$$D^{(\frac{1}{2}, 0)}(\Lambda) = e^{-i(\varphi \cdot \sigma/2 - i\zeta \cdot \sigma/2)}, \quad (4.451)$$

$$D^{(0, \frac{1}{2})}(\Lambda) = e^{-i(\varphi \cdot \sigma/2 + i\zeta \cdot \sigma/2)}. \quad (4.452)$$

An alternative decomposition that will later be useful is a factorization into rotations and subsequent boosts:

$$D^{(\frac{1}{2}, 0)}(\Lambda) = e^{-\zeta \cdot \sigma/2} e^{-i\varphi \cdot \sigma/2}, \quad (4.453)$$

$$D^{(0, \frac{1}{2})}(\Lambda) = e^{\zeta \cdot \sigma/2} e^{-i\varphi \cdot \sigma/2}. \quad (4.454)$$

The right-hand sides can easily be calculated explicitly by expanding them in a Taylor series. The expansion terms separate naturally into even and odd powers, due to the normalization property of the σ -matrices $(\hat{\varphi}\sigma)^2 = 1$ and $(\hat{\zeta}\sigma)^2 = 1$, where $\hat{\varphi}$, $\hat{\zeta}$ are the directions of rotation axis and Lorentz boost, respectively. For rotations, this implies for integer k the power laws $(\varphi\sigma)^{2k} = \varphi^{2k}$, $(\varphi\sigma)^{2k+1} = (\hat{\varphi}\sigma)\varphi^{2k+1}$, so that

$$e^{-i\varphi \cdot \sigma/2} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \left(\frac{\hat{\varphi}\sigma}{2} \right)^n = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \left(\frac{\varphi}{2} \right)^{2k} - i\hat{\varphi}\sigma \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \left(\frac{\varphi}{2} \right)^{2k+1}. \quad (4.455)$$

Summing up separately even and odd powers of the parameters φ , this becomes

$$R_{\hat{\varphi}}(\varphi) = e^{-i\varphi \cdot \sigma/2} = \cos \frac{\varphi}{2} - i\sigma \cdot \hat{\varphi} \sin \frac{\varphi}{2}. \quad (4.456)$$

Similarly we find that

$$B(\zeta) = e^{\mp \zeta \cdot \sigma/2} = \cosh \frac{\zeta}{2} \mp \sigma \cdot \hat{\zeta} \sinh \frac{\zeta}{2}. \quad (4.457)$$

When applying these representations to a particle of mass M at rest, energy and momentum are boosted from $p^\mu = (M, \mathbf{0})$ to

$$p^\mu = (p^0, \mathbf{p}) = M(\cosh \zeta, \hat{\boldsymbol{\zeta}} \sinh \zeta). \quad (4.458)$$

Using the relations

$$\begin{aligned} \cosh \frac{\zeta}{2} &= \sqrt{\frac{1}{2}(\cosh \zeta + 1)} = \sqrt{\frac{p_0 + M}{2M}}, \\ \sinh \frac{\zeta}{2} &= \sqrt{\frac{1}{2}(\cosh \zeta - 1)} = \sqrt{\frac{p_0 - M}{2M}}, \end{aligned} \quad (4.459)$$

we can express the pure Lorentz transformations of the $(\frac{1}{2}, 0)$ -representation in terms of energy and momentum of the boosted particle as follows:

$$B(\boldsymbol{\zeta}) = e^{-\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2} = \frac{1}{\sqrt{2M(p_0 + M)}}(p_0 + M - \boldsymbol{\sigma} \cdot \mathbf{p}). \quad (4.460)$$

We may also use the Einstein parameter γ to write this as

$$B(\boldsymbol{\zeta}) = \frac{1}{\sqrt{2(\gamma + 1)}}(\gamma + 1 - \gamma \boldsymbol{\sigma} \cdot \mathbf{v}/c). \quad (4.461)$$

It is convenient to introduce an extra 2×2 “Pauli matrix”:

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4.462)$$

and define a *four-vector of 2×2 matrices*:

$$\sigma^\mu \equiv (\sigma^0, \sigma^i). \quad (4.463)$$

Note that the four Pauli matrices satisfy a multiplicative algebra:

$$\sigma^0 \sigma^0 = \sigma^0, \quad \sigma^i \sigma^0 = \sigma^0 \sigma^i = \sigma^i, \quad \sigma^i \sigma^j = i\epsilon^{ijk} \sigma^k + \delta^{ij} \sigma^0. \quad (4.464)$$

With σ^μ , we can form *Lorentz-covariant matrices*:

$$p\sigma \equiv p_\mu \sigma^\mu = p^\mu \sigma_\mu. \quad (4.465)$$

This notation allows us to write the boosts in the $(\frac{1}{2}, 0)$ -representation of the Lorentz group as

$$e^{-\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2} = \frac{M + p\sigma}{\sqrt{2M(p_0 + M)}}. \quad (4.466)$$

For a corresponding expression in the $(0, \frac{1}{2})$ -representation, we define, by analogy with $\tilde{x} \equiv (x^0, -x^i)$ in Eq. (4.195), the space inverted vectors:

$$\begin{aligned} \tilde{p}^\mu &\equiv (p^0, -p^i), \\ \tilde{\sigma}^\mu &= (\sigma^0, -\sigma^i). \end{aligned} \quad (4.467)$$

Then

$$e^{\zeta \cdot \sigma / 2} = \frac{M + \tilde{p}\sigma}{\sqrt{2M(p_0 + M)}} = \frac{M + p\tilde{\sigma}}{\sqrt{2M(p_0 + M)}}. \quad (4.468)$$

For many explicit calculations to follow it is useful to realize that the boost matrices (4.466) and (4.468) may be considered as the square-root of the same expression with twice the rapidity:

$$e^{\mp \zeta \cdot \sigma} = \cosh \zeta \mp \boldsymbol{\sigma} \cdot \hat{\boldsymbol{\zeta}} \sinh \zeta. \quad (4.469)$$

Because of (4.458), the right-hand sides have simple momentum representations

$$e^{-\zeta \cdot \sigma} = \frac{p\sigma}{M}, \quad e^{\zeta \cdot \sigma} = \frac{p\tilde{\sigma}}{M}. \quad (4.470)$$

Using these, we may write the boost matrices shorter as

$$e^{-\zeta \cdot \sigma / 2} = \sqrt{\frac{p\sigma}{M}}, \quad e^{\zeta \cdot \sigma / 2} = \sqrt{\frac{p\tilde{\sigma}}{M}}, \quad (4.471)$$

a notation which will be convenient in later calculations.

Having thus succeeded in finding the smallest dimensional representations of the Lorentz group, we define fields $\xi_\alpha(x)$ and $\eta^{\dot{\alpha}}(x)$ to have the corresponding transformation laws:

$$\begin{aligned} \xi_\alpha(x) &\xrightarrow{\Lambda} \xi'_\alpha(x') = D^{(\frac{1}{2}, 0)}(\Lambda)_\alpha{}^\beta \xi_\beta(x), \\ \eta^{\dot{\alpha}}(x) &\xrightarrow{\Lambda} \eta'^{\dot{\alpha}}(x') = D^{(0, \frac{1}{2})}(\Lambda)^{\dot{\alpha}}{}_{\dot{\beta}} \eta^{\dot{\beta}}(x). \end{aligned} \quad (4.472)$$

The different transformation behavior of the two kinds of spinors is exhibited by the lower undotted and upper dotted indices. These spinors were introduced in 1929 by Hermann Weyl [6] and are referred to as *Weyl spinors* of type $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$, respectively.

Let us now see whether we can construct a Lorentz-invariant free-field action from Weyl spinors which can contain only quadratic terms in the fields and their first derivatives. First we look for invariant quadratic terms without spacetime derivatives, which are needed to describe particles with a mass. Let us begin by looking for suitable combinations of ξ and η , which are invariant only under the rotation subgroup. For this, the representation matrices $D^{(\frac{1}{2}, 0)}$ and $D^{(0, \frac{1}{2})}$ are both equal to the same unitary matrix $U = e^{-i\boldsymbol{\zeta} \cdot \boldsymbol{\sigma} / 2}$ to be applied to both ξ and η . Due to the unitarity of U , all quadratic expressions $\xi^\dagger \xi$, $\eta^\dagger \eta$, $\eta^\dagger \xi$, $\xi^\dagger \eta$ are rotationally invariant quadratic field combinations, for example,

$$\begin{aligned} \xi'^\dagger(x') \xi'(x') &= \xi^\dagger(x) U^\dagger U \xi(x) \\ &= \xi^\dagger(x) \xi(x). \end{aligned} \quad (4.473)$$

Consider now pure Lorentz transformations. Then $D^{(\frac{1}{2},0)} = e^{-\zeta \cdot \sigma/2}$ and $D^{(0,\frac{1}{2})} = e^{\zeta \cdot \sigma/2}$ are both nonunitary but Hermitian. The quadratic expressions $\xi^\dagger \xi$ and $\eta^\dagger \eta$ are no longer invariant. However, since the two representation matrices are inverse to each other,

$$D^{(\frac{1}{2},0)\dagger} = D^{(\frac{1}{2},0)} = D^{(0,\frac{1}{2})^{-1}}, \quad (4.474)$$

the mixed quadratic expressions $\eta^\dagger \xi$ and $\xi^\dagger \eta$ are invariant field combinations. Thus we conclude: If the action should contain a quadratic field combination without spacetime derivatives, then both spinors ξ, η , i.e., four field components $\xi_1, \xi_2, \eta^1, \eta^2$, are needed to form an invariant.

Let us now construct a Lorentz invariant term involving spacetime derivatives ∂_μ . It is necessary if an action is supposed to describe a particle which can move through spacetime. Consider first the spatial derivatives. It is easy to see that

$$\begin{aligned} \xi^\dagger \sigma^i \partial_i \xi, & \quad \eta^\dagger \sigma^i \partial_i \eta, \\ \xi^\dagger \sigma^i \partial_i \eta, & \quad \eta^\dagger \sigma^i \partial_i \xi \end{aligned} \quad (4.475)$$

are all rotationally invariant. Take for example

$$\xi^{\dagger'}(x') \sigma^i \partial'_i \xi'(x') = \xi^\dagger(x) U^\dagger \sigma^i \partial'_i U \xi(x). \quad (4.476)$$

From the commutation rules among the Pauli matrices σ^i it is easy to derive the transformation law

$$U^{-1} \sigma^i U = R_{\hat{\varphi}}(\varphi)^i_j \sigma^j. \quad (4.477)$$

The proof of this proceeds in the same way as in the finite transformation of the spatial vector x^i in (4.106) with the help of Lie's expansion formula (4.105). The commutation rules between $-i\sigma^3/2$ and σ^i are precisely the same as those between $\hat{L}_3$ and x^i , so that we find for a rotation around the 3-axis,

$$\begin{aligned} e^{i\sigma^3\varphi/2} \sigma^3 e^{-i\sigma^3\varphi/2} &= \sigma^3, \\ e^{i\sigma^3\varphi/2} \sigma^1 e^{-i\sigma^3\varphi/2} &= \cos \varphi \sigma^1 - \sin \varphi \sigma^2, \\ e^{i\sigma^3\varphi/2} \sigma^2 e^{-i\sigma^3\varphi/2} &= \sin \varphi \sigma^1 + \cos \varphi \sigma^2, \end{aligned} \quad (4.478)$$

corresponding precisely to (4.477) with the matrix (14.283). The 2×2 representation has the advantage, used already in (4.456), that the exponentials can be expanded into linear combinations of σ^0 and σ^i . If we do this on the left-hand sides, we can calculate the right-hand sides also using products of σ^i rather than commutators as in Lie's expansion formula (4.105).

Now, since derivatives transform like a vector,

$$\partial_i \xrightarrow{R} \partial'_i = R_{\hat{\varphi}}(\varphi)_{ij} \partial_j, \quad (4.479)$$

the expression (4.476) is indeed a rotationally invariant field combination. For the other terms in (4.475), the proof is the same.

How can we extend the expressions (4.475) to form relativistic invariants? For this we remember that in the boost matrices (4.471), the four-vector generalizations $\sigma^\mu, \tilde{\sigma}^\mu$ of the Pauli matrices appeared naturally contracted with p_μ . This suggests studying

$$\begin{aligned}\xi^\dagger \sigma^\mu \partial_\mu \xi, & \quad \eta^\dagger \sigma^\mu \partial_\mu \eta, \\ \xi^\dagger \sigma^\mu \partial_\mu \eta, & \quad \eta^\dagger \sigma^\mu \partial_\mu \xi,\end{aligned}\tag{4.480}$$

and once more the same combinations, but with σ^μ replaced by $\tilde{\sigma}^\mu$.

The additional time derivatives in (4.480) are trivially invariant under rotations and thus do not destroy the rotational invariance of the spatial parts shown in (4.476). Consequently we have to study only the behavior under pure Lorentz transformations in, say, the z -direction. Under these, the x - and y -components do not change. It is easy to verify that

$$\begin{aligned}e^{-\sigma^3 \zeta/2} \sigma^0 e^{-\sigma^3 \zeta/2} &= e^{-\sigma^3 \zeta} = \cosh \zeta \sigma^0 + \sinh \zeta (-\sigma^3), \\ e^{-\sigma^3 \zeta/2} (-\sigma^3) e^{-\sigma^3 \zeta/2} &= e^{-\sigma^3 \zeta} (-\sigma^3) = \sinh \zeta \sigma^0 + \cosh \zeta (-\sigma^3), \\ e^{\sigma^3 \zeta/2} \sigma^0 e^{\sigma^3 \zeta/2} &= e^{\sigma^3 \zeta} = \cosh \zeta \sigma^0 + \sinh \zeta \sigma^3, \\ e^{\sigma^3 \zeta/2} \sigma^3 e^{\sigma^3 \zeta/2} &= e^{\sigma^3 \zeta} \sigma^3 = \sinh \zeta \sigma^0 + \cosh \zeta \sigma^3.\end{aligned}\tag{4.481}$$

In contrast to the transformation laws (4.478), this cannot be derived with the help of Lie's expansion formula (4.105), since the exponentials on the left-hand sides have the same exponents. However, as before in the calculation of (4.457), we may use the multiplicative algebra of σ^i -matrices rather than the commutation rules between them to expand the exponentials into linear combinations of σ^0 and σ^i .

The first two lines in (4.481) show that the matrices $\tilde{\sigma}^\mu$ transform like a four-vector under $(\frac{1}{2}, 0)$ -boosts, the remaining lines σ^μ show the corresponding behavior under $(0, \frac{1}{2})$ -boosts. In combination with rotations, we thus have proved the Lorentz transformation behavior:

$$\begin{aligned}D^{(\frac{1}{2}, 0)\dagger}(\Lambda) \tilde{\sigma}^\mu D^{(\frac{1}{2}, 0)}(\Lambda) &= \Lambda^\mu{}_\nu \tilde{\sigma}^\nu, \\ D^{(0, \frac{1}{2})\dagger}(\Lambda) \sigma^\mu D^{(0, \frac{1}{2})}(\Lambda) &= \Lambda^\mu{}_\nu \sigma^\nu.\end{aligned}\tag{4.482}$$

This allows us to conclude that the quadratic field terms with a derivative

$$\xi^\dagger \tilde{\sigma}^\mu \partial_\mu \xi, \quad \eta^\dagger \sigma^\mu \partial_\mu \eta\tag{4.483}$$

are Lorentz-invariant. For instance

$$\begin{aligned}\eta'^\dagger(x') \sigma^\mu \partial'_\mu \eta'(x') &= \eta^\dagger(x) D^{(0, \frac{1}{2})\dagger}(\Lambda) \sigma^\mu \partial'_\mu D^{(0, \frac{1}{2})}(\Lambda) \eta(x) = \eta^\dagger(x) \Lambda^\mu{}_\nu \sigma^\nu \partial'_\mu \eta(x) \\ &= \eta^\dagger(x) \sigma^\nu \partial_\nu \eta(x).\end{aligned}\tag{4.484}$$

It is easy to see that the other quadratic combinations in (4.480) are not invariant.

If we allow only for these lowest-order in the derivative terms, the most general Lorentz-invariant action reads

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x (\xi^\dagger \tilde{\sigma}^\mu i \partial_\mu \xi + \eta^\dagger \sigma^\mu i \partial_\mu \eta - M_1 \xi^\dagger \eta - M_2 \eta^\dagger \xi).\tag{4.485}$$

Observe that this expression involves necessarily both two-component spinors ξ and η . Only for zero parameters $M_{1,2}$, a single species of two-component spinors, ξ or η , possesses an invariant action.

The equations of motion are obviously

$$\begin{aligned} i\tilde{\sigma}^\mu \partial_\mu \xi(x) &= M_1 \eta(x), \\ i\sigma^\mu \partial_\mu \eta(x) &= M_2 \xi(x). \end{aligned} \quad (4.486)$$

Combining the second equation with the first and vice versa we find the two second-order field equations

$$(-\partial^2 - M_1 M_2) \xi(x) = 0, \quad (4.487)$$

$$(-\partial^2 - M_1 M_2) \eta(x) = 0. \quad (4.488)$$

In deriving these, we have used the relation

$$\sigma^\mu \tilde{\sigma}^\nu + \sigma^\nu \tilde{\sigma}^\mu = 2g^{\mu\nu}, \quad (4.489)$$

by which

$$\tilde{\sigma}^\mu \partial_\mu \sigma^\nu \partial_\nu = \partial^2, \quad (4.490)$$

which is easily shown by direct evaluation. In momentum space, equations (4.487) are solved by particles of mass

$$M = \sqrt{M_1 M_2}. \quad (4.491)$$

For $M \neq 0$, it is useful to combine the two spinors ξ and η into a single four-component object, called *bispinor* or *Dirac spinor*:

$$\psi(x) = \begin{pmatrix} \xi(x) \\ \eta(x) \end{pmatrix}. \quad (4.492)$$

In terms of this, the action may be written as

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \bar{\psi}(x) \left[i\gamma^\mu \partial_\mu - \begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} \right] \psi(x), \quad (4.493)$$

where γ^μ are the 4×4 *Dirac matrices*:

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix}, \quad (4.494)$$

and $\bar{\psi}(x)$ is the *adjoint Dirac spinor* defined by

$$\bar{\psi}(x) \equiv \psi^\dagger(x) \gamma^0 = (\eta^\dagger(x), \xi^\dagger(x)). \quad (4.495)$$

The Dirac matrices satisfy the anticommutation rules

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \quad (4.496)$$

It has become customary to abbreviate the contraction of γ^μ with any vector v^μ by

$$\psi \equiv \gamma^\mu v_\mu. \quad (4.497)$$

In this notation, the derivative terms $\gamma^\mu \partial_\mu$ in (4.493) become simply ψ .

For the Dirac spinor, the equations of motion (4.486) take the form

$$\left[i\psi - \begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} \right] \psi(x) = 0. \quad (4.498)$$

This is almost, but not quite, the wave equation postulated first by Dirac for the electron. He assumed a diagonal 4×4 -mass matrix

$$\begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} = M \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4.499)$$

and proposed the *Dirac equation*

$$(i\psi - M) \psi(x) = 0 \quad (4.500)$$

corresponding to an action

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \bar{\psi}(x) (i\psi - M) \psi(x). \quad (4.501)$$

Just as in the case of a complex scalar field, there exists a four-vector quantity

$$j^\mu(x) = \bar{\psi}(x) \gamma^\mu \psi(x), \quad (4.502)$$

which by virtue of the Dirac equation satisfies a local conservation law [recall (4.171) and (4.172)]:

$$\partial_\mu j^\mu(x) = 0. \quad (4.503)$$

This four-vector will be used in Chapter 12 to couple Dirac fields to electromagnetism, thus becoming the electromagnetic current density of the Dirac field. Later in Subsection 8.11.1 we shall see that the local conservation law (4.503) is a consequence of the invariance of the Dirac action (4.501) under arbitrary changes of the phase of the field:

$$\psi(x) \rightarrow e^{-i\alpha} \psi(x). \quad (4.504)$$

It is this invariance which gives rise to a conserved current density [see (8.272), also (12.48)].

By construction, the actions (4.493) and (4.501) are invariant under the bispinor or Dirac-Lorentz transformations

$$\psi_a(x) \xrightarrow{\Lambda} \psi'_a(x') = D_a{}^b(\Lambda) \psi_b(x), \quad (4.505)$$

where the 4×4 -matrices $D(\Lambda)$ consist of rotations and pure Lorentz transformations:

$$D(R) = \begin{pmatrix} e^{-i\varphi \cdot \sigma/2} & 0 \\ 0 & e^{-i\varphi \cdot \sigma/2} \end{pmatrix}, \quad D(B) = \begin{pmatrix} e^{-\zeta \cdot \sigma/2} & 0 \\ 0 & e^{\zeta \cdot \sigma/2} \end{pmatrix}. \quad (4.506)$$

With the 2×2 matrices (4.453) and (4.454) we can write $D(\Lambda)$ in the form

$$D(\Lambda) = \begin{pmatrix} D^{(\frac{1}{2},0)}(\Lambda) & 0 \\ 0 & D^{(0,\frac{1}{2})}(\Lambda) \end{pmatrix}, \quad (4.507)$$

The invariance can be seen most directly by combining the transformation laws (4.482) with the 4×4 -relation

$$\bar{D}(\Lambda)\gamma^\mu D(\Lambda) = \Lambda^\mu{}_\nu \gamma^\nu, \quad (4.508)$$

where we define

$$\bar{D}(\Lambda) \equiv \begin{pmatrix} D^{(\frac{1}{2},0)\dagger}(\Lambda) & 0 \\ 0 & D^{(0,\frac{1}{2})\dagger}(\Lambda) \end{pmatrix} = D^{-1}(\Lambda). \quad (4.509)$$

From (4.508), the invariance of the derivative term in (4.501) follows at once, using (4.138), (4.139), and (4.44):

$$\begin{aligned} i\bar{\psi}'(x')\gamma^\mu\partial'_\mu\psi'(x') &= i\bar{\psi}(x)\bar{D}(\Lambda)\gamma^\mu D(\Lambda)\partial'_\mu\psi(x) = i\bar{\psi}(x)\Lambda^\mu{}_\nu\gamma^\nu\partial'_\mu\psi(x) \\ &= i\bar{\psi}(x)\gamma^\nu\partial_\nu\psi(x). \end{aligned} \quad (4.510)$$

In terms of Dirac matrices (4.494), the pure Lorentz transformations can also be written as

$$D(B) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0 + M)}}. \quad (4.511)$$

The representation matrices of all Lorentz transformations may be expressed in terms of covariant generators as

$$D(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}, \quad (4.512)$$

where $\omega_{\mu\nu}$ is the same antisymmetric matrix as in (4.69). They contain both the rotation and boost parameters as specified in (4.70) and (4.71). Taking the matrices (4.506) to the limit of small $\boldsymbol{\varphi}$ and $\boldsymbol{\zeta}$, we identify the 4×4 -matrix generators $S^{\mu\nu}$ as

$$S^{ij} = \epsilon_{ijk} \frac{1}{2} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \quad S^{0i} = \frac{i}{2} \begin{pmatrix} -\sigma^i & 0 \\ 0 & \sigma^i \end{pmatrix}. \quad (4.513)$$

The 4×4 -generator of the rotation group on the left-hand side contains the direct 4×4 -extension of the Pauli matrices:

$$\boldsymbol{\Sigma} \equiv \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}. \quad (4.514)$$

The spin matrix

$$\mathbf{S} \equiv \frac{1}{2} \boldsymbol{\Sigma} \quad (4.515)$$

has the components $S^i = \frac{1}{2}\epsilon_{ijk}S^{jk}$.

The generator of the pure Lorentz transformations on the right-hand side of (4.513) is also written as $S^{0i} = i\alpha^i/2$ with the matrix

$$\alpha = \begin{pmatrix} -\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}. \quad (4.516)$$

It is customary to introduce the matrices

$$\sigma^{\mu\nu} \equiv \frac{i}{2}[\gamma^\mu, \gamma^\nu]. \quad (4.517)$$

In terms of these, equations (4.513) can be summarized as

$$S^{\mu\nu} \equiv \frac{1}{2}\sigma^{\mu\nu}. \quad (4.518)$$

It is easy to check that the matrices $S^{\mu\nu}$ satisfy the same commutation rules as the defining generators of the Lorentz group in (4.87):

$$[S^{\mu\nu}, S^{\mu\lambda}] = -ig^{\mu\mu}S^{\nu\lambda}, \quad \text{no sum over } \mu. \quad (4.519)$$

Thus they are generators of a new 4×4 -representation of the Lorentz group. The 4×4 -Dirac representation matrices $D(\Lambda)$ transforming bispinors are mathematically inequivalent to the defining 4×4 -representation Λ of the Lorentz group transforming vectors.

With the gamma matrices, the generators $S^{\mu\nu}$ have the following commutation rules:

$$[S^{\mu\nu}, \gamma^\lambda] = -(L^{\mu\nu})^\lambda{}_\kappa \gamma^\kappa = -i(g^{\mu\lambda}\gamma^\nu - g^{\nu\lambda}\gamma^\mu), \quad (4.520)$$

which state that γ^μ is a vector operator in bispinor space [recall (4.99)]. The transformation law (4.508) is the global consequence of these rules.

In terms of the generators $S^{\mu\nu}$, we can write the field transformation law (4.505) more explicitly as

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda)\psi(\Lambda^{-1}x) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}\psi(\Lambda^{-1}x). \quad (4.521)$$

As in the case of the scalar field [recall (4.122)], it is useful to perform the transformation of the spacetime argument on the right-hand side in terms of the differential operator of four-dimensional angular momentum. Thus we rewrite (4.521) as

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = \hat{D}(\Lambda)D(\Lambda)\psi(x) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{J}^{\mu\nu}}\psi(x), \quad (4.522)$$

where

$$\hat{J}^{\lambda\kappa} \equiv S^{\lambda\kappa} \times \hat{1} + 1 \times \hat{L}^{\lambda\kappa} \quad (4.523)$$

are the generators of the total four-dimensional angular momentum of a Dirac field, by analogy with (4.293). The tensor products exhibits the two separate representation spaces associated with the Dirac index and the spacetime coordinates. The commutation rules between the generators $\hat{J}^{\mu\nu}$ are of course the same as in the case of the vector potential (4.295), and in fact for any spin.

4.12 Other Symmetries of the Dirac Action

As in the scalar case, the spin-1/2 action (4.501) is invariant under more than just the Lorentz group.

4.12.1 Translations and Poincaré Group

First, it is automatically invariant under translations (4.185) for which

$$\psi(x) \xrightarrow{\mu} \psi'_a(x) = \psi(x - a). \quad (4.524)$$

Together with the Lorentz transformations, these form the *inhomogeneous Lorentz group* or the *Poincaré group* (4.189). Under it, the spinor transforms as

$$\psi(x) \xrightarrow{\Lambda, a} \psi'(x) = \psi(\Lambda^{-1}(x - a)). \quad (4.525)$$

Extending (4.522), we can generate all Poincaré transformations by the operations

$$\psi(x) \xrightarrow{\Lambda, a} \psi'(x) = \hat{D}(\Lambda) D(\Lambda) \psi(x) = e^{ia^\mu \hat{p}_\mu / \hbar} e^{-i\frac{1}{2} \omega_{\mu\nu} \hat{J}^{\mu\nu}} \psi(x). \quad (4.526)$$

4.12.2 Space Inversion

In contrast to scalar fields, the Poincaré invariance does not automatically imply invariance under *parity* transformations. In the quantum theory of electrons and photons called quantum electrodynamics (QED), it is an additional requirement confirmed by all experimental data. The action of free electrons must therefore be invariant under parity transformations. To achieve this, we first have to define an appropriate way to transform a bispinor under space reflections P . The bispinor must form a representation of the Lorentz group extended by P ,

$$\psi(x) \xrightarrow{P} \psi'_P(x) = D(P) \psi(\tilde{x}), \quad (4.527)$$

where $x'_P = \tilde{x}$ as in (4.195). The representation matrices $D(P)$ must combine with the representation matrices of the Lorentz group $D(\Lambda)$ in the same way as the 4×4 -matrix of space reflections

$$P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \quad (4.528)$$

combines with the Lorentz transformations Λ . From the explicit matrices (4.54)–(4.56) and (4.60)–(4.62) we find

$$P^{-1} \mathbf{L} P = \mathbf{L}, \quad P^{-1} \mathbf{M} P = -\mathbf{M}. \quad (4.529)$$

Thus rotations commute with reflections, which is intuitively obvious since $\mathbf{x}$ and $-\mathbf{x}$ rotate both with the same 3×3 matrices. Pure Lorentz transformations, on the other hand, are space-inverted to boost into the opposite direction. Since upper and lower components in a Dirac spinor contain the boost matrices (4.471) in opposite directions, we can immediately write down the transformation law for a Dirac spinor under space inversion as

$$\psi(x) \xrightarrow{P} \psi'_P(x) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi(\tilde{x}). \quad (4.530)$$

The phase η_P is the intrinsic parity of the field $\psi(x)$. The representation matrix of the reflection P in Dirac space is denoted by

$$D(P) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \eta_P \gamma_0. \quad (4.531)$$

The property $P^2 = 1$ must be reproduced by the representation matrix $D(P)$. By applying two successive space inversions on $\psi(x)$ we can conclude that the intrinsic parity can only have the values $\eta_P = \pm 1$.

We easily check that the matrix $D(P)$ transforms the 4×4 -bispinor representation (4.513) of the generators L_i and M_i as in the defining representation (4.529):

$$D^{-1}(P)D(L_i)D(P) = D(L_i), \quad D^{-1}(P)D(M_i)D(P) = D(-M_i). \quad (4.532)$$

We now postulate Lorentz invariance of the action (4.493) under space reflection. Since

$$D^{-1}(P) \begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} D(P) = \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix}, \quad (4.533)$$

this is only possible if $M_1 = M_2$, so that the action takes the Dirac form (4.501). Also, since space inversion transforms $\xi(x)$ into $\eta(x)$, a parity-invariant theory necessarily contains both fields and thus the full bispinor $\psi(x)$.

Having set $M_1 = M_2$, the mass term of the Dirac action is parity-invariant. In order to ensure the invariance of the derivative term, we observe that the representation matrix (4.531) of P satisfies

$$D^{-1}(P)\gamma^\mu D(P) = \tilde{\gamma}^\mu. \quad (4.534)$$

Hence we calculate

$$\begin{aligned} \bar{\psi}'(x') i\gamma^\mu \partial'_\mu \psi'(x') &= \bar{\psi}'(\tilde{x}) i\gamma^\mu \tilde{\partial}_\mu \psi'(\tilde{x}) = \bar{\psi}(x) D^{-1}(P) i\gamma^\mu \tilde{\partial}_\mu D(P) \psi(x) \\ &= \bar{\psi}(x) i\gamma^\mu \partial_\mu \psi(x), \end{aligned} \quad (4.535)$$

which proves the invariance of the derivative term, and thus of the full Dirac action.

The Dirac equation

$$(i\gamma^\mu \partial_\mu - M)\psi(x) = 0 \quad (4.536)$$

can trivially be rewritten as

$$(i\gamma^\mu \tilde{\partial}_\mu - M)\psi(\tilde{x}) = 0. \quad (4.537)$$

Using (4.530) and (4.531), we can replace $\psi(\tilde{x})$ by $\eta_P \gamma_0 \psi'_P(x)$, and take the matrix γ_0 to the left of the Dirac operator with the help of (4.534). The result is

$$(i\gamma^\mu \partial_\mu - M)\psi'_P(x) = 0, \quad (4.538)$$

i.e., the Dirac equation for the mirror-reflected bispinor.

As we shall see in Chapter 12, the interactions of electrons with electromagnetism are described with extreme accuracy by the parity-invariant theory called quantum electrodynamics (QED). The electrons in this theory are described by the Dirac action (4.501).

A theory based only on a single two-component spinor field ξ or η is necessarily massless and violates parity. Such a theory was used successfully to describe *neutrino* processes. There exist several neutrinos in nature, one associated with every charged lepton e^- , μ^- , τ^- whose masses are $m_e = 0.510 \text{ MeV}$, $m_\mu = 105.66 \text{ MeV}$, $m_\tau = 1777.03 \pm 0.30 \text{ MeV}$, the latter two having finite lifetimes $\tau_\mu = (2.19703 \pm 0.00004) \times 10^{-6} \text{ sec}$ and $\tau_\tau = (290.6 \pm 1.1) \times 10^{-15} \text{ sec}$. The corresponding neutrinos are denoted by ν_e , ν_μ , ν_τ . The six leptons seem to exist in nature by complete analogy to six quarks which are the elementary building blocks of strongly interacting particles. The analogous configurations are illustrated in Fig. 4.1.

$$\begin{pmatrix} e^- & \mu^- & \tau^- \\ \nu_e & \nu_\mu & \nu_\tau \end{pmatrix} \quad \begin{pmatrix} u & c & t \\ d & s & b \end{pmatrix}$$

FIGURE 4.1 Six leptons and quarks.

The electron-neutrino was postulated in 1931 by Pauli in order to explain an apparent violation of energy conservation in the final state of the β -decay of the neutron. Energy conservation would have been violated if only the observed particles proton and electron emerged from the decay. From the energy spectrum of the electron one can deduce that the mass of the electron neutrino is extremely small, less than $2 \text{ eV}/c^2$. The most precise value is expected from an ongoing experiment performed in Karlsruhe. There one studies the beta radiation of tritium nuclei which decay in 12.3 years with a total energy release of 18.6 keV shared by an electron and a neutrino. The energy of the electron is measured in an experiment called KATRIN (acronym for the Karlsruhe Tritium Neutrino Experiment) by a giant electrostatic spectrometer of diameter 7 m and length 20 m. After this the particle identity is confirmed in a semiconducting detector. The experiment is sensitive to electron neutrino masses $\geq 0.4 \text{ eV}/c^2$. The masses of the other two neutrinos have presently the bounds $m_{\nu_\mu} < 0.19 \text{ MeV}$ and $m_{\nu_\tau} < 0.18.3 \text{ MeV}$.

In summary, in a mirror-symmetric Lorentz-invariant theory of particles with the lowest nontrivial spin 1/2, the action is given by Dirac's expression (4.501). If

parity is allowed to be violated, there are two simpler Lorentz-invariant actions of massless particles:

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \xi^\dagger(x) i \tilde{\sigma}^\mu \partial_\mu \xi(x), \quad (4.539)$$

or

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \eta^\dagger(x) i \sigma^\mu \partial_\mu \eta(x). \quad (4.540)$$

The parity-invariant action (4.501) is the correct one for electrons, while the action (4.539) describes neutrinos. For neutrinos, it has become customary to work also with four-component bispinors $\psi(x)$, but making only use of the two upper components. The upper and lower components are extracted from $\psi(x)$ by the projection matrices

$$P_{u,l} \equiv \frac{1}{2}(1 \mp \gamma_5) \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4.541)$$

where γ_5 denotes the 4×4 -matrix

$$\gamma_5 \equiv \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \gamma^5. \quad (4.542)$$

This is a Lorentz-invariant matrix, since it may also be expressed in the contracted form

$$\gamma_5 = \frac{i}{4!} \epsilon_{\mu\nu\lambda\kappa} \gamma^\mu \gamma^\nu \gamma^\lambda \gamma^\kappa \equiv \gamma^5, \quad (4.543)$$

where $\epsilon_{\mu\nu\lambda\kappa}$ is the completely antisymmetric tensor with $\epsilon_{0123} = 1$ (see [12]). Using γ_5 , the actions (4.539) and (4.540) can be written as

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \frac{1}{2} \int d^4x \bar{\psi}(x) i \gamma^\mu \partial_\mu (1 \mp \gamma_5) \psi(x). \quad (4.544)$$

From (4.534) we see that under space inversion, γ_5 transforms as follows:

$$D^{-1}(P) \gamma_5 D(P) = -\gamma_5, \quad (4.545)$$

thereby interchanging the two actions (4.544) with each other.

The parity-violating actions (4.539) and (4.540), or (4.544), have an interesting history. After having been proposed by Weyl in 1929 to describe massless spin-1/2 particles [6] it was initially rejected on theoretical grounds, since at that time all interactions were firmly believed to be invariant under space reflections. Electromagnetic and nuclear interactions had definitely displayed this property, and it was suggestive to assume that nature should follow the same principle in all its interactions. In 1956, however, Lee and Yang suggested that a violation of parity can be deduced from the existence of the two decay modes of the heavy mesons K^0 and K^+ . The first decays into $\pi^0\pi^0$ with relative s-waves, the second into $\pi^+\pi^+\pi^-$ with both $\pi^+\pi^+$ and $\pi^-\pi^+$ in relative s-waves. Since the pion has negative parity the

violation is manifest. In 1957, the above authors pointed out the relevance of measuring the β -decay from a polarized nucleus [7]. If parity was an invariance of weak interactions, the distribution of electrons would have to be symmetric with respect to the direction of spin. Indeed, since the scalar product between spin, which is an axial vector, and the momentum vector is a pseudoscalar operator, its expectation value should vanish. In 1957, Madame Wu and collaborators [8] performed the historic experiment observing a nonzero up-down asymmetry in the distribution of electrons coming from polarized $^{60}_{27}\text{Co}$ (see Fig. 4.2).⁸

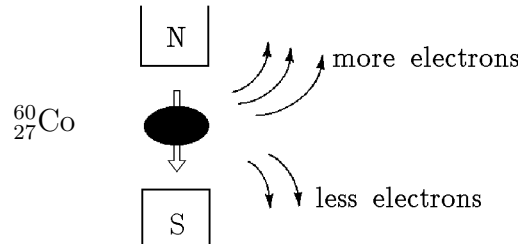


FIGURE 4.2 Asymmetry observed in the distribution of electrons from the β -decay of polarized $^{60}_{27}\text{Co}$.

The polarization of the sample was done by placing it into a strong magnetic field. By going to an extremely low temperature, a sufficient population difference between spin down and spin up was achieved that made the experiment display a clear violation of parity. In later experiments it was found that the violation is even *maximal*, in the sense that the unobserved neutrino emitted in the decay process can only have one polarization along its momentum direction, the other being *completely* forbidden. A massless neutrino possesses no mirror image in nature and can be described by a pure Weyl action with only a $\frac{1}{2}(1 - \gamma_5)\psi$ field. We shall see in Chapter 7 that also a massless antineutrino is described by the field $\frac{1}{2}(1 - \gamma_5)\psi$.

The initial $^{60}_{27}\text{Co}$ -state has a spin $s = 5$ and intrinsic parity $\eta_P = +1$, thus being a $s^P = 5^+$ -state. The β -decay transforms it into an excited state of $^{60}_{28}\text{Ni}$ with spin-parity $s^P = 4^+$. As such, it is a so-called *Gamow-Teller transition*. In this transition it can be shown that only combinations of tensor and axialvector couplings contribute (T-A). The details will be explained in Chapter 27.

A year later a crucial hypothesis was made by several authors [19] that the weak interactions are mediated by a specific combination of vector and axial vector couplings. This is the famous *V-A hypothesis* which eventually led to the present standard model of weak and electromagnetic interactions (see Chapter 27).

The bispinors $\frac{1}{2}(1 \mp \gamma^5)\psi$ are eigenvalues of the matrix γ^5 . Their eigenvalues are -1 or $+1$. They are called states of left or right *chirality*, respectively.

There exist, of course, many equivalent representations of the Lorentz group extended by the discrete transformation of space inversion on spin-1/2 fields. Instead

⁸In nuclear physics the customary notation for a nucleus X is $^A_Z X_N$, where A is the *nucleon number*, Z the number of protons or the *atomic number* (also the *charge number*), and N the number of neutrons. The last label is not really necessary since the name of the nucleus is specified uniquely by A and Z .

of the bispinors $\psi(x)$ transforming with the 4×4 -matrices (4.507), in which parity exchanges upper and lower two-component spinors in $\psi(x)$ via the matrix $D(P)$ of (4.531), consider symmetric and antisymmetric combinations

$$\psi_D(x) \equiv S_D \psi(x), \quad (4.546)$$

where S_D is the similarity transformation matrix

$$S_D \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \quad (4.547)$$

In the bispinor $\psi_D(x)$, upper and lower components are eigenstates of opposite parity. These fields transform according to the 4×4 representation

$$\begin{aligned} D_D(\Lambda) &= S_D D(\Lambda) S_D^{-1} \\ &= \begin{pmatrix} \frac{1}{2} (D^{(\frac{1}{2},0)} + D^{(0,\frac{1}{2})}) (\Lambda) & -\frac{1}{2} (D^{(\frac{1}{2},0)} - D^{(0,\frac{1}{2})}) (\Lambda) \\ -\frac{1}{2} (D^{(\frac{1}{2},0)} - D^{(0,\frac{1}{2})}) (\Lambda) & \frac{1}{2} (D^{(\frac{1}{2},0)} + D^{(0,\frac{1}{2})}) (\Lambda) \end{pmatrix}. \end{aligned} \quad (4.548)$$

When boosting a massive particle from rest to momentum p^μ this matrix becomes explicitly, with (4.471) and (4.468),

$$\begin{aligned} D_D(B(\zeta)) &= \begin{pmatrix} \frac{1}{2} (e^{-\zeta \cdot \sigma/2} + e^{\zeta \cdot \sigma/2}) & -\frac{1}{2} (e^{-\zeta \cdot \sigma/2} - e^{\zeta \cdot \sigma/2}) \\ -\frac{1}{2} (e^{-\zeta \cdot \sigma/2} - e^{\zeta \cdot \sigma/2}) & \frac{1}{2} (e^{-\zeta \cdot \sigma/2} + e^{\zeta \cdot \sigma/2}) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} (\sqrt{p\sigma/M} + \sqrt{p\tilde{\sigma}/M}) & -\frac{1}{2} (\sqrt{p\sigma/M} - \sqrt{p\tilde{\sigma}/M}) \\ -\frac{1}{2} (\sqrt{p\sigma/M} - \sqrt{p\tilde{\sigma}/M}) & \frac{1}{2} (\sqrt{p\sigma/M} + \sqrt{p\tilde{\sigma}/M}) \end{pmatrix} \\ &= \frac{1}{\sqrt{2M(M+p_0)}} \begin{pmatrix} M+p_0 & \mathbf{p} \cdot \boldsymbol{\sigma} \\ \mathbf{p} \cdot \boldsymbol{\sigma} & M+p_0 \end{pmatrix}. \end{aligned} \quad (4.549)$$

The Dirac matrices which ensure in this case the invariance of the action (4.493) are now

$$\gamma_D^\mu = S_D \gamma^\mu S_D^{-1} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix} \right\}, \quad (4.550)$$

$$\gamma_D^5 = S_D \gamma^5 S_D^{-1} = i\gamma_D^0 \gamma_D^1 \gamma_D^2 \gamma_D^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (4.551)$$

In terms of these, the boost transformation (4.549) takes the form

$$D_D(B) = \frac{M + \not{p}_D \gamma_D^0}{\sqrt{2M(p_0 + M)}}, \quad (4.552)$$

which is the same as the similarity-transformed $S_D D(B) S_D^{-1}$ of the boost matrix (4.511) in the chiral representation. The generators are

$$S_D^{ij} = S_D S^{ij} S_D^{-1} = \epsilon_{ijk} \frac{1}{2} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \quad S_D^{0i} = S_D S^{0i} S_D^{-1} = \frac{i}{2} \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad (4.553)$$

which are equal to

$$\sigma_D^{\mu\nu} \equiv S_D \sigma^{\mu\nu} S_D^{-1} = \frac{i}{2} [\gamma_D^\mu, \gamma_D^\nu], \quad (4.554)$$

as in (4.517). The generators of rotations S_D^{ij} are the same as in the chiral representation (4.513). Indeed, writing $S_D^{ij} = \epsilon_{ijk} \frac{1}{2} \Sigma_D^i$, we see that the 4×4 -generalization of the Pauli matrices (4.514) is invariant under the similarity transformation S_D :

$$\Sigma_D = S_D \Sigma S_D^{-1} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} = \Sigma, \quad (4.555)$$

so that we can write $S_D^{ij} = \epsilon_{ijk} \frac{1}{2} \Sigma^i$, as before in Eq. (4.515).

For small momenta, the boost matrix (4.549) has the limit

$$D_D(B(\boldsymbol{\zeta})) \approx \begin{pmatrix} 1 & \mathbf{p} \cdot \boldsymbol{\sigma}/2 \\ \mathbf{p} \cdot \boldsymbol{\sigma}/2 & 1 \end{pmatrix}. \quad (4.556)$$

This shows that the spinors in Dirac's representation of the gamma matrices have small lower (or upper) components for slow particles (or antiparticles). The Dirac representation is therefore useful for studying the nonrelativistic limit of Dirac particles.

For such calculations it is advantageous to state the Dirac matrices in a direct-product form

$$\gamma_D^0 = \sigma^3 \times 1, \quad \gamma_D = i\sigma^2 \times \boldsymbol{\sigma}, \quad (4.557)$$

in which $\gamma_D^5 = \sigma^1 \times 1$ and the generators of the Lorentz group (4.554) take the form

$$\sigma_D^{ij} = \epsilon_{ijk} \Sigma^k = \epsilon_{ijk} 1 \times \sigma^k, \quad \sigma_D^{0i} = i\sigma^1 \times \sigma^i. \quad (4.558)$$

In each case, the first matrix mixes upper and lower components, whereas the second matrix acts on the up and down components of the spin.

Actually, it is this representation of the Dirac matrices which was stated in his original paper [5] and later in many textbooks. This is why it is referred to as the *standard representation*. In it, the *chirality matrix* γ^5 is not diagonal, as in the representation (4.542) of Section 4.11. To emphasize this property, the 4×4 -matrices (4.494) of Section 4.11 are referred to as *chiral representation* of the gamma matrices (also called *Weyl representation*).

4.12.3 Dirac's Original Derivation

Note that Dirac did not find his matrices from group-theoretic considerations. Instead of searching for a relativistic Schrödinger equation for an electron which, in contrast to the Klein-Gordon equation, contains only a single time derivative, so that there would be no negative-energy solutions [5], he looked for a time-independent electron field that satisfies the wave equation

$$\hat{H}\psi(\mathbf{x}) = \sqrt{\hat{\mathbf{p}}^2 + M^2}\psi(\mathbf{x}) = E\psi(\mathbf{x}) \quad (4.559)$$

with only the positive square-root. Since in relativistic theories energy and momentum appear on equal footing, he searched for a way to take an explicit square-root. For this he allowed $\psi(\mathbf{x}, t)$ to consist of several components, which would somehow represent the spin degrees of freedom of the electron. So he made the ansatz

$$\hat{H}_D \psi(\mathbf{x}) = (\alpha^i \hat{p}^i + \beta M) \psi(\mathbf{x}) = E \psi(\mathbf{x}), \quad (4.560)$$

with α_i, β being unknown matrices. Then he required that applying $\hat{H}_D$ twice to $\psi(\mathbf{x})$ should give $\hat{H}_D \psi(\mathbf{x}) = (\hat{\mathbf{p}}^2 + M^2) \psi(\mathbf{x}) = E^2 \psi(\mathbf{x})$. This led him to the algebraic relations

$$\begin{aligned} \{\alpha^i, \alpha^j\} &= \delta_{ij}, \\ \{\alpha^i, \beta\} &= 0, \\ \beta^2 &= 1. \end{aligned} \quad (4.561)$$

He solved these anticommutators with the matrices

$$\beta = \beta_D \equiv \gamma_D^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\alpha} = \boldsymbol{\alpha}_D \equiv \gamma_D^0 \boldsymbol{\gamma}_D = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}. \quad (4.562)$$

He could, of course, have solved them just as well in the chiral representation by

$$\beta \equiv \gamma^0, \quad \boldsymbol{\alpha} \equiv \gamma^0 \boldsymbol{\gamma} = \begin{pmatrix} -\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}. \quad (4.563)$$

By multiplying Eq. (4.560) with β and going over to a time-dependent equation by replacing E by $\hat{p}_0 = i\partial_{x^0}$, he obtained the Dirac equation in the form

$$(\gamma_D^\mu \hat{p}_\mu - M) \psi(x) = 0 \quad (4.564)$$

with the matrices

$$\gamma_D^0 \equiv \beta, \quad \gamma_D^i \equiv \beta \alpha^i. \quad (4.565)$$

The anticommutation relations (4.561) go over into the anticommutation relations (4.496) for the Dirac matrices

$$\{\gamma_D^\mu, \gamma_D^\nu\} = 2g^{\mu\nu}. \quad (4.566)$$

Inserting the bispinor form (4.492) of $\psi(x)$ into the Dirac equation (4.564), we find for upper and lower components $\xi(x)$ and $\eta(x)$ the equations

$$\begin{aligned} i\partial_t \xi(x) + i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \eta(x) &= M \xi(x), \\ i\partial_t \eta(x) + i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \xi(x) &= -M \eta(x). \end{aligned} \quad (4.567)$$

They can be combined to a single bispinor equation

$$(\partial_t + \boldsymbol{\alpha}_D \cdot \boldsymbol{\nabla} + iM\beta_D) \psi(x) = 0. \quad (4.568)$$

The equations (4.567) should be contrasted with their chiral versions, where they are given by the two lines in (4.486) for $M_1 = M_2 = M$:

$$\begin{aligned} i\partial_t \xi(x) - i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \xi(x) &= M \xi(x), \\ i\partial_t \eta(x) + i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \eta(x) &= M \eta(x). \end{aligned} \quad (4.569)$$

4.12.4 Maxwell Equations Written à la Dirac

It is interesting to note that the Maxwell equations (4.246) and (4.247) can be brought to a similar form using a spin-1 version of the matrix α_D :

$$\alpha_M \equiv \begin{pmatrix} 0 & \mathbf{L} \\ \mathbf{L} & 0 \end{pmatrix}, \quad (4.570)$$

where $(L_i)_{jk} = -i\epsilon_{ijk}$ are the generators (4.57) of rotation for a vector field. The analog of the Dirac bispinor is the “Maxwell bivector”:

$$\psi_M \equiv \begin{pmatrix} \mathbf{E} \\ i\mathbf{B} \end{pmatrix}. \quad (4.571)$$

The analogs of the two separate spinor equations (4.567) are the equations:

$$\begin{aligned} \partial_t \mathbf{E} + \mathbf{L} \cdot \nabla (i\mathbf{B}) &= 0, \\ \partial_t (i\mathbf{B}) + \mathbf{L} \cdot \nabla \mathbf{E} &= 0. \end{aligned} \quad (4.572)$$

These coincide with the Maxwell equations (4.246) and (4.247).

Note, however, that the bivectors (4.571) *cannot* be used to set up an action analog to Dirac’s (4.493) for zero mass. That must involve the local vector potential A^μ . A formulation which incorporates the dual symmetry between electricity and magnetism is nevertheless possible by defining the two bivector components $\mathcal{B}^1 = \mathbf{E}$, $\mathcal{B}^2 = \mathbf{B}$, and an associated pair of vector potentials $\mathcal{A}^a$ ($a = 1, 2$), whose two-dimensional curls are these fields:

$$\mathcal{B}^a = (\nabla \times \mathcal{A})^a. \quad (4.573)$$

The curls are formed with the Levi-Civita tensor $\epsilon_{ab} = -\epsilon_{ba}$ and $\epsilon_{12} = 1$. Then we can write the Maxwell action as

$$\mathcal{A} = \frac{1}{2} \int d^4x \mathcal{B}^a (\epsilon_{ab} \partial_t \mathcal{A}^b - \delta_{ab} \mathcal{B}^b). \quad (4.574)$$

Indeed, a variation of this action does yield the Maxwell equations since

$$\delta \mathcal{A} = \int d^4x \delta \mathcal{B}^b (\epsilon_{ab} \partial_t \mathcal{A}^b - \delta_{ab} \mathcal{B}^b), \quad (4.575)$$

which, after an integration by parts, becomes

$$\delta \mathcal{A} = \int d^4x \delta \mathcal{A}^a (\epsilon_{ab} \partial_t \mathcal{B}^b - \delta_{ab} \nabla \times \mathcal{B}^b). \quad (4.576)$$

The vanishing of the variation $\delta \mathcal{A}$ produces the equations

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \quad \partial_t \mathbf{E} - \nabla \times \mathbf{B} = 0, \quad (4.577)$$

which are precisely the Maxwell equations (4.246) and (4.247) [20].

These are invariant under the duality transformation

$$\delta \mathbf{E} = \alpha \mathbf{B}, \quad \delta \mathbf{B} = -\alpha \mathbf{E}, \quad (4.578)$$

and so is the action (4.576).

The second of the duality transformations (4.578) corresponds to a *nonlocal* transformation of the vector potential:

$$\delta \mathbf{A} = \alpha \nabla \times (\nabla^2)^{-1} \mathbf{E}. \quad (4.579)$$

When calculating the small-momentum limit (4.556) we have noted that the Dirac representation is most convenient for studying the nonrelativistic limit. This limit, in which $Mc^2 \rightarrow \infty$, corresponds in natural units to letting $M \rightarrow \infty$. The energies of slowly moving particles are very close to M , so that $(i\partial_t - M)\chi(x)$ is much smaller than $(i\partial_t + M)\eta(x)$, which can be approximated by $2M\eta(x)$. The lower equation in (4.567) can therefore be solved approximately by the relation between lower and upper spinor

$$\eta(x) \approx -i \frac{\boldsymbol{\sigma} \cdot \nabla}{2M} \xi(x). \quad (4.580)$$

We can also remove the fast temporal oscillations as in (4.156) and replace

$$\begin{pmatrix} \xi(x) \\ \eta(x) \end{pmatrix} \rightarrow e^{-iMc^2 t/\hbar} \frac{1}{\sqrt{2M}} \begin{pmatrix} \Psi(x) \\ \Phi(x) \end{pmatrix}. \quad (4.581)$$

If we solve again the lower equation by a relation like (4.580), the upper equation reduces to the Schrödinger equation for each spinor component:

$$i\partial_t \Psi(x) = -\frac{1}{2M} (\boldsymbol{\sigma} \cdot \nabla)^2 \Psi(x). \quad (4.582)$$

Using

$$(\boldsymbol{\sigma} \cdot \nabla)^2 = \sigma^i \sigma^j \nabla_i \nabla_j = [\delta^{ij} + i\epsilon_{ijk} \sigma^k] \nabla_i \nabla_j = \nabla^2, \quad (4.583)$$

this becomes

$$i\partial_t \Psi(x) = -\frac{1}{2M} \nabla^2 \Psi(x). \quad (4.584)$$

In the presence of electromagnetic interactions, the last step is nontrivial, yielding the nonrelativistic *Pauli equation* (6.114) with the correct magnetic moment of a Dirac particle.

In both representations, we can insert one equation into the other and find that $\xi(x)$ and $\eta(x)$ satisfy the Klein-Gordon equations (4.487) with $M_1 = M_2 = M$:

$$\begin{aligned} (-\partial^2 - M^2)\xi(x) &= 0, \\ (-\partial^2 - M^2)\eta(x) &= 0. \end{aligned} \quad (4.585)$$

This follows simply from the Dirac equation (4.500) upon multiplication by $(i\partial\!\!\!/ + M)$ and working out

$$(i\partial\!\!\!/ + M)(i\partial\!\!\!/ - M)\psi(x) = (-\partial^2 - M^2)\psi(x) = (-\partial^2 - M^2)\psi(x). \quad (4.586)$$

In the massless case, the Dirac equations (4.567) have a very similar structure to Maxwell's equations (4.246) and (4.247):

$$\begin{aligned}\partial_t \mathbf{B} + \nabla \times \mathbf{E} &= 0, \\ \partial_t \mathbf{E} - \nabla \times \mathbf{B} &= 0.\end{aligned}\tag{4.587}$$

To see this similarity we rewrite the cross product with the help of the 3×3 -generators (4.57) of the rotation group, $(L_i)_{jk} = -i\epsilon_{ijk}$, where they read

$$\begin{aligned}i\partial_t \mathbf{E} + i(\mathbf{L} \cdot \nabla)(i\mathbf{B}) &= 0, \\ i\partial_t(i\mathbf{B}) + i(\mathbf{L} \cdot \nabla)\mathbf{E} &= 0,\end{aligned}\tag{4.588}$$

thus becoming quite similar to the Dirac equations (4.567) derived from Dirac's representation of γ -matrices. The reader is encouraged to discuss the analogy between the transformation properties of (ξ, η) in Dirac's representation and $(\mathbf{E}, i\mathbf{B})$ and the generators $\boldsymbol{\sigma}$ and $\mathbf{L}$.

4.12.5 Pauli-Villars Equation for the Klein-Gordon Field

It is worth mentioning that Dirac's procedure of deducing a matrix version of the relativistic Schrödinger equation (4.559) has other solutions that is not linear in the momentum as $\hat{H}_D$ in (4.560), for example:

$$\hat{H}_{\text{FV}} = \frac{\hat{p}^2}{2M}(\sigma_3 + i\sigma_2) + M\sigma_3.\tag{4.589}$$

The subscript FV indicates that this Hamiltonian was first proposed by Feshbach and Villars [17]. Here Pauli matrices have no relation to spin. They are merely employed to specify the 2×2 -matrix $\hat{H}_{\text{FV}}$. By using the multiplication rules (4.464), it is easy to verify that the 2×2 -matrix $\hat{H}_{\text{FV}}^2$ has the same square $\hat{H}_{\text{FV}}^2 = \hat{\mathbf{p}}^2 + M^2$ as the 4×4 Dirac matrix H_D of Eq. (4.560). Thus the solutions of the equation $\hat{H}_{\text{FV}}\psi(\mathbf{x}) = E\psi(\mathbf{x})$ have again the proper relativistic energy-momentum relation. However, contrary to the solutions of the Dirac equation (4.560), they carry no spin. In fact, a field theory based on the Lagrangian density

$$\mathcal{L} = \psi^*(\mathbf{x}, t)(i\partial_t - \hat{H}_{\text{FV}})\psi(\mathbf{x}, t)\tag{4.590}$$

is completely equivalent to the Klein-Gordon theory of scalar particles.

4.12.6 Charge Conjugation

In Section 4.5.4 we observed that the action of a scalar field was invariant under an extra discrete symmetry not related to the Lorentz group, namely charge conjugation. It consisted of a simple exchange of the scalar field by its complex conjugate. A similar invariance can be found for the action of the Dirac field. There is only one complication: We must make sure that this operation commutes with the Lorentz

group. Thus we must form linear combinations of the components of the conjugate bispinor $\psi^*(x)$ which transform again like the original bispinor $\psi(x)$. Let us call this new bispinor

$$\psi^c(x) \equiv C\bar{\psi}^T(x), \quad (4.591)$$

where the superscript T on the right-hand side indicates a transposition of the row vector $\bar{\psi}$, which makes ψ^c a column vector. The operation of charge conjugation is then defined by

$$\psi(x) \xrightarrow{C} \psi'_C(x) = \eta_C \psi^c(x), \quad (4.592)$$

with a phase

$$\eta_C = \pm 1. \quad (4.593)$$

The matrix C is determined by the requirement that $\psi'_C(x)$ must satisfy the Dirac equation:

$$(i\cancel{\partial} - M)\psi'_C(x) = 0. \quad (4.594)$$

Inserting the right-hand side of (4.592), this reads

$$(i\cancel{\partial} - M)C\bar{\psi}^T(x) = 0, \quad (4.595)$$

or

$$[iC^{-1}\gamma^\mu C\partial_\mu - M]\bar{\psi}^T(x) = 0. \quad (4.596)$$

Its transposed form is

$$\bar{\psi}(x)[i(C^{-1}\gamma^\mu C)^T \overleftarrow{\partial}_\mu - M] = 0. \quad (4.597)$$

Consider, on the other hand, the adjoint of the Dirac equation

$$(i\gamma^\mu\partial_\mu - M)\psi(x) = 0, \quad (4.598)$$

which is

$$\psi^\dagger(x)(-i\gamma^{\mu\dagger} \overleftarrow{\partial}_\mu - M) = 0. \quad (4.599)$$

Multiplying this by γ^0 from the right and using the fact that

$$(\gamma_0)^{-1}\gamma^{\mu\dagger}\gamma^0 = \gamma^\mu, \quad (4.600)$$

we see that

$$\bar{\psi}(x)(-i\gamma^\mu \overleftarrow{\partial}_\mu - M) = 0. \quad (4.601)$$

Comparing this with (4.597) we conclude that $\psi'_T(x)$ satisfies the Dirac equation if the matrix C fulfills the identity

$$C^{-1}\gamma^\mu C = -\gamma^{\mu T}. \quad (4.602)$$

In both the chiral and the Dirac representation, the transposition of γ^μ changes only the sign of γ^2 . A matrix C with this property in the chiral representation is given by

$$C = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}, \quad (4.603)$$

where c is the 2×2 matrix

$$c = -i\sigma^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (4.604)$$

This matrix is the two-dimensional representation of rotation around the 2-axis by an angle π :

$$c = e^{-i\pi\sigma^2/2}, \quad (4.605)$$

as can easily be verified by using (4.456) [or by a direct power series expansion as in (4.455)]. From this rotation property it follows directly [or via Lie's expansion formula (4.105) as in (4.478)] that

$$c^{-1} \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix} c = \begin{pmatrix} -\sigma^1 \\ \sigma^2 \\ -\sigma^3 \end{pmatrix}, \quad (4.606)$$

and we find

$$\begin{aligned} \begin{pmatrix} c^{-1} & 0 \\ 0 & -c^{-1} \end{pmatrix} \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix} \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} &= \begin{pmatrix} 0 & -c^{-1}\sigma^\mu c \\ -c^{-1}\tilde{\sigma}^\mu c & 0 \end{pmatrix} \\ &= (-\gamma^0, \gamma^1, -\gamma^2, \gamma^3) = -\gamma^{\mu T}, \end{aligned} \quad (4.607)$$

so that (4.602) is fulfilled.

Note that the 2×2 -matrix c satisfies the identities

$$c = -c^T = -c^{-1} = -c^\dagger, \quad (4.608)$$

which also hold for the 4×4 -matrices C :

$$C = C^* = -C^T = -C^{-1} = -C^\dagger. \quad (4.609)$$

Using these properties, we find that the conjugate Dirac field behaves under the transformation (4.592) as

$$\bar{\psi}(x) \xrightarrow{C} \bar{\psi}'_C(x) = -\eta_C^* \bar{\psi}^c(x), \quad (4.610)$$

with

$$\bar{\psi}^c(x) \equiv \psi^T(x)C. \quad (4.611)$$

This follows from the simple calculation:

$$\bar{\psi} = \psi^{*T} \gamma^0 \rightarrow (C\bar{\psi}^T)^{*T} \gamma^0 = (C\gamma^{0T} \psi^*)^{*T} \gamma^0 = \psi^T \gamma^0 C^T \gamma^0 = -\psi^T C = -\bar{\psi}^c. \quad (4.612)$$

Note that

$$\bar{\psi}^c(x) = \overline{\psi^c(x)}, \quad (4.613)$$

since

$$\bar{\psi}^c = \psi^{c\dagger} \gamma^0 = (C\bar{\psi}^T)^\dagger \gamma^0 = (\bar{\psi}^T)^\dagger C^\dagger \gamma^0 = (\psi^\dagger \gamma^0)^{T\dagger} C^\dagger \gamma^0 = \psi^T \gamma^{0T\dagger} C^\dagger \gamma^0 = \psi^T C. \quad (4.614)$$

The minus sign on the right-hand side of Eq. (4.610) will be seen in Chapter 7 to have the important consequence that antiparticles have the opposite intrinsic parity of particles.

By writing the charge conjugation matrix (4.603) as

$$C = i\gamma^0\gamma^2, \quad (4.615)$$

we can take the result directly to the Dirac representation (4.550) where⁹

$$C_D \equiv -i\gamma_D^0\gamma_D^2 = -S_D \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} S_D^{-1} = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}. \quad (4.616)$$

The reason for the name *charge conjugation* is the same as for the scalar field in (4.227). In contrast to the scalar case, however, this cannot simply be seen by studying the effect of charge conjugation upon the conserved particle current. In contrast to Eq. (4.229) which shows that the current reverses its sign under charge conjugation, the operation (4.591) with C satisfying (4.602) leaves the current density (4.502) unchanged:

$$j^\mu(x) \xrightarrow{C} j^{\mu'}(x) = j^\mu(x). \quad (4.617)$$

This follows directly from

$$\begin{aligned} j^\mu(x) &= \bar{\psi}(x)\gamma^\mu\psi(x) \xrightarrow{C} -\psi^T(x)C^{-1}\gamma^\mu C\bar{\psi}^T(x) \\ &= \psi^T(x)\gamma^{\mu T}\bar{\psi}^T(x) = \bar{\psi}(x)\gamma^\mu\psi(x) = j^\mu(x). \end{aligned} \quad (4.618)$$

The proper physical effect will only be reached after field quantization. This turns the fields into anticommuting fermion operators which produce a sign change in the last step of the transformation (4.618), thus justifying the name *charge conjugation* for the operation (4.591).

It is possible to imitate this effect of quantization at the classical level by imagining the classical fields to be *anticommuting* or *Grassmann variables*. Such fields will be introduced in Chapter 14 and used in Chapter 25.

4.12.7 Time Reversal

Let us now see how time reversal acts upon the Dirac field. Under time reversal, the direction of a particle momentum and angular momentum are both reversed, and the generators of the Lorentz group are subject to an automorphism (4.132). The same automorphism is now applied to the 4×4 bispinor representation $D(T)$. Writing $D(T) = \eta_T D_T$, we must have

$$D_T^{-1}D(L_i)D_T = -D(L_i)^*, \quad D_T^{-1}D(M_i)D_T = -D(M_i)^*. \quad (4.619)$$

⁹The minus sign is added to agree with Dirac's sign convention for C_D .

The explicit form of the transformation matrix D_T is now determined by the requirement that the time-reversed field $\psi'_T(x)$ defined by

$$\psi(x) \xrightarrow{T} \psi'_T(x) = D(T)\psi^*(x_T), \quad (4.620)$$

with $x_T = -\tilde{x}$ has to satisfy the Dirac equation

$$(i\gamma^\mu \partial_\mu - M)\psi'^*_T(x) = 0. \quad (4.621)$$

The reason for the complex conjugation of the field on the right-hand side of (4.620) was discussed in Subsection 4.5.3, where it was shown that the Schrödinger equation for the time-reversed Schrödinger operator carries a complex conjugation [see Eq. (4.222)]. This is needed to keep the energy in the time-dependent phase factor $e^{ip^0 t}$ positive for $t \rightarrow -t$.

Inserting (4.620) into (4.621) we obtain

$$D^{-1}(T)(i\gamma^\mu \partial_\mu - M)D(T)\psi^*(-\tilde{x}) = 0. \quad (4.622)$$

From the original Dirac equation we know that

$$(-i\tilde{\gamma}^\mu \partial_\mu - M)\psi(-\tilde{x}) = 0, \quad (4.623)$$

or

$$(i\tilde{\gamma}^{\mu*} \partial_\mu - M)\psi^*(-\tilde{x}) = 0. \quad (4.624)$$

To be compatible with (4.622), the matrix $D(T)$ has to satisfy

$$D^{-1}(T)\gamma^{\mu*}D(T) = \tilde{\gamma}^\mu. \quad (4.625)$$

In both the chiral and the Dirac representation, the γ^μ -matrices have the property

$$\gamma^{\mu*} = \tilde{\gamma}^{\mu T}. \quad (4.626)$$

Using the property (4.602) of the matrix C , we can substitute

$$\gamma^{\mu T} = -C\gamma^\mu C^{-1}, \quad (4.627)$$

and the condition (4.625) becomes

$$D^{-1}(T)C\tilde{\gamma}^\mu C^{-1}D(T) = -\tilde{\gamma}^\mu. \quad (4.628)$$

This is satisfied by

$$D(T) = \eta_T C \gamma_5. \quad (4.629)$$

It is easy to verify that this matrix transforms the generators of the Lorentz group for Dirac spinors (4.518) in the way required by (4.619):

$$D^{-1}(T)S^{\mu\nu}D(T) = -S^{\mu\nu*}. \quad (4.630)$$

4.12.8 Transformation Properties of Currents

An important role in interacting field theory is played by bilinear combinations of the Dirac field formed with 16 combinations of Dirac matrices, collectively called Γ , which are all selfadjoint under the Dirac conjugation (4.495):

$$\bar{\Gamma} = \gamma_0 \Gamma^\dagger \gamma_0. \quad (4.631)$$

These are the scalar, vector, tensor, axialvector, and pseudoscalar matrices:

$$\Gamma_S \equiv 1, \quad \Gamma_V^\mu \equiv \gamma^\mu, \quad \Gamma_T^{\mu\nu} \equiv \sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu], \quad \Gamma_A^\mu \equiv \gamma^\mu \gamma_5, \quad \Gamma_P \equiv i\gamma_5, \quad (4.632)$$

which form a so-called *Clifford algebra*. They are used to define corresponding *current densities*. The most important of these is the *vector current density*

$$j_V^\mu(x) = \bar{\psi}(x) \gamma^\mu \psi(x), \quad (4.633)$$

which is the source of electromagnetism (see Chapter 12). By sandwiching the other Γ -matrices between two Dirac fields, one obtains fields which transform under the Lorentz group as scalar, tensor, axialvector, and pseudoscalar fields. For instance,

$$j_A^\mu(x) = \bar{\psi}(x) \gamma^\mu \gamma_5 \psi(x) \quad (4.634)$$

is an axial vector current which, together with the vector current, is responsible for weak interactions. The combination

$$j_T^{\mu\nu}(x) = \frac{i}{2} \bar{\psi}(x) [\gamma^\mu, \gamma^\nu] \psi(x) \quad (4.635)$$

is a tensor current related to the current spin density to be introduced in Section 8.6.2. The different possible current densities are shown in Table 4.12.8, which also lists the behavior of these currents under the discrete transformations T, C, P , and their various combinations.

TABLE 4.1 Transformation properties of various composite fields $j_S = \bar{\psi}\psi$, $j_V^\mu = \bar{\psi}\gamma^\mu\psi$, $j_T^{\mu\nu} = \bar{\psi}\frac{i}{2}[\gamma^\mu, \gamma^\nu]\psi$, $j_A^\mu = \bar{\psi}\gamma^\mu\gamma_5\psi$, $P = \bar{\psi}i\gamma_5\psi$. The wiggles on vectors and tensors denote the parity transformed objects for each index. For the charge-conjugated composites we have inserted the minus-sign arising after second quantization explained after Eq. (4.618).

	$j_S(x)$ $\bar{\psi}\psi$	$j_V(x)$ $\bar{\psi}\gamma^\mu\psi$	$j_T(x)$ $\bar{\psi}\frac{i}{2}[\gamma^\mu, \gamma^\nu]\psi$	$j_A^\mu(x)$ $\bar{\psi}\gamma^\mu\gamma_5\psi$	$j_P(x)$ $\bar{\psi}i\gamma_5\psi$
P	$j_S(\tilde{x})$	$\tilde{j}_V(\tilde{x})$	$\tilde{j}_T(\tilde{x})$	$-\tilde{j}_A(\tilde{x})$	$-j_P(\tilde{x})$
C	$j_S(x)$	$-j_V(x)$	$-j_T(x)$	$j_A(x)$	$j_P(x)$
T	$j_S(-\tilde{x})$	$\tilde{j}_V(\tilde{x})$	$-\tilde{j}_T(-\tilde{x})$	$\tilde{j}_A(-\tilde{x})$	$-j_P(-\tilde{x})$
PCT	$j_S(-x)$	$-j_V(-x)$	$j_T(-x)$	$-j_A(-x)$	$j_P(-x)$

4.13 Majorana Fields

In the chiral and Dirac representations of γ^μ -matrices used so far, the bispinor fields $\psi(x)$ are necessarily complex since only σ^2 , and thus γ^2 , is imaginary, whereas $\sigma^0, \sigma^1, \sigma^3$ and thus $\gamma^0, \gamma^1, \gamma^3$ are real. One may then wonder whether the Dirac equation $(i\partial\!\!\!/ - M)\psi(x) = 0$, and thus the Lorentz transformations $e^{-i\omega_{\mu\nu}S^{\mu\nu}}$, necessarily mix real and imaginary parts of a spin-1/2 field. It can easily be seen that this is not so. The complex conjugate Dirac fields are transformed by the 4×4 -representation matrices

$$D^*(\Lambda) = \begin{pmatrix} D^{(\frac{1}{2},0)*} & 0 \\ 0 & D^{(0,\frac{1}{2})*} \end{pmatrix}. \quad (4.636)$$

As far as rotations are concerned, $D^{(\frac{1}{2},0)*}$ and $D^{(0,\frac{1}{2})*}$ are equivalent to the original representations by a similarity transformation:

$$\begin{aligned} D^{(\frac{1}{2},0)*} &= c^{-1} D^{(\frac{1}{2},0)} c, \\ D^{(0,\frac{1}{2})*} &= c^{-1} D^{(0,\frac{1}{2})} c, \end{aligned} \quad (4.637)$$

with $c = -i\sigma^2$. This follows directly by writing the 2×2 rotation matrices in the explicit form

$$(e^{-i\varphi \cdot \sigma/2})^* = e^{i\varphi \cdot \sigma^*/2}. \quad (4.638)$$

The complex conjugation reverses the 1- and 3-components in the exponent, since σ^1, σ^3 are real, while preserving the 1-component, since σ^2 is imaginary. Using (4.606) we see that

$$c^{-1} \boldsymbol{\sigma} c = -\boldsymbol{\sigma}^*, \quad (4.639)$$

so that the right-hand side of (4.638) becomes

$$e^{i\varphi \cdot \sigma^*} = c^{-1} e^{-i\varphi \cdot \sigma/2} c, \quad (4.640)$$

which is the same as (4.637). Therefore, the charge-conjugated bispinor

$$\psi^c(x) \equiv C \bar{\psi}^T(x) = C \gamma^{0T} \psi^*(x) = \begin{pmatrix} 0 & -c \\ c & 0 \end{pmatrix} \psi^*(x) \quad (4.641)$$

transforms under rotations just as $\psi(x)$ itself.

Consider now pure Lorentz transformations of the complex-conjugate bispinor $\psi^*(x)$:

$$\psi^*(x) \xrightarrow{B} \psi^{*'}(x') = \begin{pmatrix} e^{-\zeta \cdot \sigma^*/2} & 0 \\ 0 & e^{\zeta \cdot \sigma^*/2} \end{pmatrix} \psi^*(x). \quad (4.642)$$

With (4.639), the right-hand side becomes

$$\begin{pmatrix} c^{-1} e^{\zeta \cdot \sigma/2} c & 0 \\ 0 & c^{-1} e^{-\zeta \cdot \sigma/2} c \end{pmatrix} \psi^*(x). \quad (4.643)$$

Writing $\psi(x)$ as in (4.492) we see that the upper complex conjugate components $c\xi^*(x)$ transform like the lower components η , whereas the lower components $c\eta^*(x)$ transform like $\xi(x)$. Hence also under Lorentz transformations, $\psi^c(x)$ behaves like ψ , and we can write for the entire proper Lorentz group the transformation law

$$\psi^c(\Lambda x) = D(\Lambda)\psi^c(x), \quad (4.644)$$

with the transformation matrix $D(\Lambda)$ satisfying the relation

$$C^{-1}\gamma^{0-1}D^*(\Lambda)\gamma^0C = C^{-1}\bar{D}(\Lambda)C = D(\Lambda) \quad (4.645)$$

[recalling the definition of Dirac-adjoint matrices (4.495)]. Since ψ and ψ^c both transform in the same way under $D(\Lambda)$ we may form the combinations

$$\begin{aligned} \chi &\equiv \frac{1}{\sqrt{2}}(\psi + \psi^c), \\ \chi' &\equiv \frac{1}{\sqrt{2}i}(\psi - \psi^c), \end{aligned} \quad (4.646)$$

which are separately irreducible representations of the Lorentz group and eigenstates of charge conjugation with charge parity $\pm\eta_C$. Since the original field had 4 complex degrees of freedom, these combinations can only have half as many degrees of freedom, i.e., four real degrees of freedom. Explicitly, the components of the bispinors (4.646) satisfy, in the chiral representation, the relations:

$$\chi_1^* = -\chi_4, \quad \chi_2^* = \chi_3, \quad (4.647)$$

$$\chi_1' = -\chi_4'^*, \quad \chi_2' = \chi_3'^*. \quad (4.648)$$

We may now ask whether there are γ -matrices which make these real degrees of freedom explicit. This would be the case if we would find a representation of the γ -matrices in which $C\gamma^0$ is the unit matrix. Then ψ^c would be equal to ψ^* and the fields χ, χ' would be purely real. Such a representation does indeed exist. It is given by the γ -matrices in the so-called *Majorana representation*:

$$\begin{aligned} \gamma_M^0 &= \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, & \gamma_M^1 &= \begin{pmatrix} i\sigma^3 & 0 \\ 0 & i\sigma^3 \end{pmatrix}, \\ \gamma_M^2 &= \begin{pmatrix} 0 & -\sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, & \gamma_M^3 &= \begin{pmatrix} -i\sigma^1 & 0 \\ 0 & -i\sigma^1 \end{pmatrix}. \end{aligned} \quad (4.649)$$

They are obtained from γ^μ in the chiral representation (4.494) by a similarity transformation

$$\gamma_M^\mu = S_M \gamma^\mu S_M^{-1}, \quad (4.650)$$

with the transformation matrix

$$S_M = \frac{1}{4} \begin{pmatrix} 1 - \sigma^2 & 1 + \sigma^2 \\ 1 + \sigma^2 & -1 + \sigma^2 \end{pmatrix}. \quad (4.651)$$

The action expressed with Majorana matrices γ_M^μ is invariant under Lorentz transformations

$$D_M(\Lambda) = S_M D(\Lambda) S_M^{-1}. \quad (4.652)$$

In the Majorana representation (4.649), all γ -matrices are purely imaginary, so that the Dirac equation

$$(i\gamma_M^\mu \partial_\mu - M)\chi(x) = 0 \quad (4.653)$$

is purely real. The complex conjugate field satisfies the same equation as χ itself:

$$(i\gamma_M^\mu \partial_\mu - M)\chi^*(x) = 0. \quad (4.654)$$

A matrix C of complex-conjugation satisfying (4.602) is now given by

$$C_M = \gamma_M^0 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} = i \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}. \quad (4.655)$$

In contrast to the other two representations, the normalization is $C_M^2 = 1$ rather than $C^2 = -1$, satisfying

$$C_M = -C_M^T = C_M^{-1} = C_M^\dagger \quad (4.656)$$

rather than (4.609). This is more convenient here since we want two successive applications of the operations (4.641) to produce the identity operation $(\psi^c)^c = \psi$. That requires $(C_M \gamma^{0T})^2 = 1$. In the other two representations of the gamma matrices where C anticommutes with γ^0 , one has $C^2 = -1$. In the Majorana representation where C_M and γ^0 commute, one has $C_M^2 = 1$. Note that up to a factor i , the matrix C_M happens to coincide with C_D of Eq. (4.616).

It should be pointed out that C_M is not related to C by a similarity transformation $S_M C S_M^{-1} = i\gamma_M^0 \gamma_M^2$, since γ_M^μ does not have the same sign changes under transposition as γ^μ and γ_D^μ : Whereas $\gamma^{\mu T} = (\gamma^0, -\gamma^1, \gamma^2, -\gamma^3)$ holds also for the Dirac matrices γ_D^μ , the Majorana matrices satisfy $\gamma_M^{\mu T} = (-\gamma^0, \gamma^1, \gamma^2, \gamma^3)$.

According to (4.936), $C\gamma^0$ is equal to the unit matrix, so that

$$\psi^C = \psi^*. \quad (4.657)$$

The bispinors (4.646) reduce to

$$\chi \equiv \frac{1}{\sqrt{2}}(\psi + \psi^*), \quad \chi' \equiv \frac{1}{\sqrt{2}i}(\psi - \psi^*), \quad (4.658)$$

which are now real fields transforming irreducibly under the Lorentz group. They are called *Majorana spinors*.

Under the operation of charge conjugation they transform into themselves

$$\chi(x) \xrightarrow{C} \chi'_C(x) = \eta_C \chi(x), \quad (4.659)$$

with a charge parity $\eta_C = \pm 1$.

Note that between Majorana spinors $\chi(x)$, the quadratic expressions $\bar{\chi}\gamma_M^\mu\chi$ and $\bar{\chi}\gamma_M^\mu\gamma_M^\nu\chi$ are identically zero.

The γ^5 -matrix (4.542) has now the form

$$\gamma_{5M} = i\gamma_M^0\gamma_M^1\gamma_M^2\gamma_M^3 = \begin{pmatrix} \sigma^2 & 0 \\ 0 & -\sigma^2 \end{pmatrix} = i \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} \equiv \gamma_M^5. \quad (4.660)$$

In recent years solutions of the Majorana type have become relevant for describing electrons in condensed matter and this has led to a resurgence of applications of this subject [9].

4.13.1 Plane-Wave Solutions of Dirac Equation

By analogy with the scalar case we now seek for all plane-wave solutions of the Dirac equation (4.500):

$$(i\partial - M)\psi(x) = 0. \quad (4.661)$$

We make an ansatz

$$f_{\mathbf{p}s_3}(x) \equiv u(\mathbf{p}, s_3) \frac{e^{-ipx}}{\sqrt{Vp^0/M}}, \quad f_{\mathbf{p}s_3}^c(x) \equiv v(\mathbf{p}, s_3) \frac{e^{ipx}}{\sqrt{Vp^0/M}}, \quad (4.662)$$

thereby distinguishing, as in (4.180), waves with positive and negative frequencies, and allowing for a spin orientation index s_3 . Due to the presence of Dirac indices, the solutions will no longer be merely the complex-conjugates of each other, as in (4.152). The superscript of $f_{\mathbf{p}s_3}^c(x)$ indicates the appropriate generalization of complex conjugation.

If the wave functions in (4.662) are supposed to solve the Dirac equation (4.661), the bispinors $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$ in momentum space have to satisfy the Dirac equations in momentum space

$$(\not{p} - M)u(\mathbf{p}, s_3) = 0, \quad (\not{p} + M)v(\mathbf{p}, s_3) = 0. \quad (4.663)$$

The normalization of these wave functions will be chosen as in the scalar case by requiring the charge (4.175) of these solutions to be of unit size, with the charge density $j^0(x)$ of Eq. (4.502).

In Section 4.4 we have introduced scalar products for solutions of the Klein-Gordon equation (4.177) with the help of the zeroth component of the conserved particle current. This is generalized to the Dirac case by introducing the scalar products

$$\begin{aligned} (f_{\mathbf{p}'s'_3}, f_{\mathbf{p}s_3}) &\equiv \int d^3x \bar{f}_{\mathbf{p}'s'_3}(\mathbf{x}, t) \gamma^0 f_{\mathbf{p}s_3}(\mathbf{x}, t) = \delta_{\mathbf{p}', \mathbf{p}} \delta_{s'_3, s_3}, \\ (f_{\mathbf{p}'s'_3}^c, f_{\mathbf{p}s_3}^c) &\equiv \int d^3x \bar{f}_{\mathbf{p}'s'_3}^c(\mathbf{x}, t) \gamma^0 f_{\mathbf{p}s_3}^c(\mathbf{x}, t) = \delta_{\mathbf{p}', \mathbf{p}} \delta_{s'_3, s_3}, \\ (f_{\mathbf{p}'s'_3}^c, f_{\mathbf{p}s_3}) &\equiv \int d^3x \bar{f}_{\mathbf{p}'s'_3}^c(\mathbf{x}, t) \gamma^0 f_{\mathbf{p}s_3}(\mathbf{x}, t) = 0, \\ (f_{\mathbf{p}'s'_3}, f_{\mathbf{p}s_3}^c) &\equiv \int d^3x \bar{f}_{\mathbf{p}'s'_3}(\mathbf{x}, t) \gamma^0 f_{\mathbf{p}s_3}^c(\mathbf{x}, t) = 0. \end{aligned} \quad (4.664)$$

From these we deduce the orthonormality conditions for the bispinors:

$$\begin{aligned}\bar{u}(\mathbf{p}, s'_3)\gamma^0 u(\mathbf{p}, s_3) &= \frac{p^0}{M}\delta_{s'_3, s_3}, & \bar{v}(\mathbf{p}, s'_3)\gamma^0 v(\mathbf{p}, s_3) &= \frac{p^0}{M}\delta_{s'_3, s_3}, \\ \bar{u}(\mathbf{p}, s'_3)\gamma^0 v(-\mathbf{p}, s_3) &= 0, & \bar{v}(-\mathbf{p}, s'_3)\gamma^0 u(\mathbf{p}, s_3) &= 0.\end{aligned}\quad (4.665)$$

The reversal of the momentum in $v(-\mathbf{p}, s_3)$ appears in the second line since the spatial integrals in (4.665) enforce opposite momenta in scalar products between solutions of positive and negative frequency. According to this, vanishing scalar products in bispinor space are necessary to produce orthogonality.

In contrast to the scalar product (4.177) for Klein-Gordon wave functions, both positive- and negative-frequency solutions have now a positive charge, since for any spinor, $\bar{\psi}(x)\gamma^0\psi(x) = \psi^\dagger(x)\psi(x)$ is positive definite.

The explicit form of the bispinors $u(\mathbf{p})$ and $v(\mathbf{p})$ depends on the representation employed for the matrices γ^μ . The different cases will be discussed separately. In an infinite volume we use plane wave functions analogous to (4.181):

$$f_{\mathbf{p} s_3}(x) \equiv u(\mathbf{p}, s_3)e^{-ipx}, \quad f_{\mathbf{p} s_3}^c(x) \equiv v(\mathbf{p}, s_3)e^{ipx}. \quad (4.666)$$

They satisfy the Lorentz-invariant orthonormality conditions:

$$\begin{aligned}(f_{\mathbf{p}' s'_3}, f_{\mathbf{p} s_3}) &\equiv \int d^3x \bar{f}_{\mathbf{p}' s'_3}(\mathbf{x}, t)\gamma^0 f_{\mathbf{p} s_3}(\mathbf{x}, t) = 2p^0 \delta(\mathbf{p}' - \mathbf{p})\delta_{s'_3, s_3}, \\ (f_{\mathbf{p}' s'_3}^c, f_{\mathbf{p} s_3}^c) &\equiv \int d^3x \bar{f}_{\mathbf{p}' s'_3}^c(\mathbf{x}, t)\gamma^0 f_{\mathbf{p} s_3}^c(\mathbf{x}, t) = 2p^0 \delta(\mathbf{p}' - \mathbf{p})\delta_{s'_3, s_3}, \\ (f_{\mathbf{p}' s'_3}^c, f_{\mathbf{p} s_3}) &\equiv \int d^3x \bar{f}_{\mathbf{p}' s'_3}^c(\mathbf{x}, t)\gamma^0 f_{\mathbf{p} s_3}(\mathbf{x}, t) = 0, \\ (f_{\mathbf{p}' s'_3}, f_{\mathbf{p} s_3}^c) &\equiv \int d^3x \bar{f}_{\mathbf{p}' s'_3}(\mathbf{x}, t)\gamma^0 f_{\mathbf{p} s_3}^c(\mathbf{x}, t) = 0.\end{aligned}\quad (4.667)$$

Spinors in Chiral Representation

Using the chiral representation (4.494) for γ^μ , Eqs. (4.663) take the form

$$\begin{pmatrix} 0 & p\sigma \\ p\tilde{\sigma} & 0 \end{pmatrix} u(\mathbf{p}, s_3) = M u(\mathbf{p}, s_3), \quad \begin{pmatrix} 0 & p\sigma \\ p\tilde{\sigma} & 0 \end{pmatrix} v(\mathbf{p}, s_3) = -M v(\mathbf{p}, s_3). \quad (4.668)$$

We can immediately write down 4×2 -matrices solving these equations. The first is solved by

$$u(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix}, \quad (4.669)$$

and the second by

$$v(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix}. \quad (4.670)$$

This follows from the matrix identities

$$p\sigma\sqrt{\frac{p\tilde{\sigma}}{M}} \equiv M\sqrt{\frac{p\tilde{\sigma}^2}{M}}\sqrt{\frac{p\tilde{\sigma}}{M}} = M\sqrt{\frac{p\tilde{\sigma}}{M}}\sqrt{\frac{p\sigma}{M}\frac{p\tilde{\sigma}}{M}} \quad (4.671)$$

and

$$p\sigma p\tilde{\sigma} = \frac{1}{2}(p_\mu p_\nu \sigma^\mu \tilde{\sigma}^\nu + p_\mu p_\nu \tilde{\sigma}^\mu \sigma^\nu) = p_\mu p_\nu = M^2, \quad (4.672)$$

the latter being a direct consequence of (4.489).

The 4×2 -matrices (4.669) and (4.670) can be multiplied by an arbitrary 2×2 -matrix from the right, and they will still solve the equations (4.668). There are several convenient choices for such a matrix with different advantages, as we shall see below. The two-column vectors in the 4×2 -matrices form independent bispinor solutions of Eqs. (4.668). The projection into these is accomplished by multiplication from the right with two unit spinors, the Pauli spinors (4.446)

$$\chi(\tfrac{1}{2}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi(-\tfrac{1}{2}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (4.673)$$

By multiplying the 4×2 -matrices (4.669) with the unit spinors (4.673), we obtain the *canonical bispinors*

$$u(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3). \quad (4.674)$$

The unit spinors (4.673) are eigenvectors of the spin-1/2 generator $L_3 = \sigma^3/2$ of the rotation group:

$$L_3 \chi(\tfrac{1}{2}) = \tfrac{1}{2} \chi(\tfrac{1}{2}), \quad L_3 \chi(-\tfrac{1}{2}) = -\tfrac{1}{2} \chi(-\tfrac{1}{2}). \quad (4.675)$$

The associated bispinors at rest:

$$u(\mathbf{0}, \tfrac{1}{2}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(\tfrac{1}{2}) \\ \chi(\tfrac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad u(\mathbf{0}, -\tfrac{1}{2}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(-\tfrac{1}{2}) \\ \chi(-\tfrac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \quad (4.676)$$

are eigenstates of the 4×4 bispinor representation of the generator of rotations around the z -axis [recall (4.514)–(4.518)]:

$$S^3 = S^{12} = \frac{1}{2} \sigma^{12} = \frac{1}{2} \Sigma^3 = \frac{1}{2} \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}. \quad (4.677)$$

In order to construct explicit bispinors $v(\mathbf{p}, s_3)$ we do not directly multiply them with the unit spinors (4.673) from the right-hand side, as we did to obtain $u(\mathbf{p}, s_3)$ in (4.674), but we first use the above-observed freedom of multiplying (4.670) by an arbitrary 2×2 -matrix from the right. This is necessary to construct a spinor $v(\mathbf{p}, s_3)$

with the physically most appropriate transformation properties under Lorentz transformations.

From the 4×2 -matrices (4.670) it is possible to find directly the solutions $v(\mathbf{p}, s_3)$ of the second equation in (4.668). We simply define $v(\mathbf{p}, s_3)$ as the charge-conjugated spinor of $u(\mathbf{p}, s_3)$ by an operation of the form (4.591), i.e.,

$$v(\mathbf{p}, s_3) = C \bar{u}^T(\mathbf{p}, s_3). \quad (4.678)$$

It is easy to verify that this $v(\mathbf{p}, s_3)$ solves (4.668). For a proof we take

$$\bar{u}(\mathbf{p}, s_3) = u^\dagger(\mathbf{p}, s_3) \gamma^0 = \frac{1}{\sqrt{2}} \chi^\dagger(s_3) \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} & \sqrt{\frac{p\sigma}{M}} \end{pmatrix}, \quad (4.679)$$

and form

$$\bar{u}^T(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}}^T \\ \sqrt{\frac{p\sigma}{M}}^T \end{pmatrix} \chi^*(s_3). \quad (4.680)$$

Multiplying this by the charge-conjugation matrix C of (4.603) yields

$$C \bar{u}^T(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} c \sqrt{\frac{p\bar{\sigma}}{M}}^T \\ -c \sqrt{\frac{p\sigma}{M}}^T \end{pmatrix} \chi(s_3), \quad (4.681)$$

with $c = -i\sigma^2$ of Eq. (4.604). At this place we realize that due to the hermiticity property of the Pauli matrices (8.158) and (4.462), one has

$$\sigma^{\mu*} = \sigma^{\mu T}, \quad (4.682)$$

such that relation (4.639) implies the four-component relation

$$c \sigma^{\mu*} c^{-1} = c \sigma^{\mu T} c^{-1} = \tilde{\sigma}^\mu. \quad (4.683)$$

With this, the charge-conjugated spinor $u^c(\mathbf{p}, s_3) = C \bar{u}^T(\mathbf{p}, s_3)$ goes directly over into the bispinor

$$v(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} c \chi^*(s_3). \quad (4.684)$$

Thus, while the 4×2 -solutions $u(\mathbf{p})$ of Eq. (4.669) are multiplied by the Pauli spinors $\chi(s_3)$ of Eq. (4.673), the 4×2 -solutions $v(\mathbf{p})$ of Eq. (4.670) are multiplied from the right by the spinors

$$\chi^c(s_3) \equiv c \chi(s_3) = \chi(-s_3) (-1)^{s-s_3}. \quad (4.685)$$

These are called *charge-conjugated Pauli spinors*. Their explicit form is

$$\chi^c(s_3) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix}. \quad (4.686)$$

This construction is necessary to ensure that the Pauli spinors $v(\mathbf{p}, s_3)$ at rest have the same transformation behavior under rotations as the spinors $u(\mathbf{p}, s_3)$ at rest.

Under rotation, the original basis spinors $\chi(s_3)$ are multiplied by the 2×2 rotation matrix $e^{-i\phi \cdot \sigma/2}$:

$$\chi(s_3) \xrightarrow{R} \chi'(s_3) = e^{-i\phi \cdot \sigma/2} \chi(s_3) = \sum_{s'_3=-1/2}^{1/2} \chi(s'_3) \left(e^{-i\phi \cdot \sigma/2} \right)_{s_3, s'_3}. \quad (4.687)$$

The last step follows from the specific form (4.673) of the unit spinors. The same mixing occurs in the charge-conjugated spinors:

$$\chi^c(s_3) \xrightarrow{R} \chi'^c(s_3) = c\chi'^*(s_3) = ce^{i\phi \cdot \sigma^*/2} \chi^*(s_3). \quad (4.688)$$

Using (4.639), we see that

$$c^{-1} e^{-i\phi \cdot \sigma/2} c = e^{i\phi \cdot \sigma^*/2}, \quad (4.689)$$

so that the right-hand side becomes

$$e^{-i\phi \cdot \sigma/2} c\chi^*(s_3) = e^{-i\phi \cdot \sigma/2} \chi^c(s_3) = \sum_{s'_3=-1/2}^{1/2} \chi^c(s'_3) \left(e^{-i\phi \cdot \sigma/2} \right)_{s_3, s'_3}. \quad (4.690)$$

Thus $\chi^c(s_3)$ is indeed rotated precisely like $\chi(s_3)$.

At rest, the 4×2 -matrices (4.669) and (4.670) become

$$u(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix}, \quad v(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix}. \quad (4.691)$$

Hence the rotation properties of the bispinors $u(\mathbf{p}, s_3) = u(\mathbf{p})\chi(s_3)$ and $v(\mathbf{p}, s_3) = v(\mathbf{p})\chi^c(s_3)$ at rest are the same as those of $\chi(s_3)$ and $\chi^c(s_3)$. Explicitly, the bispinors $v(\mathbf{p}, s_3)$ at rest become

$$v(\mathbf{0}, \tfrac{1}{2}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(\tfrac{1}{2}) \\ -\chi^c(\tfrac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \quad v(\mathbf{0}, -\tfrac{1}{2}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(-\tfrac{1}{2}) \\ -\chi^c(-\tfrac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad (4.692)$$

to be compared with (4.676) for $u(\mathbf{0}, s_3)$.

For the bispinors at rest in Eqs. (4.676) and (4.692), the Dirac equations in momentum space (4.663) take the simple form

$$M(\gamma^0 - 1)u(\mathbf{0}, s_3) = 0, \quad M(\gamma^0 + 1)v(\mathbf{0}, s_3) = 0. \quad (4.693)$$

By applying the boost matrix (4.511), we find the alternative expression for the bispinors with momentum $\mathbf{p}$:

$$u(\mathbf{p}, s_3) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(s_3) \\ \chi(s_3) \end{pmatrix}, v(\mathbf{p}, s_3) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(s_3) \\ -\chi^c(s_3) \end{pmatrix}. \quad (4.694)$$

Since γ^0 is a simple off-diagonal unit matrix, we can replace it by ± 1 in the left and right equation, respectively, and write just as well

$$u(\mathbf{p}, s_3) = \frac{M + \not{p}}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(s_3) \\ \chi(s_3) \end{pmatrix}, v(\mathbf{p}, s_3) = \frac{M - \not{p}}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(s_3) \\ -\chi^c(s_3) \end{pmatrix}. \quad (4.695)$$

The two sets of bispinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ satisfy the orthonormality conditions (4.665). Using (4.674) and (4.684), we find

$$\begin{aligned} u^\dagger(\mathbf{p}, s_3)u(\mathbf{p}, s'_3) &= \frac{1}{2}\chi^T(s_3) \begin{pmatrix} \sqrt{\frac{p\sigma}{M}}, \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s'_3) \\ &= \chi^T(s_3) \frac{1}{2} \left(\frac{p\sigma}{M} + \frac{p\tilde{\sigma}}{M} \right) \chi(s'_3) \\ &= \frac{p^0}{M} \chi^T(s_3) \chi(s'_3) = \frac{p^0}{M} \delta_{s_3, s'_3}, \end{aligned} \quad (4.696)$$

$$\begin{aligned} v^\dagger(-\mathbf{p}, s_3)v(-\mathbf{p}, s'_3) &= \frac{1}{2}\chi^{cT}(s_3) \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}}, -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s'_3) \\ &= \frac{p^0}{M} \delta_{s_3, s'_3}, \end{aligned} \quad (4.697)$$

$$\begin{aligned} u^\dagger(\mathbf{p}, s_3)v(-\mathbf{p}, s'_3) &= \frac{1}{2}\chi^T(s_3) \begin{pmatrix} \sqrt{\frac{p\sigma}{M}}, -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s'_3) \\ &= 0, \end{aligned} \quad (4.698)$$

$$v^\dagger(-\mathbf{p}, s_3)u(\mathbf{p}, s'_3) = 0. \quad (4.699)$$

The reason for the appearance of the negative momenta in the bispinors $v(-\mathbf{p}, s_3)$ is that the plane wave solutions $f_{\mathbf{p}s_3}^c(x)$ in (4.662) carry negative momenta, so that states of a fixed momentum $\mathbf{p}$ are associated with $f_{\mathbf{p}s_3}(x)$ and $f_{-\mathbf{p}s_3}^c(x)$. The momentum reversal in the conjugate wave functions goes along with the reversal of the spin orientation in the charge-conjugated Pauli spinors in Eq. (4.685). The

physical reason for these two reversals will be understood after field quantization in Section 7.4.3.

Inserting a matrix γ^0 between the bispinors in (4.696)–(4.699) we may also derive orthonormality relations between bispinors $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$:

$$\begin{aligned}\bar{u}(\mathbf{p}, s_3)u(\mathbf{p}, s'_3) &= \delta_{s_3, s'_3}, \\ \bar{v}(\mathbf{p}, s_3)v(\mathbf{p}, s'_3) &= -\delta_{s_3, s'_3}, \\ \bar{u}(\mathbf{p}, s_3)v(\mathbf{p}, s'_3) &= 0, \\ \bar{v}(\mathbf{p}, s_3)u(\mathbf{p}, s'_3) &= 0.\end{aligned}\tag{4.700}$$

The two sets of spinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ span the spinor space at a fixed momentum. This may be expressed by a completeness relation

$$\sum_{s_3} [u(\mathbf{p}, s_3)u^\dagger(\mathbf{p}, s_3) + v(-\mathbf{p}, s_3)v^\dagger(-\mathbf{p}, s_3)] = \frac{p^0}{M}.\tag{4.701}$$

To prove this 4×4 -matrix equation in Dirac space, we derive the separate polarization sums¹⁰ for u - and v -spinors. These can be calculated directly from (4.674) and (4.684) as follows:

$$\begin{aligned}\sum_{s_3} u(\mathbf{p}, s_3)\bar{u}(\mathbf{p}, s_3) &= \frac{1}{2} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \sum_{s_3} \chi(s_3)\chi^\dagger(s_3) \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} & \sqrt{\frac{p\sigma}{M}} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & \frac{p\sigma}{M} \\ \frac{p\tilde{\sigma}}{M} & 1 \end{pmatrix} = \frac{\not{p} + M}{2M},\end{aligned}\tag{4.702}$$

$$\begin{aligned}\sum_{s_3} v(\mathbf{p}, s_3)\bar{v}(\mathbf{p}, s_3) &= \frac{1}{2} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \sum_{s_3} \chi^c(s_3)\chi^{c\dagger}(s_3) \begin{pmatrix} -\sqrt{\frac{p\tilde{\sigma}}{M}} & \sqrt{\frac{p\sigma}{M}} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} -1 & \frac{p\sigma}{M} \\ \frac{p\tilde{\sigma}}{M} & -1 \end{pmatrix} = \frac{\not{p} - M}{2M}.\end{aligned}\tag{4.703}$$

Combining the two polarization sums for $\mathbf{p}$ and $-\mathbf{p}$, respectively, and multiplying them by the Dirac matrix γ^0 from the right, proves their completeness.

Subtracting the two polarization sums from each other yields another relation that is the Dirac-adjoint version of the completeness relation (4.701) [recall (4.495)]:

$$\sum_{s_3} [u(\mathbf{p}, s_3)\bar{u}(\mathbf{p}, s_3) - v(\mathbf{p}, s_3)\bar{v}(\mathbf{p}, s_3)] = 1.\tag{4.704}$$

¹⁰They may be called *semi-completeness relations*.

This contains a minus sign in the second sum which reflects the minus sign in the second orthogonality relation (4.700). This sign will be important in Section 7.10 to prove a famous theorem on the relation between spin and statistics of fundamental particles.

Polarization sums will frequently be needed later, in particular in the process of field quantization. We introduce the sums

$$P(p) \equiv \sum_{s_3} u(\mathbf{p}, s_3) u^\dagger(\mathbf{p}, s_3), \quad \bar{P}(p) \equiv \sum_{s_3} v(\mathbf{p}, s_3) v^\dagger(\mathbf{p}, s_3), \quad (4.705)$$

defined only for p^0 on the mass shell, $p^0 = \omega_{\mathbf{p}}$. They satisfy the relation $\bar{P}(p) = -P(-p)$. Similar polarization sums exist for plane-wave solutions for any spin. In general, the polarization sums $P(p)$ and $\bar{P}(p)$ of positive and negative energies of momenta $\mathbf{p}$ and $-\mathbf{p}$, respectively, fulfill the relation

$$\bar{P}(p) = \pm P(-p), \quad (4.706)$$

where the upper sign holds for integer spin, and the lower for half-integer spin. The matrices $P(p)$ and $P(-p)$ are projection matrices onto solutions of momenta $\mathbf{p}$ and $-\mathbf{p}$ with energies $p^0 = \omega_{\mathbf{p}}$ and $p^0 = -\omega_{\mathbf{p}}$, respectively. As such they satisfy

$$P(\pm p)^2 = P(\pm p). \quad (4.707)$$

It is always possible to find a single covariant expression for $P(p)$ defined for arbitrary off-shell values of p^0 which, for the on-shell values $p^0 = \pm\omega_{\mathbf{p}}$, reduces to the above projections $P(p)$ and $P(-p)$. In the Dirac case, where $P(p) = (\not{p} - M)\gamma^0/2M$, we verify that (4.707) is true for $p^0 = \pm\omega_{\mathbf{p}}$.

Spinors in Dirac Representation

Let us also write down the bispinors in the Dirac representation (4.550) of the γ -matrices. The rest bispinors are solutions of equations (4.693), where

$$\gamma_D^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Thus we have

$$u(\mathbf{0}, \tfrac{1}{2}) = \begin{pmatrix} \chi^{(\frac{1}{2})} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u(\mathbf{0}, -\tfrac{1}{2}) = \begin{pmatrix} \chi^{(-\frac{1}{2})} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \quad (4.708)$$

and

$$v(\mathbf{0}, \tfrac{1}{2}) = \begin{pmatrix} 0 \\ \chi^{c(\frac{1}{2})} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad v(\mathbf{0}, -\tfrac{1}{2}) = \begin{pmatrix} 0 \\ \chi^{c(-\frac{1}{2})} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}. \quad (4.709)$$

The bispinors at finite momentum are obtained from these by applying the 4×4 boost matrix (4.511), yielding

$$u(\mathbf{p}, s_3) = \frac{M + \not{p}_D}{\sqrt{2M(p_0 + M)}} \begin{pmatrix} \chi(s_3) \\ 0 \end{pmatrix}, \quad v(\mathbf{p}, s_3) = \frac{M - \not{p}_D}{\sqrt{2M(p_0 + M)}} \begin{pmatrix} 0 \\ \chi^c(s_3) \end{pmatrix}. \quad (4.710)$$

Since γ_D^0 has a simple diagonal form with eigenvalues ± 1 for upper and lower spinor components [see Eq. (4.562)], we have replaced γ_D^0 directly by its eigenvalues when going from (4.511) to (4.710) [as we did from (4.694) to (4.695)]. More explicitly, we can write

$$u(\mathbf{p}, s_3) = \begin{pmatrix} \sqrt{\frac{p_0 + M}{2M}} \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{\sqrt{2M(p_0 + M)}} \end{pmatrix} \chi(s_3), \quad v(\mathbf{p}, s_3) = \begin{pmatrix} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{\sqrt{2M(p_0 + M)}} \\ \sqrt{\frac{p_0 + M}{2M}} \end{pmatrix} \chi^c(s_3). \quad (4.711)$$

In this representation, the bispinors $u(\mathbf{p}, s_3)$ of slowly moving particles have large upper and small lower spinor components. The converse is true for the bispinors $v(\mathbf{p}, s_3)$. This is what makes the original Dirac spinors useful for discussing the nonrelativistic limit of spin-1/2 particles, as observed before in the boost matrix (4.556) and in x -space equations (4.569).

The Dirac spinors possess, of course, the same polarization sums (4.705) as in the chiral case, if the appropriate Dirac matrices γ_D^μ are used on the right-hand side.

Helicity Spinors

Sometimes, the choice of the spinors (4.673) with the particle spins quantized along the z -axis is not the most convenient basis in spinor space. Instead of the z -axis, one may choose any quantization direction, in particular, the direction of the momentum of the particle. This amounts to multiplying the 4×2 -matrix solutions (4.669) by a 2×2 rotation matrix from the right:

$$R(\hat{\mathbf{p}}) \equiv e^{-i\phi\sigma^3/2} e^{-i\theta\sigma^2/2}, \quad (4.712)$$

where θ, ϕ are the spherical angles of the momentum $\mathbf{p}$. In contrast to the notation of Eq. (4.9), the rotation matrix carries now an argument indicating that the z -direction is rotated into the momentum direction $\hat{\mathbf{p}}$.¹¹ Equivalently, we may choose in the bispinors (4.674), instead of $\chi(s_3)$, a basis $\chi_h(\hat{\mathbf{p}}, \lambda)$ with $\lambda = \pm 1/2$, defined by

$$\chi_h(\hat{\mathbf{p}}, \lambda) \equiv R(\hat{\mathbf{p}}) \chi(s_3) \equiv e^{-i\phi\sigma^3/2} e^{-i\theta\sigma^2/2} \chi(\lambda). \quad (4.713)$$

¹¹As before in this sections, hats on vectors denote unit vectors, not Schrödinger operators.

The explicit components are

$$\chi_h(\hat{\mathbf{p}}, \tfrac{1}{2}) = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi/2} \\ \sin \frac{\theta}{2} e^{i\phi/2} \end{pmatrix}, \quad \chi_h(\hat{\mathbf{p}}, -\tfrac{1}{2}) = \begin{pmatrix} -\sin \frac{\theta}{2} e^{-i\phi/2} \\ \cos \frac{\theta}{2} e^{i\phi/2} \end{pmatrix}. \quad (4.714)$$

They diagonalize the projection of the angular momentum in the rest frame along the direction of motion of the particle $\hat{\mathbf{p}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, the so-called *helicity*:

$$h(\hat{\mathbf{p}}) \equiv \mathbf{L} \cdot \hat{\mathbf{p}} = \frac{1}{2} \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} = \frac{1}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}. \quad (4.715)$$

The eigenvalues are

$$h(\mathbf{p})\chi(\hat{\mathbf{p}}, \lambda) = \lambda\chi(\hat{\mathbf{p}}, h), \quad \lambda = \pm \frac{1}{2}. \quad (4.716)$$

The eigenstates $\chi_h(\hat{\mathbf{p}}, \lambda)$ are called *helicity spinors*. The associated bispinors are, as in (4.674) and (4.684),

$$u_h(\mathbf{p}, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(\hat{\mathbf{p}}, \lambda), \quad v_h(\mathbf{p}, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(\hat{\mathbf{p}}, \lambda), \quad (4.717)$$

with the charge-conjugated helicity spinors

$$\chi^c(\hat{\mathbf{p}}, \lambda) = c\chi^*(\hat{\mathbf{p}}, \lambda). \quad (4.718)$$

These diagonalize the 4×4 bispinor representation of the helicity:

$$H(\hat{\mathbf{p}}) \equiv \mathbf{S} \cdot \hat{\mathbf{p}} = \frac{1}{2} \boldsymbol{\Sigma} \cdot \hat{\mathbf{p}} = \frac{1}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \cdot \hat{\mathbf{p}}. \quad (4.719)$$

This is a direct consequence of the fact that $H(\hat{\mathbf{p}})$ commutes with the boost matrix (4.511).

Alternatively, we can obtain the helicity bispinors (4.717) by first boosting the bispinors at rest (4.713), (4.714) into the z -direction, and rotating them afterwards into the $\hat{\mathbf{p}}$ -direction:

$$u_h(\hat{\mathbf{p}}, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} R(\hat{\mathbf{p}}) \sqrt{\frac{p^0 \sigma^0 - |\mathbf{p}| \sigma^3}{M}} \chi(h) \\ R(\hat{\mathbf{p}}) \sqrt{\frac{p^0 \sigma^0 + |\mathbf{p}| \sigma^3}{M}} \chi(h) \end{pmatrix}, \quad (4.720)$$

and

$$v_h(\hat{\mathbf{p}}, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} R(\hat{\mathbf{p}}) \sqrt{\frac{p^0 \sigma^0 + |\mathbf{p}| \sigma^3}{M}} \chi^c(h) \\ -R(\hat{\mathbf{p}}) \sqrt{\frac{p^0 \sigma^0 - |\mathbf{p}| \sigma^3}{M}} \chi^c(h) \end{pmatrix}. \quad (4.721)$$

The equality with (4.717) follows from the transformation law (4.477), according to which

$$R(\hat{\mathbf{p}})|\mathbf{p}|\sigma^3 = \mathbf{p} \cdot \boldsymbol{\sigma} R(\hat{\mathbf{p}}). \quad (4.722)$$

One of the important advantages of the helicity spinor is that it has a smooth limit as the particle mass M tends to zero. Indeed, by expanding

$$p^0 = \sqrt{\mathbf{p}^2 + M^2} = |\mathbf{p}| + \frac{M^2}{2|\mathbf{p}|} + \dots \quad (4.723)$$

we see that

$$\begin{aligned} \frac{p^0 \sigma^0 - |\mathbf{p}| \sigma^3}{M} &\xrightarrow{M \rightarrow 0} \frac{2}{M} \begin{pmatrix} 0 & 0 \\ 0 & |\mathbf{p}| \end{pmatrix}, \\ \frac{p^0 \sigma^0 + |\mathbf{p}| \sigma^3}{M} &\xrightarrow{M \rightarrow 0} \frac{2}{M} \begin{pmatrix} |\mathbf{p}| & 0 \\ 0 & 0 \end{pmatrix}. \end{aligned} \quad (4.724)$$

Thus the massless helicity spinors $u_h(\mathbf{p}, \lambda)$ and $v_h(\mathbf{p}, \lambda)$ have only two nonzero components. We shall normalize them to

$$u_h^\dagger(\mathbf{p}, \lambda) u(\mathbf{p}, \lambda) = 2p^0 = 2|\mathbf{p}|, \quad v_h^\dagger(\mathbf{p}, \lambda) v(\mathbf{p}, \lambda) = 2p^0 = 2|\mathbf{p}|, \quad (4.725)$$

as opposed the normalization to p^0/M of the massive spinors (4.717). The explicit form is

$$\begin{aligned} u_h(\mathbf{p}, \tfrac{1}{2}) &= \sqrt{|\mathbf{p}|} \begin{pmatrix} 0 \\ 0 \\ R(\hat{\mathbf{p}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} \equiv u_R(\mathbf{p}), \\ u_h(\mathbf{p}, -\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|} \begin{pmatrix} R(\hat{\mathbf{p}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0 \\ 0 \end{pmatrix} \equiv u_L(\mathbf{p}), \end{aligned} \quad (4.726)$$

and

$$\begin{aligned} v_h(\mathbf{p}, \tfrac{1}{2}) &= \sqrt{|\mathbf{p}|} \begin{pmatrix} 0 \\ 0 \\ -R(\hat{\mathbf{p}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = v_R(\mathbf{p}) \\ v_h(\mathbf{p}, -\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|} \begin{pmatrix} -R(\hat{\mathbf{p}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \\ 0 \end{pmatrix} = v_L(\mathbf{p}). \end{aligned} \quad (4.727)$$

The helicity bispinors $u_h(\mathbf{p}, \lambda)$ and $v_h(\mathbf{p}, \lambda)$ are eigenstates of the chirality matrix

$$\gamma_5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4.728)$$

with the eigenvalue 2λ . By applying the 4×4 projection matrix $\frac{1-\gamma_5}{2}$ to the bispinors $u_h(\mathbf{p}, \lambda)$, forming

$$\frac{1-\gamma_5}{2}u_h(\mathbf{p}, \lambda), \quad (4.729)$$

we obtain a negative helicity state. Such projected bispinors are used for the description of neutrinos which only exist with negative helicity (*left-handed neutrinos*). As we shall see later in Section 27, weak interactions involve also the orthogonally projected bispinors

$$\frac{1+\gamma_5}{2}v_h(\mathbf{p}, \lambda) \quad (4.730)$$

which describe antineutrinos. These exist only with positive helicity (*right-handed antineutrinos*).

4.14 Lorentz Transformation of Spinors

Let us study the behavior of the bispinors $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$ under Lorentz transformations. This will be most straightforward in the chiral representation, where we may focus our attention upon the upper components only, which will be denoted by $\xi(\mathbf{p}, s_3)$. The properties of the lower components, to be denoted by $\eta(\mathbf{p}, s_3)$, can be obtained by a simple change in the direction of the momentum. The upper components can be written explicitly as

$$\xi(\mathbf{p}, s_3) = B(\zeta)\chi(s_3) = e^{-\zeta \cdot \sigma/2}\chi(s_3). \quad (4.731)$$

Applying to this a general Lorentz transformation $D^{(\frac{1}{2},0)}(\Lambda)$, the momentum $\mathbf{p}$ is changed to some other vector $\mathbf{p}'$, which is the spatial part of the four-vector $\Lambda^\mu{}_\nu p^\nu$. The transformation can be done in three steps: First, deboost the particle by applying a boost opposite to the particle's momentum which brings it to rest, with the four-momentum p^μ becoming $p_R^\mu = (M, \mathbf{0})$. Second, perform a rotation, and third, boost the particle to its final four-momentum p'^μ . Thus we can write the general Lorentz transformations as

$$D^{(\frac{1}{2},0)}(\Lambda) = B(\zeta')W(p', \Lambda, p)B_\zeta^{-1}(\zeta) \equiv e^{-\zeta' \cdot \sigma/2}e^{-i\alpha \cdot \sigma/2}e^{\zeta \cdot \sigma/2}. \quad (4.732)$$

The rotation $W(p', \Lambda, p)$ in the middle is called a *Wigner rotation*. It is an element of the little group of the massive particle acting only in its rest frame [see the earlier short discussion on p. 35].

Let p' be the momentum reached from the momentum p after a Lorentz transformation Λ . Then the spinor (4.731) changes as follows:

$$\xi(\mathbf{p}, s_3) \xrightarrow{\Lambda} \xi'(\mathbf{p}', s_3) = D^{(\frac{1}{2},0)}(\Lambda)\xi(\mathbf{p}, s_3) = e^{-\zeta' \cdot \sigma/2}e^{-i\alpha \cdot \sigma/2}\chi(s_3)$$

$$\begin{aligned}
&= e^{-\zeta' \cdot \sigma / 2} \sum_{s'_3 = -1/2}^{1/2} \chi(s'_3) \left(e^{-i\alpha \cdot \sigma / 2} \right)_{s'_3, s_3} \\
&= \sum_{s'_3 = -1/2}^{1/2} \xi(\mathbf{p}', s'_3) W_{s'_3, s_3}(p', \Lambda, p), \tag{4.733}
\end{aligned}$$

where we have used the rotation property (4.687) of the spinors $\chi(s_3)$, which amounts here to

$$W(p', \Lambda, p) \chi(s_3) = \sum_{s'_3 = -1/2}^{1/2} \chi(s'_3) W_{s'_3, s_3}(p', \Lambda, p). \tag{4.734}$$

By analogy, the spinor $\eta(\mathbf{p}, s_3)$ transforms like

$$\eta(\mathbf{p}, s_3) \xrightarrow{\Lambda} \eta'(\mathbf{p}', s_3) = D^{(0, \frac{1}{2})}(\Lambda) \eta(\mathbf{p}, s_3) = \sum_{s'_3 = -1/2}^{1/2} \eta(\mathbf{p}', s'_3) W_{s'_3, s_3}(p', \Lambda, p), \tag{4.735}$$

implying for the Dirac spinor $u(\mathbf{p}, s_3)$ the transformation law

$$u(\mathbf{p}, s_3) \xrightarrow{\Lambda} u'(\mathbf{p}', s_3) = D(\Lambda) u(\mathbf{p}, s_3) = \sum_{s'_3 = -1/2}^{1/2} u(\mathbf{p}', s'_3) W_{s'_3, s_3}(p', \Lambda, p). \tag{4.736}$$

The result can be expressed most compactly in terms of the 4×2 -matrix form (4.670) for the bispinor solutions as

$$u(\mathbf{p}) \xrightarrow{\Lambda} u'(\mathbf{p}') = D(\Lambda) u(\mathbf{p}) = u(\mathbf{p}') W(p', \Lambda, p). \tag{4.737}$$

We are now prepared to understand the group-theoretic reason for the occurrence of the rotation matrix $c = e^{-i\pi\sigma_2/2}$ in the charge-conjugated bispinor $v(\mathbf{p})$ of Eq. (4.684). The 4×2 solutions $v(\mathbf{p})$ of (4.670) transform in the same way as $u(\mathbf{p})$ of (4.669):

$$v(\mathbf{p}) \xrightarrow{\Lambda} v'(\mathbf{p}') = D(\Lambda) v(\mathbf{p}) = v(\mathbf{p}') W(p', \Lambda, p). \tag{4.738}$$

The behavior of the Dirac spinors $v(\mathbf{p}, s_3)$ is found by multiplying this equation from the right-hand side with $c\chi^*(s_3)$ [recall (4.684)], leading to

$$v(\mathbf{p}, s_3) \xrightarrow{\Lambda} v'(\mathbf{p}', s_3) = D(\Lambda) v(\mathbf{p}, s_3) = v(\mathbf{p}') W(p', \Lambda, p) c\chi^*(s_3). \tag{4.739}$$

Now we use the fact that the 2×2 -Wigner rotation can be written as $e^{-i\alpha \cdot \sigma / 2}$, which satisfies the relation (4.689), so that

$$c^{-1} W(p', \Lambda, p) c = W^*(p', \Lambda, p), \tag{4.740}$$

to rewrite on the right-hand side

$$W(p', \Lambda, p) c\chi^*(s_3) = c W^*(p', \Lambda, p) \chi^*(s_3) = c\chi^*(s'_3) W_{s'_3, s_3}^*. \tag{4.741}$$

We obtain the transformation law for the bispinors $v(\mathbf{p}, s_3)$:

$$v(\mathbf{p}, s_3) \xrightarrow{\Lambda} v'(\mathbf{p}', s_3) = D(\Lambda)v(\mathbf{p}, s_3) = \sum_{s'_3=-1/2}^{1/2} v(\mathbf{p}', s'_3) W_{s'_3 s_3}^*(p', \Lambda, p). \quad (4.742)$$

Thus we find that under Lorentz transformations, the spin orientations of the bispinors $v(\mathbf{p}, s_3)$ are linearly recombined with each other by the complex-conjugate Wigner rotations $W_{s'_3 s_3}^*(p', \Lambda, p)$. This is a consequence of the presence of the matrix c in the 4×2 -matrices (4.670) for $v(\mathbf{p})$, which has reversed canonical spin indices.

Had we used the bispinors $v(\mathbf{p}, s_3)$ in the form (4.684), the same result would have been obtained from the observation (4.688), that the spin indices of the charge-conjugated Pauli spinors $\chi^c(s_3)$ are linearly recombined with each other by the complex-conjugate rotation matrix.

The transformation properties (4.737) and (4.738) can be verified most easily in an infinitesimal form for spinors at rest. If Λ is an infinitesimal rotation R with the 4×4 -matrix $R^\mu{}_\nu = \delta^\mu{}_\nu - i\boldsymbol{\varphi} \cdot \mathbf{L}^\mu{}_\nu$, the left-hand sides must be multiplied by $D(\Lambda) = R = 1 - i\boldsymbol{\varphi} \cdot \boldsymbol{\Sigma}/2$, where Σ^i is given by (4.514). This produces the same infinitesimal Wigner rotation $1 - i\boldsymbol{\varphi} \cdot \boldsymbol{\sigma}/2$ on the right-hand sides. Thus we have the relations

$$i\Sigma^i u(\mathbf{0}) = u(\mathbf{0}) i\sigma^i, \quad i\Sigma^i v(\mathbf{0}) = v(\mathbf{0}) i\sigma^i. \quad (4.743)$$

Using (4.669) and (4.670), these become explicitly

$$i\Sigma^i \begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix} i\sigma^i, \quad i\Sigma^i \begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix} c(-i\sigma^i)^*. \quad (4.744)$$

Let us also write down the Wigner rotations for the helicity spinors (4.717). Since they arise from the 4×2 -matrix solutions (4.669) by a multiplication from the right with the 2×2 rotation matrix (4.712), a Lorentz transformation of $u_h(\mathbf{p}, \lambda)$ yields obviously

$$u_h(\mathbf{p}, \lambda) \xrightarrow{\Lambda} u'_h(\mathbf{p}', \lambda) = D(\Lambda)u_h(\mathbf{p}, \lambda) = \sum_{\lambda'=-1/2}^{1/2} u_h(\mathbf{p}', \lambda') W_{h\lambda'\lambda}(p', \Lambda, p), \quad (4.745)$$

with the helicity form of the Wigner rotation

$$W_h(p', \Lambda, p) = R^{-1}(\hat{\mathbf{p}}') W(p', \Lambda, p) R(\hat{\mathbf{p}}). \quad (4.746)$$

Similarly,

$$v_h(\mathbf{p}, \lambda) \xrightarrow{\Lambda} v'_h(\mathbf{p}', \lambda) = D(\Lambda)v_h(\mathbf{p}, \lambda) = \sum_{\lambda'=-1/2}^{1/2} v_h(\mathbf{p}', \lambda') W_{\lambda'\lambda}^{H*}(p', \Lambda, p), \quad (4.747)$$

with

$$W^{H*}(p', \Lambda, p) = R^{-1*}(\hat{\mathbf{p}}') W^*(p', \Lambda, p) R^*(\hat{\mathbf{p}}). \quad (4.748)$$

4.15 Precession

The properties of relativistic spinors under Lorentz transformations are crucial for a phenomenon known in atomic physics as *Thomas precession*. The Thomas precession is a direct consequence of what may be called *Wigner precession*.

4.15.1 Wigner Precession

Consider an electron moving around an atomic nucleus. In each time interval Δt , it receives a small centripetal Lorentz boost changing its momentum. Let us see what happens to the upper two components of the canonical bispinors $u(\mathbf{p}, s_3)$ which are explicitly

$$\xi(\mathbf{p}, s_3) = B(\boldsymbol{\zeta})\chi(s_3) \equiv e^{-\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2} \chi(s_3). \quad (4.749)$$

At an instance of time t , the electron moves with a certain velocity through space. Its state can be described by the two-component spinor $\xi(\mathbf{p}, s_3)$ defined in Eq. (4.731). As the atomic force acts on the electron, it is accelerated towards the nucleus. Thus, after a small time interval dt , the electron will have a new momentum and a spinor $\xi(\mathbf{p}', s_3)$ which can be obtained from the first by applying a small Lorentz boost

$$B(d\boldsymbol{\epsilon}) = e^{-d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/2} \quad (4.750)$$

to the spinor $\xi(\mathbf{p}, s_3)$, which changes its momentum from $\mathbf{p}$ to $\mathbf{p}'$. The resulting transformation is split into three factors, as in (4.732). The first is a pure boost in the $-\mathbf{p}$ direction, which brings the four-momentum p to its rest frame where it is $p_R = (M, \mathbf{0})$. The second factor is a rotation, and the third is a boost into the final four-momentum p' . In this process, the spin indices of the spinor $\xi(\mathbf{p}, s_3)$ are linearly recombined with each other by a Wigner rotation according to Eq. (4.733). Let us calculate this, taking advantage of the fact that $d\boldsymbol{\epsilon}$ is very small. Then $\boldsymbol{\zeta}'$ differs very little from $\boldsymbol{\zeta}$, say $\boldsymbol{\zeta}' = \boldsymbol{\zeta} + d\boldsymbol{\zeta}$, where $d\boldsymbol{\zeta}$ is another small rapidity of the order of $d\boldsymbol{\epsilon}$. To indicate the smallness of the associated rotation vector in the Wigner rotation we shall denote it by $d\boldsymbol{\alpha}_W$. Its size is calculated from the equation

$$e^{-id\boldsymbol{\alpha}_W \cdot \boldsymbol{\sigma}/2} = e^{(\boldsymbol{\zeta} + d\boldsymbol{\zeta}) \cdot \boldsymbol{\sigma}/2} e^{-d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/2} e^{-\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2}. \quad (4.751)$$

Before calculating $d\boldsymbol{\alpha}_W$ exactly, let us estimate it for slowly moving particles where $d\boldsymbol{\epsilon}$, $d\boldsymbol{\zeta}$, and $\boldsymbol{\zeta}$ are all of the same order. Then we may expand both sides of (4.751) up to the second order in all quantities as follows:

$$\begin{aligned} 1 - id\boldsymbol{\alpha}_W \cdot \boldsymbol{\sigma}/2 &\approx \left[1 + (\boldsymbol{\zeta} + d\boldsymbol{\zeta}) \cdot \boldsymbol{\sigma}/2 + (\boldsymbol{\zeta} + d\boldsymbol{\zeta})^2/4 \right] \\ &\times \left[1 - d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/2 + (d\boldsymbol{\epsilon})^2/4 \right] \left[1 - \boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2 + \boldsymbol{\zeta}^2/4 \right]. \end{aligned} \quad (4.752)$$

In the product on the right-hand side, we set $d\boldsymbol{\zeta} \approx d\boldsymbol{\epsilon}$ to cancel the first-order terms. The second-order terms decompose into Hermitian and antihermitian parts. Since we are interested only in $d\boldsymbol{\alpha}$, we must extract the antihermitian part. Using the identity

$$\mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma} = \mathbf{a} \cdot \mathbf{b} + i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}, \quad (4.753)$$

we find

$$\begin{aligned} 1 - id\alpha_W \cdot \sigma/2 &\approx 1 - i \{[(\zeta + d\zeta) \times d\zeta] + [(\zeta + d\zeta) \times \zeta] - [d\zeta \times \zeta]\} \cdot \sigma/4 \\ &\approx 1 + i(d\zeta \times \zeta) \cdot \sigma/4, \end{aligned} \quad (4.754)$$

so that we obtain the rotation vector for small ζ :

$$d\alpha_W \approx \frac{1}{2}\zeta \times d\zeta. \quad (4.755)$$

The spin matrix is rotated under a Wigner rotation as follows:

$$\sigma \rightarrow \sigma' = W^{-1}\sigma W. \quad (4.756)$$

For an infinitesimal $W \approx 1 - id\alpha_W \cdot \sigma/2$ this yields

$$d\sigma = i[d\alpha_W \cdot \sigma, \sigma] = d\alpha_W \times \sigma. \quad (4.757)$$

An accelerated point particle receives a small boost $d\epsilon$ in each small time interval dt . In this time interval, the spin precesses at an angular velocity $d\alpha_W/dt$. In the limit $dt \rightarrow 0$, Eq. (4.755) implies an angular velocity of Wigner rotations

$$\Omega_W \approx \frac{1}{2}\zeta \times \dot{\zeta} \approx \frac{1}{2c^2}\mathbf{v} \times \dot{\mathbf{v}}. \quad (4.758)$$

4.15.2 Thomas Precession

A relative of the Wigner precession is observable in atomic physics as a *Thomas precession*. In an atom, the small additional boost acts on the electron moving with momentum $\mathbf{p}$ in its rest frame. This implies that the small boost (4.750) has to be replaced by

$$\tilde{B}(d\epsilon) = B(\zeta)B(d\epsilon)B^{-1}(\zeta) = e^{-\zeta \cdot \sigma/2}e^{-d\epsilon \cdot \sigma/2}e^{\zeta \cdot \sigma/2}, \quad (4.759)$$

and (4.751) becomes

$$e^{-id\alpha_T \cdot \sigma/2} = e^{(\zeta + d\zeta) \cdot \sigma/2}e^{-\zeta \cdot \sigma/2}e^{-d\epsilon \cdot \sigma/2}. \quad (4.760)$$

The small-velocity calculation (4.752) becomes now

$$\begin{aligned} 1 - id\alpha_T \cdot \sigma/2 &\approx \left[1 + (\zeta + d\zeta) \cdot \sigma/2 + (\zeta + d\zeta)^2/4\right] \\ &\times \left[1 - \zeta \cdot \sigma/2 + \zeta^2/4\right] \left[1 - d\epsilon \cdot \sigma/2 + (d\epsilon)^2/4\right], \end{aligned} \quad (4.761)$$

leading with $d\zeta \approx d\epsilon$ to

$$\begin{aligned} 1 - id\alpha_R \cdot \sigma/2 &\approx 1 - i \{[(\zeta + d\zeta) \times \zeta] + [(\zeta + d\zeta) \times d\zeta] - [\zeta \times d\zeta]\} \cdot \sigma/4 \\ &\approx 1 + i(\zeta \times d\zeta) \cdot \sigma/4. \end{aligned} \quad (4.762)$$

The resulting small Thomas rotation vector:

$$d\boldsymbol{\alpha}_T \approx -\frac{1}{2}\boldsymbol{\zeta} \times d\boldsymbol{\zeta} \quad (4.763)$$

is exactly the opposite of the Wigner rotation vector in Eq. (4.755). Of course, the same thing is true for the rate of the Thomas precession

$$\boldsymbol{\Omega}_T \approx -\frac{1}{2}\boldsymbol{\zeta} \times \dot{\boldsymbol{\zeta}} \approx \frac{1}{2c^2}\mathbf{v} \times \dot{\mathbf{v}}. \quad (4.764)$$

For the spin vector $\mathbf{S}$, which is the total angular momentum in the electron's rest frame, this amounts to the equation of motion

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\Omega}_T \times \mathbf{S} \approx -\frac{1}{2c^2}(\mathbf{v} \times \dot{\mathbf{v}}) \times \mathbf{S}. \quad (4.765)$$

For finite $\boldsymbol{\zeta}$, this equation will acquire relativistic correction factors and become

$$\boldsymbol{\Omega}_T = \frac{1}{c^2} \frac{\gamma^2}{\gamma + 1} \mathbf{v} \times \dot{\mathbf{v}}. \quad (4.766)$$

The derivation of this expression is somewhat tedious and will therefore be given in Appendix 4B.

The angular velocity of the Wigner rotation has observable consequences in atomic physics, where it is seen as a Thomas precession. This will be discussed in more detail in Subsection 6.1.3. It is a purely kinematic effect, caused entirely by the structure of the Lorentz group. Mathematically speaking, it is due to the fact that pure Lorentz transformations do not form a subgroup of the full Lorentz group. When performing pure Lorentz transformations one after another in such a way that the final frame is again at rest with respect to the initial one, the result is always a *Wigner rotation*.

4.15.3 Spin Four-Vector and Little Group

The working of the Wigner rotations in the little group found in Section 4.14 can be understood independently of the particular spinors. For any massive elementary or composite physical system we introduce a quantity called *total spin four-vector*. It is a combination of the total angular momentum $\hat{J}^{\mu\nu} = \hat{L}^{\mu\nu} + S^{\mu\nu}$ with the total momentum operator $\hat{p}$ which together form a vector

$$\hat{S}_\mu = \frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\hat{J}^{\nu\lambda}\hat{p}^\kappa, \quad (4.767)$$

where $\epsilon_{\mu\nu\lambda\kappa}$ is the totally antisymmetric unit matrix with $\epsilon^{0123} = 1$ (see [12]).

For massive elementary particles of momentum p^μ , the time and space components of the spin four-vector become explicitly

$$\hat{S}^0 = \mathbf{p} \cdot \hat{\mathbf{J}}, \quad \hat{\mathbf{S}} = p^0 \hat{\mathbf{J}} - \mathbf{p} \times \hat{\mathbf{K}}, \quad (4.768)$$

where $\hat{\mathbf{J}} = (\hat{J}^{23}, \hat{J}^{31}, \hat{J}^{12})$ and $\hat{\mathbf{K}} = (\hat{J}^{01}, \hat{J}^{02}, \hat{J}^{03})$. Studying particles at fixed momenta, we have dropped operator hats on the momenta in (4.768), and the generators of orbital angular momentum $\hat{L}_{\mu\nu}$ become differential operators in momentum space, where they read explicitly [compare (4.92)]

$$\hat{L}_{\mu\nu} \equiv i(p_\mu \partial_\nu - p_\nu \partial_\mu), \quad (4.769)$$

with $\partial_\mu \equiv \partial/\partial p^\mu$.

Using the commutation relations (4.295) and (4.99), the components of $\hat{S}^\mu$ in (4.767) can be shown to satisfy the commutation rules

$$[\hat{S}^\mu, \hat{S}^\nu] = i\epsilon^{\mu\nu\lambda\kappa} \hat{S}^\lambda \hat{p}^\kappa. \quad (4.770)$$

The proof makes use of the tensor identity (4.242) which, after taking advantage of the antisymmetry of $\hat{J}^{\lambda\lambda'}$ in the indices λ and λ' , and the symmetry of $p^\kappa p^{\kappa'}$ in κ and κ' , leads to

$$\epsilon_{\mu\nu\lambda\kappa} \epsilon^{\mu\lambda'\kappa'\nu'} \hat{J}^{\lambda\lambda'} p^\kappa p^{\kappa'} = \frac{1}{2} \epsilon_{\mu\kappa}{}^{\nu\nu'} \epsilon^{\mu\lambda\lambda'\kappa'} \hat{J}^{\lambda\lambda'} p^\kappa p^{\kappa'}, \quad (4.771)$$

and thus to the right-hand side of (4.770).

The same result can of course be derived without the lengthy identity (4.242) by considering time and space components in (4.768) separately, using the commutators (4.76), (4.78), and (4.99). Then we find

$$\begin{aligned} [\hat{L}_i, p^0] &= 0, & [\hat{L}_i, p^j] &= i\epsilon_{ijk} p^k, \\ [\hat{M}_i, p^0] &= -ip^i, & [\hat{M}_i, p^j] &= -i\delta_{ij} p^0. \end{aligned} \quad (4.772)$$

For a free particle, p^μ is independent of time, and so is $\hat{S}^\mu$. By definition, the spin four-vector $\hat{S}^\mu$ is orthogonal to the four-momentum:

$$\hat{S}^\mu p_\mu = 0. \quad (4.773)$$

The physical significance of $\hat{S}^\mu$ becomes clear by going into the rest frame of a massive particle where the system has no velocity, so that [recall (14.291)]

$$p_R^\lambda = Mc(1, 0, 0, 0). \quad (4.774)$$

Then

$$\hat{S}_R^0 = 0, \quad \hat{S}_R^i = Mc \frac{1}{2} \epsilon^{ijk} \hat{J}^{jk} \equiv Mc \hat{J}_i. \quad (4.775)$$

Removing an overall factor Mc , we define the operators of Wigner rotations

$$\hat{W}^i \equiv \hat{S}_R^i / Mc, \quad (4.776)$$

satisfying the commutation relations

$$[\hat{W}^i, \hat{W}^j] = i\epsilon_{ijk} \hat{W}^k. \quad (4.777)$$

Thus the total spin four-vector has the property that its spatial components coincide in the rest frame with the total angular momentum of the system. This is certainly time independent due to angular momentum conservation.

Moreover, at zero momentum, the orbital part of $\hat{J}^i$ vanishes, so that only the spin part S^i of $\hat{J}^i$ survives, and we can drop the hats on top of S_R^i which indicate the presence of differential operators. Then we obtain pure spin matrices for the operators $\hat{W}^i$:

$$W^i \equiv S_R^i/Mc, \quad (4.778)$$

satisfying the same commutation relations as the operators in (4.777). They will be called *spin three-vectors*.

The relation between the spin three-vector and the spin four-vector is obtained by applying the pure Lorentz transformation matrix (4.18) to (4.775), yielding

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_R + \frac{\gamma^2}{\gamma + 1} \frac{1}{c^2} (\hat{\mathbf{S}}_R \cdot \mathbf{v}) \mathbf{v}, \quad \hat{S}^0 = \frac{1}{c} \mathbf{S} \cdot \mathbf{v}. \quad (4.779)$$

The inverse relations are

$$\hat{\mathbf{S}}_R = \hat{\mathbf{S}} - \frac{\gamma}{\gamma + 1} \frac{1}{c} \hat{S}^0 \mathbf{v} = \hat{\mathbf{S}} - \frac{\gamma}{\gamma + 1} \frac{1}{c^2} (\hat{\mathbf{S}} \cdot \mathbf{v}) \mathbf{v}, \quad \hat{S}_R^0 = 0, \quad (4.780)$$

as can be verified with the help of the relation

$$\frac{v^2}{c^2} = \frac{\gamma^2 - 1}{\gamma^2}, \quad (4.781)$$

which implies that $\gamma/(\gamma - 1)c^2 = (\gamma - 1)/\gamma v^2$. Note that

$$\hat{S}_0 = \frac{1}{c} \hat{\mathbf{S}} \cdot \mathbf{v} = \frac{\gamma}{c} \hat{\mathbf{S}}_R \cdot \mathbf{v}. \quad (4.782)$$

For massless particles, the Wigner rotations have quite different properties from those of massive particles. In the special reference frame in which the massless particle runs along the z -axis with a reference momentum $p_R^\mu = (1, 0, 0, 1)p$ introduced in (14.295), these components become

$$\hat{S}^0 = p \hat{J}^3, \quad \hat{S}^1 = p (J^1 + K^2), \quad \hat{S}^2 = p (\hat{J}^2 - \hat{K}^1), \quad \hat{S}^3 = p \hat{J}^3. \quad (4.783)$$

The three independent components

$$\hat{W}^3 \equiv \hat{S}^0 = \hat{S}^3, \quad \hat{W}^1 \equiv \hat{S}^1, \quad \hat{W}^2 \equiv \hat{S}^2 \quad (4.784)$$

satisfy the commutation relations

$$[\hat{W}^3, \hat{W}^1] = i\hat{W}^2, \quad [\hat{W}^3, \hat{W}^2] = -i\hat{W}^1, \quad [\hat{W}^1, \hat{W}^2] = 0. \quad (4.785)$$

These generate a *euclidean group* in a plane. Recall the definition of this group. In D dimensions, it consists of $D(D - 1)$ generators L_{ij} of the D -dimensional rotation group:

$$[L_{ij}, L_{ik}] = iL_{jk}, \quad (4.786)$$

and D generators of translation p_i , which commute with each other and are vector operators under rotations:

$$[p_i, p_j] = 0, \quad [L_{ij}, p_k] = i(\delta_{ik}p_j - \delta_{jk}p_i). \quad (4.787)$$

These commutation rules can be obtained from those of the Lorentz group in D -dimensions [see Eqs. (4.76)–(4.78)] by setting $p_i = M_i/c$ and letting c go to infinity. This construction is called *group contraction*.

The commuting generators $\hat{W}^1$ and $\hat{W}^2$ can be diagonalized simultaneously like commuting momentum operators in a plane with arbitrary continuous eigenvalues w^1 and w^2 , respectively. The third generator $\hat{W}^3$ generates rotations in this plane with discrete eigenvalues $w^3 = \lambda$, where λ are azimuthal quantum numbers which can be equal to an integer or a half-integer number. In mirror-symmetric theories, both signs have to occur. In an arbitrary reference frame, $\hat{W}^0$ is given, according to (4.768), by the operator $\hat{W}^0 = \mathbf{p} \cdot \mathbf{J}/p$. This shows that the eigenvalues λ measure the angular momentum around the momentum direction, i.e., the helicity of the particle.

It turns out that in nature, all massless particles happen to follow a representation of the Wigner algebra which have only trivial eigenvalues $w^1 = w^2 = 0$. They are characterized completely by the helicity, which is unchanged under Wigner rotations. It merely receives a pure phase factor multiplying the helicity spinors or massless polarization vectors.

The occurrence of only such a subset of all possible zero-mass representations can be understood by a limiting process such as the one performed in the derivation of the massless spinors (4.726) and (4.727). We imagine for a moment that all massless particles carry a small mass which we let go to zero. It can then be verified that the limiting spinors change under a Lorentz transformation merely by a phase factor associated with helicity $\lambda = \pm 1/2$:

$$\begin{aligned} D(\Lambda)u_R(\mathbf{p}) &= u_R(\mathbf{p})e^{i\omega(p', \Lambda, p)/2}, & D(\Lambda)u_L(\mathbf{p}) &= u_L(\mathbf{p})e^{-i\omega(p', \Lambda, p)/2}, \\ D(\Lambda)v_R(\mathbf{p}) &= u_R(\mathbf{p})e^{-i\omega(p', \Lambda, p)/2}, & D(\Lambda)u_L(\mathbf{p}) &= u_L(\mathbf{p})e^{i\omega(p', \Lambda, p)/2}. \end{aligned} \quad (4.788)$$

For the polarization vectors of electromagnetism $\epsilon^\mu(\mathbf{k}, \lambda)$ in (4.319), and the tensors $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ of gravity in (4.416) we have, similarly,

$$\Lambda^\mu{}_\nu \epsilon^\nu(\mathbf{p}, \lambda) = \epsilon^\mu(\mathbf{p}, \lambda)e^{i\lambda\omega(p', \Lambda, p)}, \quad \Lambda^\mu{}_\nu \Lambda^{\mu'}{}_{\nu'} \epsilon^{\nu\nu'}(\mathbf{p}, \lambda) = \epsilon^{\mu\mu'}(\mathbf{p}, \lambda)e^{i\lambda\omega(p', \Lambda, p)}. \quad (4.789)$$

The reader is invited to derive this directly from the explicit expressions for these objects.

4.16 Weyl Spinor Calculus

Weyl has devised a simple calculus for constructing spinor invariants of the Lorentz group. It is very similar to the tensor calculus. The spinor in the upper two components of the Dirac field, which transforms under boosts via the matrix $e^{-\zeta \cdot \sigma/2}$,

was previously denoted by ξ_α , while the spinor in the lower components, transforming via $e^{\zeta \cdot \sigma / 2}$, was previously denoted by $\eta^{\dot{\beta}}$. Complex conjugation brings ξ_α into a spinor $(\xi_\alpha)^*$ which transforms via $e^{-\zeta \cdot \sigma^* / 2}$. Such a spinor is given a lower dotted index, i.e., we write

$$(\xi_\alpha)^* \equiv \xi^*_{\dot{\alpha}}. \quad (4.790)$$

Similarly, we define $(\eta^{\dot{\beta}})^*$ which transforms via $e^{\zeta \cdot \sigma^* / 2}$ as

$$(\eta^{\dot{\beta}})^* \equiv \eta^{*\beta}. \quad (4.791)$$

From the earlier discussion in Section 4.11 we know that

$$(\eta^{\dot{\alpha}})^* \xi_\alpha, \quad (\xi_\beta)^* \eta^{\dot{\beta}} \quad (4.792)$$

are Lorentz invariants. With the above notation, these can be viewed as

$$\eta^{*\alpha} \xi_\alpha, \quad \xi^*_{\dot{\beta}} \eta^{\dot{\beta}}. \quad (4.793)$$

Thus the invariants arise by simple contractions of equal upper and lower indices.

A further invariant can be constructed from two spinors which both have lower indices α and β , namely

$$\xi'_\beta c^{\beta\alpha} \xi_\alpha, \quad (4.794)$$

with the 2×2 -charge conjugation matrix $c = -i\sigma^2$ of (4.604). Writing (4.794) in matrix notation as $\xi'^T c \xi$, it goes under rotations over into

$$\xi'^T e^{-i\varphi \cdot \sigma^T / 2} c e^{-i\varphi \cdot \sigma / 2} \xi. \quad (4.795)$$

Since $\sigma^T = \sigma^*$ [see (8.158)] and $\sigma^* c = -c \sigma$ from (4.639), this is obviously invariant. A similar manipulation shows invariance under boosts. Thus the matrix $c^{\alpha\beta}$ constitutes an antisymmetric (or symplectic) metric in spinor space. Accordingly, we define

$$\xi^\beta \equiv c^{\beta\alpha} \xi_\alpha. \quad (4.796)$$

Then the invariant (4.794) arises by a contraction of equal upper and lower indices, just as in the notation in Minkowski space:

$$\xi'_\beta c^{\beta\alpha} \xi_\alpha = \xi'^\alpha \xi_\alpha. \quad (4.797)$$

Similarly, we can form an invariant from two $\eta^{\dot{\beta}}$ -spinors:

$$\eta'^{\dot{\beta}} (c^{-1})_{\dot{\beta}\dot{\alpha}} \eta^{\dot{\alpha}}, \quad (4.798)$$

defining

$$\eta_{\dot{\beta}} \equiv (c^{-1})_{\dot{\beta}\dot{\alpha}} \eta^{\dot{\alpha}}, \quad (4.799)$$

which makes the contraction $\eta'_{\dot{\beta}} \eta^{\dot{\beta}}$ Lorentz-invariant.

The Lorentz transformation matrices associated with ξ_α and $\eta^{\dot{\beta}}$ are $D^{(\frac{1}{2},0)}(\Lambda)$ and $D^{(0,\frac{1}{2})}(\Lambda)$, respectively. They carry Weyl indices $D^{(\frac{1}{2},0)}(\Lambda)_{\alpha}{}^{\alpha'}$ and $D^{(0,\frac{1}{2})}(\Lambda)^{\dot{\beta}}{}_{\dot{\beta}'}$.

It is possible to combine Weyl spinors to vectors rather than scalars with the help of the σ^μ -matrices (8.156) and of $\tilde{\sigma}^\mu$. They may be thought of as carrying Weyl labels

$$(\sigma^\mu)_{\alpha\dot{\beta}}, \quad (4.800)$$

and

$$(\tilde{\sigma}^\mu)^{\dot{\beta}\alpha}. \quad (4.801)$$

Then the indices show directly which spinors are required to form vectors:

$$\xi^* \tilde{\sigma}^\mu \xi = \xi^*_{\dot{\beta}} (\tilde{\sigma}^\mu)^{\dot{\beta}\alpha} \xi_\alpha, \quad \eta^* \sigma^\mu \eta = \eta^{*\alpha} (\sigma^\mu)_{\alpha\dot{\beta}} \eta^{\dot{\beta}}. \quad (4.802)$$

The vector nature of these combinations is proved by rewriting the transformation law (4.508) in a 2×2 -form as

$$\begin{aligned} D^{(\frac{1}{2},0)}(\Lambda)^{-1} \sigma^\mu D^{(0,\frac{1}{2})}(\Lambda) &= \Lambda^\mu{}_\nu \sigma^\nu, \\ D^{(0,\frac{1}{2})}(\Lambda)^{-1} \tilde{\sigma}^\mu D^{(\frac{1}{2},0)}(\Lambda) &= \Lambda^\mu{}_\nu \tilde{\sigma}^\nu. \end{aligned} \quad (4.803)$$

Written with Weyl indices, this reads

$$\begin{aligned} [D^{(\frac{1}{2},0)}(\Lambda)^{-1}]'_\beta{}^\alpha (\sigma^\mu)_{\alpha\dot{\beta}} D^{(0,\frac{1}{2})}(\Lambda)^{\dot{\beta}}{}_{\dot{\beta}'} &= (\sigma^\mu)_{\beta\dot{\beta}'}, \\ [D^{(0,\frac{1}{2})}(\Lambda)^{-1}]^{\dot{\alpha}}{}_{\dot{\alpha}'} (\tilde{\sigma}^\mu)^{\dot{\alpha}\beta} D^{(\frac{1}{2},0)}(\Lambda)_{\beta}{}^{\beta'} &= (\tilde{\sigma}^\mu)^{\dot{\alpha}\beta'}. \end{aligned} \quad (4.804)$$

In Weyl's calculus, the Dirac equation reads

$$(i\not{\partial} - M)\psi(x) = \begin{pmatrix} -M\delta_{\alpha}{}^{\alpha'} & (i\sigma^\mu\partial_\mu)_{\alpha\dot{\beta}'} \\ (i\tilde{\sigma}^\mu\partial_\mu)^{\dot{\beta}\alpha'} & -M\delta^{\dot{\beta}}{}_{\dot{\beta}'} \end{pmatrix} \begin{pmatrix} \xi_{\alpha'} \\ \eta^{\dot{\beta}'} \end{pmatrix} = 0. \quad (4.805)$$

4.17 Massive Vector Fields

In order to understand weak interactions and some strongly interacting particles, we must also learn to describe massive vector fields. They can be electrically neutral or carry electric charges ± 1 .

4.17.1 Action and Field Equations

The action of a neutral massive vector field $V^\mu(x)$ can be obtained by writing down an action like the electromagnetic one in (4.237), and simply adding a mass term:

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} M^2 V_\mu V^\mu \right), \quad (4.806)$$

where the field tensor is now

$$F_{\mu\nu}(x) \equiv \partial_\mu V_\nu(x) - \partial_\nu V_\mu(x). \quad (4.807)$$

Charged vector fields are described by the action

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left(-\frac{1}{2} F_{\mu\nu}^* F^{\mu\nu} + M^2 V_\mu^* V^\mu \right). \quad (4.808)$$

In either case, the equation of motion reads

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu = 0, \quad (4.809)$$

or more explicitly

$$[(-\partial^2 - M^2)g_{\mu\nu} + \partial_\mu \partial_\nu] V^\mu(x) = 0. \quad (4.810)$$

As for electromagnetic fields, the Euler-Lagrange equation for the zeroth component $V^0(x)$ does not involve the time derivative of $V^0(x)$ and is therefore not a dynamical equation, but it relates $V^0(x)$ to the spatial components $V^i(x)$ and their time derivatives via

$$V^0(x) = -\partial_\mu F^{\mu 0}/M^2 = \frac{1}{M^2} [\nabla \cdot \dot{\mathbf{V}}(x) + \nabla^2 V^0(x)]. \quad (4.811)$$

In the limit $M \rightarrow 0$, this gives rise to Coulomb's law (4.267). Taking the four-divergence of (4.809), we see that it vanishes:

$$\partial_\mu V^\mu(x) = 0. \quad (4.812)$$

Physically, this eliminates any scalar content $\partial^\mu s(x)$ from the vector potential. In contrast to the electromagnetic vector field $A^\mu(x)$, the zero four-divergence is not a matter of choice as in the Lorenz condition (4.252), but it follows here from the Euler-Lagrange equations. Inserting (4.812) back into (4.810), we find that the four components of $V^\mu(x)$ satisfy the Klein-Gordon equation

$$(-\partial^2 - M^2)V^\mu(x) = 0, \quad (4.813)$$

which is the massive version of the electromagnetic field equations (4.253) in the Lorenz gauge.

4.17.2 Plane Wave Solutions for Massive Vector Fields

The plane-wave solutions look the same as in Eqs. (4.309) and (4.310) for the electromagnetic vector potential. The mass of the vector field modifies only the possible polarization vectors $\epsilon^\mu(\mathbf{k}, \lambda)$. As in the electromagnetic case, the zero divergence property (4.812) eliminates one degree of freedom in the polarization vectors. It is, however, impossible to eliminate more, since there exists no gauge invariance, and thus no analog of the restricted gauge transformations (4.255). Adding to $V^\mu(x)$ a gradient $\partial^\mu \Lambda(x)$ and inserting the new field into the field equation (4.809) produces the condition $M^2 \partial_\mu \Lambda(x) = 0$, admitting only a trivial constant for $\Lambda(x)$. The polarization vector has therefore three independent components. Physically this reflects

the fact that a massive vector particle can be studied in its rest frame. There the third component of angular momentum L_3 , and the square $\mathbf{L}^2$ have three eigenstates corresponding to three linear combinations of the spatial vector components. With the restriction (4.812), the polarization vectors must satisfy $k_\mu \epsilon^\mu(\mathbf{k}, s_3) = 0$. For particles at rest only three polarization vectors are allowed:

$$\epsilon^\mu(\mathbf{0}, \pm 1) = \mp \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}, \quad \epsilon^\mu(\mathbf{0}, 0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (4.814)$$

These are obviously eigenstates of the 4×4 -angular momentum matrices L_3 and $\mathbf{L}^2$ in the defining representation (4.54)–(4.56). The relative phases have been chosen as in (4.321) to comply with the Condon-Shortley convention as on p. 284. Recall that this means that by applying L_+ to $\epsilon^\mu(\mathbf{0}, \lambda)$, one obtains the states with $\lambda' = \lambda \pm 1$, multiplied by positive matrix elements $\sqrt{2}$. The polarization vectors of momentum $\mathbf{k}$ are obtained from those at rest by applying the boost matrices (4.24):

$$\epsilon^\mu(\mathbf{k}, s_3) = B(\boldsymbol{\zeta}) \epsilon^\mu(\mathbf{0}, s_3). \quad (4.815)$$

The zero-helicity polarization vector $\epsilon^\mu(\mathbf{k}, 0)$ is also called *longitudinal polarization vector*, that exists for vector particles if these have a mass. The three boosted polarization vectors satisfy the orthogonality relations

$$\epsilon_\mu(\mathbf{k}, s_3)^* \epsilon^\mu(\mathbf{k}, s'_3) = -\delta_{s_3 s'_3}. \quad (4.816)$$

In order to find the completeness relations, we boost the polarization vectors at rest (4.814) to a final momentum $k^\mu \equiv (\omega_{\mathbf{k}}, 0, 0, k^3)$ in the z -direction using the matrix (14.286), and we obtain

$$\epsilon_H^\mu(k^3 \hat{\mathbf{z}}, \pm 1) = \mp \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}, \quad \epsilon_H^\mu(k^3 \hat{\mathbf{z}}, 0) = \frac{1}{M} \begin{pmatrix} k^3 \\ 0 \\ 0 \\ \omega_{\mathbf{k}} \end{pmatrix}, \quad (4.817)$$

where $\hat{\mathbf{z}}$ is the unit vector in the z -direction. We can now calculate the completeness sum

$$\sum_{s_3} \epsilon^\mu(k^3 \hat{\mathbf{z}}, s_3) \epsilon^\nu(k^3 \hat{\mathbf{z}}, s_3)^* = \frac{1}{M^2} \begin{pmatrix} k^{32} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \omega_{\mathbf{k}}^2 \end{pmatrix}. \quad (4.818)$$

By rewriting the right-hand side in the form

$$-g^{\mu\nu} + \frac{1}{M^2} \begin{pmatrix} k^0 k^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & k^3 k^3 \end{pmatrix}, \quad (4.819)$$

we recognize the general covariant form for any direction of the momentum $\mathbf{k}$:

$$\sum_{s_3} \epsilon^\mu(\mathbf{k}, s_3) \epsilon^\nu(\mathbf{k}, s_3)^* = P^{\mu\nu}(k) \equiv - \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2} \right). \quad (4.820)$$

If the vectors are first boosted into the z -direction and then rotated into the direction of their momentum:

$$\hat{\mathbf{k}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad (4.821)$$

with the polar angles θ, ϕ , we obtain the polarization vectors in the helicity basis. The subsequent rotation into the direction $\mathbf{k}$ by the four-dimensional extension of the matrix (4.328) leads to the polarization vectors of helicities $\lambda = \pm 1$ and 0:

$$\epsilon_H^\mu(\mathbf{k}, \pm 1) = \begin{pmatrix} 0 \\ \boldsymbol{\epsilon}(\mathbf{k}, \pm 1) \end{pmatrix}, \quad \epsilon_H^\mu(\mathbf{k}, 0) = \frac{1}{M} \begin{pmatrix} |\mathbf{k}| \\ \omega_{\mathbf{k}} \hat{\mathbf{k}} \end{pmatrix}, \quad (4.822)$$

where $\boldsymbol{\epsilon}(\mathbf{k}, \pm 1)$ are the three-dimensional polarization vectors (4.331). The four-dimensional polarization vectors $\epsilon_H^\mu(\mathbf{k}, \pm 1)$ agree with (4.318), and the vector $\epsilon_H^\mu(\mathbf{k}, 0)$ denotes the longitudinal polarization vector associated with the three-dimensional $\epsilon_H^i(\mathbf{k}, 0) = \omega_{\mathbf{k}} k^i / M$. The covariant completeness sum (4.820) can be derived directly from the general polarization vectors (4.822). It reads explicitly

$$\sum_{s_3} \epsilon^\mu(\hat{\mathbf{k}}, s_3) \epsilon^\nu(\hat{\mathbf{k}}, s_3)^* = \left(\frac{|\mathbf{k}|^2 / M^2}{k^i k^0 / M^2} \middle| \frac{k^0 k^i}{\delta^{ij} + k^i k^j / M^2} \right), \quad (4.823)$$

which is the rotated version of (4.819).

It will sometimes be convenient to view the photon as an $M \rightarrow 0$ -limit of a massive vector meson. For this purpose we have to add a gauge fixing term to the Lagrangian to allow for a proper limit. The extended action reads

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} M^2 V_\mu V^\mu - \frac{1}{2\alpha} (\partial_\mu V^\mu)^2 \right], \quad (4.824)$$

resulting in the field equation

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu + \frac{1}{\alpha} \partial^\nu \partial_\mu V^\mu = 0, \quad (4.825)$$

which reads more explicitly

$$\left[(-\partial^2 - M^2) g_{\mu\nu} + \left(1 - \frac{1}{\alpha} \right) \partial_\mu \partial_\nu \right] V^\mu(x) = 0. \quad (4.826)$$

Multiplying (4.825) with ∂_ν from the left gives, for the divergence $\partial_\nu V^\nu$, the Klein-Gordon equation

$$(\partial^2 + \alpha M^2) \partial_\nu V^\nu(x) = 0, \quad (4.827)$$

from which the constraint (4.812) follows in the limit of large α .

4.18 Higher-Spin Representations

Given the fundamental spin-1/2 field, it is very simple to generalize the transformation matrices to higher spins. A system with two spin-1/2 particles can have spin 1 or 0. Similarly, n spin-1/2 particles can couple to spin $n/2, n-1/2, \dots$ down to 1/2 or 0. Thus in order to build an arbitrary spin s , all we have to do is put $2s$ spin-1/2 representations together in an appropriate fashion. The problem is completely analogous to the previous extension in Section 2.5 of the one-particle Schrödinger equation to an arbitrary n -particle equation. Thus we shall construct representations of arbitrary spin by a “second quantization” of spin, and further of the generators of the entire Lorentz group.

4.18.1 Rotations

If the particle is at rest, spin is defined by the rotation subgroup. The 2×2 Hermitian generators

$$\mathbf{L} = \frac{1}{2} \boldsymbol{\sigma} \quad (4.828)$$

may be considered as the analog of the single-particle Schrödinger operator $-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + V_1(\mathbf{x}; t)$ in Eq. (2.93), or as the matrix M_i in the commutation rules (2.99). According to (2.101), the second quantized version of $\mathbf{L}$ reads

$$\hat{L}_i = \frac{1}{2} \hat{a}^\dagger \sigma^i \hat{a}, \quad (4.829)$$

where $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$ with $\alpha = 1, 2$ are two bosonic creation and annihilation operators. As proved in general in (2.102), these operators satisfy the same commutation rules as the Pauli matrices σ^i :

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k. \quad (4.830)$$

The states

$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle \equiv \hat{a}_1^\dagger |0\rangle, \quad |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \equiv \hat{a}_2^\dagger |0\rangle \quad (4.831)$$

may be identified as the two basis states of the fundamental spin-1/2 representation. The effect of the three operators $\hat{L}_i$ is, as in the general Eq. (2.103):

$$\begin{aligned} [\hat{L}_i, \hat{a}_\alpha^\dagger] &= \hat{a}_{\alpha'}^\dagger \frac{1}{2} \sigma_{\alpha'\alpha}^i, \\ [\hat{a}_{\alpha'}, \hat{L}_i] &= \frac{1}{2} \sigma_{\alpha'\alpha}^i \hat{a}_\alpha. \end{aligned} \quad (4.832)$$

On these states, the second-quantized operators (4.829) have eigenvalues

$$\hat{\mathbf{L}}|s, s_3\rangle = s(s+1)|s, s_3\rangle, \quad \hat{L}_3|s, s_3\rangle = s_3|s, s_3\rangle. \quad (4.833)$$

In the present restriction to the rotation group we shall use only lower indices 1 and 2 rather than Weyl indices of the previous section.

As in Section 2.5, we may now compose all higher representations of the rotation group by combining many of these fundamental representations, and forming states such as

$$\prod_{i=1}^{2s} (a_{\alpha_i}^\dagger) |0\rangle. \quad (4.834)$$

It is easy to see that linear combinations of such states with a fixed number of $a^\dagger$ form an invariant representation space of the rotation group. The reason is that the three generators $\hat{L}_i$ commute with the "particle" number operator

$$N = \hat{a}^\dagger \hat{a}. \quad (4.835)$$

In fact, a little algebra shows that the *Casimir operator* of the rotation group $\hat{\mathbf{L}}^2$, which characterizes an irreducible representation, is equal to

$$\hat{\mathbf{L}}^2 = \frac{1}{4} (\hat{a}^\dagger \sigma^i \hat{a})^2 = \frac{1}{2} \hat{N} \left(\frac{1}{2} \hat{N} + 1 \right), \quad (4.836)$$

showing explicitly that under rotations, states built from a fixed number $2s$ of spin creation operators $a^\dagger$ always maintain the same number $2s$, and that the eigenvalue of the Casimir operator in the space of $2s$ particles is $s(s+1)$. Thus the space is indeed *invariant* under rotations.

But it is also an irreducible representation of spin s . To see this take the complete set of basis states in the space

$$|n_1, n_2\rangle = \frac{1}{\sqrt{n_1! n_2!}} (\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} |0\rangle, \quad (4.837)$$

which diagonalize the occupation numbers of the two operators $a_1^\dagger$ and $a_2^\dagger$, and which are normalized to unity. Applying to these the operator

$$\hat{L}_3 = \hat{a}^\dagger \frac{\sigma^3}{2} \hat{a} = \frac{1}{2} (\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2), \quad (4.838)$$

we see that it measures the difference in the number of "spin up" and "spin down" particles created by $a_1^\dagger$ and $a_2^\dagger$, respectively:

$$L_3 |n_1, n_2\rangle = \frac{1}{2} (n_1 - n_2) |n_1, n_2\rangle \equiv m |n_1, n_2\rangle. \quad (4.839)$$

Thus the state has the azimuthal ("magnetic") quantum number $m = n_1 - n_2$. The operators

$$\hat{L}_+ \equiv \hat{L}_1 + i\hat{L}_2, \quad \hat{L}_- \equiv \hat{L}_1 - i\hat{L}_2, \quad (4.840)$$

on the other hand, have the form

$$\begin{aligned} \hat{L}_+ &= \hat{a}^\dagger \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \hat{a} = \hat{a}_1^\dagger \hat{a}_2, \\ \hat{L}_- &= \hat{a}^\dagger \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \hat{a} = \hat{a}_2^\dagger \hat{a}_1. \end{aligned} \quad (4.841)$$

Among each other and with $\hat{L}_3$, they satisfy the commutation rules

$$\begin{aligned} [\hat{L}_-, \hat{L}_+] &= 2\hat{L}_3, \\ [\hat{L}_3, \hat{L}_+] &= \hat{L}_+, \\ [\hat{L}_3, \hat{L}_-] &= -\hat{L}_-. \end{aligned} \quad (4.842)$$

They remove a spin down while adding a spin up and vice versa. Their matrix elements are

$$\begin{aligned} \hat{L}_+ |n_1, n_2\rangle &= \sqrt{(n_1 + 1)n_2} |n_1 + 1, n_2 - 1\rangle, \\ \hat{L}_- |n_1, n_2\rangle &= \sqrt{n_1(n_2 + 1)} |n_1 - 1, n_2 + 1\rangle. \end{aligned} \quad (4.843)$$

It is now obvious that starting from an arbitrary state, say $|n, 0\rangle$ with no number of spin-down particles and eigenvalue $n/2$ of $\hat{L}_3$, we can reach every other state $|n - k, k\rangle$ with $k = 1, \dots, n$ by repeated application of $\hat{L}_-$. The process ends at $|0, n\rangle$, where $\hat{L}_- |n, 0\rangle = 0$. This proves the irreducibility of the representation.

Conventionally, the highest eigenvalue of $\hat{L}_3$ is referred to as the value s of angular momentum:

$$s = n/2. \quad (4.844)$$

It appears in the eigenvalue (4.836) of $\hat{\mathbf{L}}^2$ as

$$\hat{\mathbf{L}}^2 |n - k, k\rangle = s(s + 1) |n - k, k\rangle. \quad (4.845)$$

Hence the states may be reexpressed in terms of the numbers s and m as

$$|s, m\rangle = |s + m, s - m\rangle = \frac{1}{\sqrt{(s - m)!(s + m)!}} (\hat{a}_1^\dagger)^{s+m} (\hat{a}_2^\dagger)^{s-m} |0\rangle, \quad (4.846)$$

and the matrix elements (4.839) and (4.843) read

$$\hat{L}_3 |s, m\rangle = m |s, m\rangle, \quad (4.847)$$

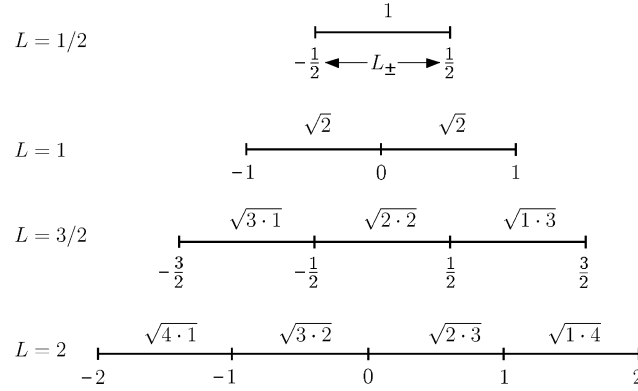
$$\hat{L}_+ |s, m\rangle = \sqrt{(s - m)(s + m + 1)} |s, m + 1\rangle, \quad (4.848)$$

$$\hat{L}_- |s, m\rangle = \sqrt{(s + m)(s - m + 1)} |s, m - 1\rangle. \quad (4.849)$$

For smaller spin values the effect of the raising and lowering operators $\hat{L}_+$ and $\hat{L}_-$ upon the states $|s, m\rangle$ is illustrated in Fig. 4.3.

Note that we could have defined the states (4.846) with arbitrary phase factors $e^{i\phi_1}$ and $e^{i\phi_2}$ accompanying $\hat{a}_1^\dagger$ and $\hat{a}_2^\dagger$. Then the application of L_+ and L_- would produce phase factors $e^{-i(\phi_1 - \phi_2)}$ and $e^{i(\phi_1 - \phi_2)}$ in (4.848) and (4.849), respectively. It is easy to verify that these phases drop out in the commutation rules (4.842) of the rotation group, and thus in (4.830).

The choice of a positive square-root in (4.848) and (4.849) without such extra phase factors is known as the *Condon-Shortley phase convention*.

FIGURE 4.3 Effect of raising and lowering operators $\hat{L}_+$ and $\hat{L}_-$ upon the states $|s, m\rangle$.

4.18.2 Extension to Lorentz Group

It is now quite simple to extend this construction of spin representations of the rotations to the entire Lorentz group. For this we deduce from the commutation rules between the generators L_i and M_i in Eq. (4.76)–(4.78) that the combinations

$$\begin{aligned}\hat{\mathbf{J}}^1 &= (\hat{\mathbf{L}} + i\hat{\mathbf{M}})/2, \\ \hat{\mathbf{J}}^2 &= (\hat{\mathbf{L}} - i\hat{\mathbf{M}})/2\end{aligned}\quad (4.850)$$

have the commutation rules

$$\begin{aligned}[\hat{J}_i^1, \hat{J}_j^2] &= 0, \\ [\hat{J}_i^1, \hat{J}_j^1] &= i\epsilon_{ijk}\hat{J}_k^1, \\ [\hat{J}_i^2, \hat{J}_j^2] &= i\epsilon_{ijk}\hat{J}_k^2.\end{aligned}\quad (4.851)$$

Therefore they generate two independent sets of rotations. Extending the previous construction, we now form the second-quantized operators

$$\begin{aligned}\hat{\mathbf{J}}^{(1)} &= \hat{a}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{a}, \\ \hat{\mathbf{J}}^{(2)} &= \hat{b}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{b},\end{aligned}\quad (4.852)$$

and obtain

$$\hat{\mathbf{L}} = \hat{\mathbf{J}}^{(1)} + \hat{\mathbf{J}}^{(2)} = \hat{a}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{a} + \hat{b}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{b}, \quad (4.853)$$

$$\hat{\mathbf{M}} = \frac{1}{i}(\hat{\mathbf{J}}^{(1)} - \hat{\mathbf{J}}^{(2)}) = \frac{1}{i} \left(\hat{a}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{a} - \hat{b}^\dagger \frac{\boldsymbol{\sigma}}{2} \hat{b} \right). \quad (4.854)$$

These operators correspond to forming the second-quantized operators

$$\hat{\mathbf{L}} = \frac{1}{2}(\hat{a}^\dagger, \hat{b}^\dagger) \boldsymbol{\Sigma} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix}, \quad (4.855)$$

$$\hat{\mathbf{M}} = \frac{1}{2}(\hat{a}^\dagger, \hat{b}^\dagger) i\boldsymbol{\alpha} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix}, \quad (4.856)$$

with the 4×4 -representation matrices (4.514) and (4.516) of the Lorentz group.

For a clearer display of the Lorentz transformation properties one may take advantage of the Weyl notation. From (4.853) and (4.854) we see that the operators $a^\dagger$ and $b^\dagger$ transform according to the fundamental representations $D^{(\frac{1}{2}, 0)}$ and $D^{(0, \frac{1}{2})}$, since the 2×2 -matrices between them are for rotations $\boldsymbol{\sigma}/2$, $-i\boldsymbol{\sigma}/2$ and for Lorentz boosts $\boldsymbol{\sigma}/2$, $i\boldsymbol{\sigma}/2$, respectively. Thus we may write them in the Weyl notation as $a_\alpha^\dagger$ and $b^{\dagger\dot{\beta}}$. By applying to the operators $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$ the same arguments as to the rotation group, we can now easily see that the set of states

$$|n_1^a, n_2^a, n_1^b, n_2^b\rangle = \frac{1}{\sqrt{n_1^a! n_2^a! n_1^b! n_2^b!}} (\hat{a}_1^\dagger)^{n_1^a} (\hat{a}_2^\dagger)^{n_2^a} (\hat{b}^{\dagger\dot{1}})^{n_1^b} (\hat{b}^{\dagger\dot{2}})^{n_2^b} |0\rangle \quad (4.857)$$

for fixed numbers $n^a = n_1^a + n_2^a$ and $n^b = n_1^b + n_2^b$ are irreducible representation spaces of the whole Lorentz group. They are denoted by

$$(s_1, s_2) \equiv \left(\frac{n^a}{2}, \frac{n^b}{2} \right). \quad (4.858)$$

The states (4.857) live in the direct-product space of the two operators $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$. They may be relabeled by the quantum numbers of the two rotation subgroups as in (4.846):

$$|s_1, m_1; s_2, m_2\rangle = \frac{1}{\sqrt{(s_1 - m_1)!(s_1 + m_1)!(s_2 - m_2)!(s_2 + m_2)!}} \times (\hat{a}_1^\dagger)^{s_1+m_1} (\hat{a}_2^\dagger)^{s_1-m_1} (\hat{b}^{\dagger\dot{1}})^{s_2+m_2} (\hat{b}^{\dagger\dot{2}})^{s_2-m_2} |0\rangle. \quad (4.859)$$

Since by (4.853) the operator of angular momentum $\hat{\mathbf{L}}$ is the direct sum of those of the two rotation subgroups, an irreducible representation $D^{(s_1, s_2)}(\Lambda)$ of the Lorentz group contains different irreducible representations of the rotation subgroup generated by $\hat{\mathbf{L}}$. They are obtained from the rules of addition of angular momenta. The operator $\hat{\mathbf{L}}^2$ and the third component $\hat{L}_3$ can be diagonalized with eigenvalues $s(s+1)$ and m by forming the linear combination

$$|s, m\rangle = \sum_{m_1, m_2} |s_1, m_1; s_2, m_2\rangle \langle s_1, m_1; s_2, m_2 | s, m\rangle, \quad (4.860)$$

where $\langle s_1, m_1; s_2, m_2 | s, m\rangle$ are Clebsch-Gordan coefficients [18]. Their calculation and properties are recalled in Appendix 4E. The values of total angular momentum s occurring in the decomposition (4.860) are

$$|s_1 - s_2| \leq s \leq s_1 + s_2. \quad (4.861)$$

The Clebsch-Gordan coefficients are orthogonal and complete, so that (4.860) can be inverted to

$$|s_1, m_1; s_2, m_2\rangle = \sum_{s, m} |s, m\rangle \langle s, m | s_1, m_1; s_2, m_2\rangle. \quad (4.862)$$

4.18.3 Finite Representation Matrices

To complete this discussion let us calculate the finite representation matrices. Due to the decompositions (4.853) and (4.854) into generators of rotations, we only need those of the rotation group.

Rotation Group

We first observe that every 3×3 -rotation matrix $R_{\hat{\varphi}}(\varphi)$ in Eq. (4.9) can be decomposed into Euler angles

$$R_{\hat{\varphi}}(\varphi) = e^{-i\varphi \cdot \mathbf{L}} = e^{-i\alpha L_3} e^{-i\beta L_2} e^{-i\gamma L_3} \equiv R(\alpha, \beta, \gamma), \quad (4.863)$$

and so can the general rotation operator

$$e^{-i\varphi \cdot \hat{\mathbf{L}}} = e^{-i\alpha \hat{L}_3} e^{-i\beta \hat{L}_2} e^{-i\gamma \hat{L}_3} \equiv \hat{R}(\alpha, \beta, \gamma). \quad (4.864)$$

Since $\hat{L}_3$ is diagonal on the states $|jm\rangle$, the finite rotation $e^{-i\varphi \cdot \hat{\mathbf{L}}}$ acts on the states $|jm\rangle$ as

$$\begin{aligned} \hat{R}(\alpha, \beta, \gamma)|jm\rangle &= \sum_{m'=-j}^j |jm'\rangle e^{-i(m'\alpha+m\gamma)} \langle jm'|e^{-i\beta \hat{L}_2}|jm\rangle \\ &\equiv \sum_{m'=-j}^j |jm'\rangle D_{m',m}^j(\alpha, \beta, \gamma), \end{aligned} \quad (4.865)$$

so that the only nontrivial matrix elements are

$$d_{m'm}^j(\beta) = \langle jm'|e^{-i\beta \hat{L}_2}|jm\rangle. \quad (4.866)$$

For a single creation operator $\hat{a}^\dagger$, we have from (4.832):

$$\begin{aligned} [\hat{L}_2, \hat{a}_1^\dagger] &= \frac{1}{2i} [\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1, \hat{a}_1^\dagger] = \frac{i}{2} \hat{a}_2^\dagger, \\ [\hat{L}_2, \hat{a}_2^\dagger] &= \frac{1}{2i} [\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1, \hat{a}_2^\dagger] = -\frac{i}{2} \hat{a}_1^\dagger, \end{aligned} \quad (4.867)$$

and therefore

$$\begin{aligned} e^{-i\beta \hat{L}_2} \hat{a}_1^\dagger e^{i\beta \hat{L}_2} &= \hat{a}_1^\dagger \cos \frac{\beta}{2} + \hat{a}_2^\dagger \sin \frac{\beta}{2}, \\ e^{-i\beta \hat{L}_2} \hat{a}_2^\dagger e^{i\beta \hat{L}_2} &= -\hat{a}_1^\dagger \sin \frac{\beta}{2} + \hat{a}_2^\dagger \cos \frac{\beta}{2}. \end{aligned} \quad (4.868)$$

Of course, this is just the statement that $\hat{a}_1^\dagger|0\rangle$ and $\hat{a}_2^\dagger|0\rangle$ are transformed according to the spin-1/2-representation of the rotation group [recall (4.456)]:

$$\begin{aligned} e^{-i\beta \hat{L}_2} a_{\alpha}^\dagger e^{i\beta \hat{L}_2} &= a_{\alpha'}^\dagger \begin{pmatrix} \cos \frac{\beta}{2} & -\sin \frac{\beta}{2} \\ \sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix}_{\alpha}^{\alpha'} \\ &= a_{\alpha'}^\dagger (e^{-i\beta \sigma^2/2})_{\alpha}^{\alpha'}. \end{aligned} \quad (4.869)$$

An arbitrary state (4.846) goes over into

$$e^{-\beta L_2} |jm\rangle = \frac{1}{\sqrt{(j-m)!(j+m)!}} \times \left(\hat{a}_1^\dagger \cos \frac{\beta}{2} + \hat{a}_2^\dagger \sin \frac{\beta}{2} \right)^{j+m} \left(-\hat{a}_1^\dagger \sin \frac{\beta}{2} + \hat{a}_2^\dagger \cos \frac{\beta}{2} \right)^{j-m} |0\rangle. \quad (4.870)$$

We now expand the right-hand side into a sum of products of two creation operators. After ordering the terms, we rewrite the rotated state as

$$e^{-\beta L_2} |jm\rangle = \sum_{m'} \frac{1}{\sqrt{(j-m')!(j+m')!}} (\hat{a}_1^\dagger)^{j+m'} (\hat{a}_2^\dagger)^{j-m'} |0\rangle d_{m'm}^j(\beta). \quad (4.871)$$

This defines the matrix elements of the rotations around the second axis by an angle β :

$$d_{m'm}^j(\beta) = \sqrt{\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}} \sum_{k=0}^{\infty} \binom{j+m}{j-m'-k} \binom{j-m}{k} \times (-1)^{j-m-k} \left(\cos \frac{\beta}{2} \right)^{2k+m'+m} \left(\sin \frac{\beta}{2} \right)^{2j-2k-m'-m}. \quad (4.872)$$

The sum can be expressed in terms of hypergeometric functions

$$F(a, b, c; z) \equiv 1 + \frac{ab}{c} z + \frac{a(a+1)b(b+1)}{c(c+1)} \frac{z^2}{2!} + \dots, \quad (4.873)$$

in terms of which they read

$$d_{m'm}^j(\beta) = \frac{(-1)^{m'-m}}{(m'-m)!} \sqrt{\frac{(j-m)!(j+m')!}{(j+m)!(j-m')!}} \left(\cos \frac{\beta}{2} \right)^{m'+m} \left(\sin \frac{\beta}{2} \right)^{m'-m} \times F\left(-j+m', j+m'+1; m'-m+1; \sin^2 \frac{\beta}{2}\right). \quad (4.874)$$

This formula is directly applicable for $m' \geq m$, where the hypergeometric function is regular at the origin. For $m' < m$ we use the property

$$d_{m'm}^j(\beta) = (-1)^{m'-m} d_{mm'}^j(\beta) = (-1)^{m'-m} d_{-m'-m}^j(\beta) \quad (4.875)$$

to exchange the order. Additional useful relations are

$$d_{m'm}^j(\beta - \pi) = (-1)^{j-m'} d_{-m'm}^j(\beta) \quad (4.876)$$

and

$$d_{m'm}^j(\pi) = (-1)^{j+m'} \delta_{m', -m}. \quad (4.877)$$

The hypergeometric functions can also be expressed in terms of Jacobi polynomials:

$$\begin{aligned} F\left(-j+m', j+m'+1; m'-m+1; \sin^2 \frac{\beta}{2}\right) \\ = \frac{(j-m')!}{(j-m)!} (m'-m)! P_{j-m'}^{(m'-m, m'+m)}(\cos \beta). \end{aligned} \quad (4.878)$$

The matrix elements $d_{00}^l(\beta)$ coincide with the Legendre polynomials,

$$d_{00}^l(\beta) = P_l(\cos \beta), \quad (4.879)$$

and the matrix elements $d_{m0}^l(\beta)e^{i\gamma}$ are proportional to the spherical harmonics $Y_{lm}(\beta, \gamma)$:

$$d_{m0}^l(\beta)e^{i\gamma} = (-1)^m d_{0m}^l(\beta)e^{i\gamma} = \sqrt{\frac{4\pi}{2l+1}} Y_{lm}(\beta, \gamma). \quad (4.880)$$

For $j = \frac{1}{2}$ we reobtain the spinor representation of the rotation group

$$d_{m'm}^{1/2}(\beta) = \begin{pmatrix} \cos \beta/2 & -\sin \beta/2 \\ \sin \beta/2 & \cos \beta/2 \end{pmatrix} = e^{-i\beta\sigma^2/2}, \quad (4.881)$$

while for $j = 1$ we find the vector representation

$$d_{m'm}^1(\beta) = \begin{pmatrix} \frac{1}{2}(1+\cos \beta) & -\sin \beta/\sqrt{2} & \frac{1}{2}(1-\cos \beta) \\ \sin \beta/\sqrt{2} & \cos \beta & -\sin \beta/\sqrt{2} \\ \frac{1}{2}(1-\cos \beta) & \sin \beta/\sqrt{2} & \frac{1}{2}(1+\cos \beta) \end{pmatrix}. \quad (4.882)$$

The indices have the order $+1/2, -1/2$ and $+1, 0, -1$, respectively.

The representation functions (4.865) of all rotations

$$D_{m,m'}^j(\alpha, \beta, \gamma) = e^{-i(m\alpha+m'\gamma)} d_{m,m'}^j(\beta) \quad (4.883)$$

have the following orthonormality properties:

$$\frac{2j+1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^\pi d\beta \int_0^{2\pi} d\gamma D_{m_1,m'_1}^{j_1}(\alpha, \beta, \gamma) D_{m_2,m'_2}^{j_2}(\alpha, \beta, \gamma) = \delta_{j_1,j_2} \delta_{m_1,m_2} \delta_{m'_1,m'_2}. \quad (4.884)$$

At equal $m'_1 = m'_2$, these yield the integrals

$$\frac{2j+1}{4\pi} \int_0^{2\pi} d\alpha \int_0^\pi d\beta D_{m_1,m'_1}^{j_1}(\alpha, \beta, 0) D_{m_2,m'_1}^{j_2}(\alpha, \beta, 0) = \delta_{j_1,j_2} \delta_{m_1,m_2}. \quad (4.885)$$

The representation matrices $D_{m,m'}^j(\alpha, \beta, \gamma)$ with $j = 1$ are related to the original 3×3 -rotations $R(\alpha, \beta, \gamma)$ of Eq. (4.863) by a similarity transformation. It is the same transformation which relates the three spherical components $\mathfrak{e}(\lambda)$ in Eq. (4.321) to

the unit vectors (4.325). The eigenvectors (4.321) supply us with the matrix elements of the desired similarity transformation. Identifying the scalar products $\langle i|1, m\rangle$ as spherical components of a vector:

$$\langle i|1, m\rangle \equiv \epsilon^i(m), \quad (4.886)$$

we can write, using the 3×3 matrices (4.54)

$$\begin{aligned} (L_3)_{jk} &= \sum_{m=-1}^1 \langle j|1, m\rangle m \langle 1, m|k\rangle, \\ (L_{\pm})_{jk} &= \langle j|1, \pm 1\rangle \sqrt{2} \langle 1, 0|k\rangle + \langle j|1, 0\rangle \sqrt{2} \langle 1, \mp 1|k\rangle. \end{aligned} \quad (4.887)$$

In Dirac's bracket notation, the original 3×3 -matrices $R(\alpha, \beta, \gamma)$ in (4.863) may be considered as matrix elements of the general rotation operator $\hat{R}(\alpha, \beta, \gamma)$ in (4.864) between the basis states $|i\rangle$:

$$R_{ij}(\alpha, \beta, \gamma) = \langle i|\hat{R}(\alpha, \beta, \gamma)|j\rangle. \quad (4.888)$$

From the manipulation rules of Dirac brackets it is then obvious that the matrix elements transform under finite rotations as

$$\begin{aligned} \sum_{j=1}^3 R_{ij} \langle j|1, m\rangle &= \sum_{j=1}^3 \langle i|\hat{R}(\alpha, \beta, \gamma)|j\rangle \langle j|1, m\rangle \\ &= \sum_{j=1}^3 \sum_{m'=-1}^1 \langle i|1, m'\rangle \langle 1, m'|\hat{R}(\alpha, \beta, \gamma)|j\rangle \langle j|1, m\rangle \\ &= \sum_{m'=-1}^1 \langle i|1, m'\rangle \langle 1, m'|\hat{R}(\alpha, \beta, \gamma)|1, m\rangle = \sum_{m'=-1}^1 \langle i|1, m'\rangle D_{m',m}^1(R), \end{aligned} \quad (4.889)$$

which may also be written in a matrix form as¹²

$$R \epsilon(m) = \sum_{m'=-1}^1 \epsilon(m') D_{m',m}^1(R). \quad (4.890)$$

In Eq. (4.112) we stated the transformation law of a vector operator [see also Eq. (2.113)]:

$$[\hat{L}_i, \hat{v}_k] = \hat{v}_j (L_i)_{jk}, \quad (4.891)$$

With the help of the above similarity transformation, we find the spherical components of the vector operator $\hat{v}_i$:

$$\hat{v}(m) \equiv \sum_{i=1}^3 \hat{v}_i \langle i|1, m\rangle, \quad (4.892)$$

¹²Note that the spinor transformation laws (4.745) and (4.747) are a generalization of this relation.

or, explicitly,

$$\hat{v}(\pm 1) \equiv \mp \frac{1}{\sqrt{2}}(\hat{v}_1 \pm i\hat{v}_2), \quad \hat{v}(0) \equiv \hat{v}_3. \quad (4.893)$$

For these components, the commutation rules (4.891) become

$$[\hat{L}_i, \hat{v}(m)] = \sum_{m'=-1}^1 \hat{v}(m') \langle 1, m' | \hat{L}_i | 1, m \rangle. \quad (4.894)$$

They may be generalized to an arbitrary *spherical tensor operator* $\hat{v}(j, m)$ of spin j :

$$[\hat{L}_i, \hat{v}(j, m)] = \sum_{m'=-1}^1 \hat{v}(j, m') \langle j, m' | \hat{L}_i | j, m \rangle. \quad (4.895)$$

For $\hat{L}_3$ and $\hat{L}_{\pm}$, these commutation relations become

$$[\hat{L}_3, \hat{v}(j, m)] = \hat{v}(j, m) m, \quad [\hat{L}_{\pm}, \hat{v}(j, m)] = \hat{v}(j, m \pm 1) \sqrt{(j \mp m)(j \pm m + 1)}. \quad (4.896)$$

They are in one-to-one correspondence with the relations (4.847), (4.848), and (4.849) for the states $|j, m\rangle$.

For finite rotations, they give rise to the transformation behavior

$$\hat{R} \hat{v}(j, m) \hat{R}^{-1} = \hat{v}(j, m') D_{m'm}^j(R). \quad (4.897)$$

The use of defining such spherical tensor operators lies in the fact that all their matrix elements are related to each other by Clebsch-Gordan coefficients (4.860) via the so-called *Wigner-Eckart theorem*. Applying $\hat{v}(j, m)$ to a state $|j', m'\rangle$, we obtain a state $\hat{v}(j, m)|j', m'\rangle$, which transforms by a direct product of the representation matrices (4.865) and (4.897) like a state $|j, m; j', m'\rangle$. Its irreducible contents can be obtained with the help of the Clebsch-Gordan series (4.860). If we therefore expand

$$\hat{v}(j, m)|j', m'\rangle = \sum_{j'', m''} |j'', m''\rangle \langle j'', m'' | \hat{v}(j, m) | j', m' \rangle, \quad (4.898)$$

the matrix elements $\langle j'', m'' | \hat{v}(j, m) | j', m' \rangle$ must be proportional to the associated Clebsch-Gordan coefficients:

$$\langle j'', m'' | \hat{v}(j, m) | j', m' \rangle = \langle j'' || v(j) || j' \rangle \langle j'', m'' | j, m; j', m' \rangle. \quad (4.899)$$

The proportionality constants $\langle j'' || v(j) || j' \rangle$ are independent of the azimuthal quantum numbers m, m', m'' . They are called the *reduced matrix elements* of the spherical tensor operator $\hat{v}(j, m)$. They vanish if j'' does not satisfy the vector coupling condition $|j - j'| \leq j'' \leq j + j'$.

For $j = 1/2$, the matrix $d_{m'm}^j(\pi)$ is equal to $e^{-i\sigma^2\pi/2} = -i\sigma^2$. It is therefore the spin- j representation of the matrix c of (4.604), and will therefore be denoted by

$$c^{(j)} \equiv d_{m'm}^j(c) = (-1)^{j+m'} \delta_{m', -m}. \quad (4.900)$$

When applied to the representation matrix $D_{m'm}^j(\alpha, \beta, \gamma)$ as a similarity transformation, we find a spin- j generalization of the important 2×2 -relation (4.689):

$$[c^{(j)}]^{-1} D^j(\alpha, \beta, \gamma) c^{(j)} = D^{j*}(\alpha, \beta, \gamma). \quad (4.901)$$

The matrix $c^{(j)}$ gives rise to an invariant bilinear form for any pair of spherical tensor operators $\hat{v}(j, m)$ and $\hat{v}'(j, m)$:

$$(\hat{v}, \hat{v}') \equiv \sum_{m, m'=-j}^j \hat{v}(j, m) c_{mm'}^{(j)} \hat{v}'(j, m') = \sum_{m=-j}^j (-1)^{j+m} \hat{v}(j, m) \hat{v}(j, -m). \quad (4.902)$$

This product remains invariant under rotations, since

$$D^{jT}(\alpha, \beta, \gamma) c^{(j)} D^j(\alpha, \beta, \gamma) = c^{(j)}. \quad (4.903)$$

The invariance of (4.902) is a generalization to spin- j operators of the Weyl invariance of the spinor product $\xi'_\beta c^{\beta\alpha} \xi_\alpha$ of (4.794).

For $j = 1$, the invariant product (4.902) is equivalent to the ordinary scalar product. This is seen by replacing the spherical components $\hat{v}(1, m)$ by the cartesian ones on the right-hand side of (4.902) according to (4.893), yielding

$$(\hat{v}, \hat{v}') = -\delta_{ij} \hat{v}_i \hat{v}'_j. \quad (4.904)$$

Also for $j = 1$, the spherical relation (4.903) is equivalent to the invariance of the Kronecker symbol δ_{ij} under rotations in the 3×3 defining representation:

$$R_{i_1 i'_1} R_{i_2 i'_2} \delta_{i'_1 i'_2} = \delta_{i_1 i_2}. \quad (4.905)$$

The invariance of scalar products (4.902) formed with $c^{(j)}$ can be used to extend the Weyl calculus to spin- j objects as follows: The spherical tensor operator $\hat{v}(j, m)$ is written as $\hat{v}(\begin{smallmatrix} j \\ m \end{smallmatrix})$, and a contravariant spherical tensor operator is introduced as follows:

$$\hat{v}(\begin{smallmatrix} m \\ j \end{smallmatrix}) \equiv \sum_{m'=-j}^j c_{m, m'}^{(j)} \hat{v}(\begin{smallmatrix} j \\ m' \end{smallmatrix}) = (-1)^{j+m} \hat{v}(\begin{smallmatrix} j \\ -m \end{smallmatrix}). \quad (4.906)$$

Then the invariant form (4.902) can simply be written as

$$(\hat{v}, \hat{v}') = \hat{v}(\begin{smallmatrix} j \\ m \end{smallmatrix}) \hat{v}'(\begin{smallmatrix} m \\ j \end{smallmatrix}), \quad (4.907)$$

with the convention that pairs of upper and lower indices m are assumed to be summed.

The relation between the axis-angle representation and the Euler-angle form of the rotations on the two sides of (4.863) is easily found by comparing the explicit 2×2 -representations (4.469) of the two forms:

$$\begin{aligned} & e^{-i\alpha\sigma^3/2} e^{-i\beta\sigma^2/2} e^{-i\gamma\sigma^3/2} \\ &= \left(\cos \frac{\alpha}{2} - i\sigma^3 \sin \frac{\alpha}{2} \right) \left(\cos \frac{\beta}{2} - i\sigma^2 \sin \frac{\beta}{2} \right) \left(\cos \frac{\gamma}{2} - i\sigma^3 \sin \frac{\gamma}{2} \right) \\ &= \cos \frac{\beta}{2} \cos \frac{\alpha + \gamma}{2} + \sin \frac{\beta}{2} \frac{\alpha - \gamma}{2} i\sigma^1 \\ &\quad - \sin \frac{\beta}{2} \cos \frac{\alpha - \gamma}{2} i\sigma^2 - \sin \frac{\beta}{2} \sin \frac{\alpha + \gamma}{2} i\sigma^3. \end{aligned} \quad (4.908)$$

Comparing the coefficients of $(\sigma^1, \sigma^2, \sigma^3) = \boldsymbol{\sigma}$ and $\sigma^0 = 1$ gives

$$\begin{aligned}\hat{\boldsymbol{\varphi}} \sin \frac{\varphi}{2} &= \left(-\sin \frac{\alpha - \gamma}{2}, \cos \frac{\alpha - \gamma}{2}, \sin \frac{\alpha + \gamma}{2} \right) \sin \frac{\beta}{2}, \\ \cos \frac{\varphi}{2} &= \cos \frac{\beta}{2} \cos \frac{\alpha + \gamma}{2}.\end{aligned}\quad (4.909)$$

More details on the rotation group can be found in the textbook Ref. [18].

Lorentz Group

To extend these results to the Lorentz group we make use of the fact that due to the decompositions (4.853) and (4.854), pure rotations can be decomposed as

$$e^{-i\boldsymbol{\varphi} \cdot \hat{\mathbf{L}}} = e^{-i\boldsymbol{\varphi} \cdot \hat{\mathbf{J}}^{(1)}} e^{-i\boldsymbol{\varphi} \cdot \hat{\mathbf{J}}^{(2)}}, \quad (4.910)$$

where $\mathbf{J}^{(1)}$ and $\mathbf{J}^{(2)}$ are the matrices (4.850). The pure Lorentz transformations are

$$e^{-i\boldsymbol{\zeta} \cdot \hat{\mathbf{M}}} = e^{-\boldsymbol{\zeta} \cdot \hat{\mathbf{J}}^{(1)}} e^{\boldsymbol{\zeta} \cdot \hat{\mathbf{J}}^{(2)}}, \quad (4.911)$$

with $e^{-\boldsymbol{\zeta} \cdot \hat{\mathbf{J}}^{(1)}} e^{\boldsymbol{\zeta} \cdot \hat{\mathbf{J}}^{(2)}}$ having again matrix elements of rotations, as calculated above. Thus, given the parameters $\boldsymbol{\varphi}$ and $\boldsymbol{\zeta}$ of the Lorentz transformation in question, we merely have to find the corresponding Euler angles and take the corresponding rotation matrices from (4.865) and (4.874).

Note that for pure Lorentz transformations the rotation parameters are imaginary so that the trigonometric functions become hyperbolic. For pure Lorentz transformations with imaginary angles, the relation between the axis-angle and the Euler representations corresponding to the two sides of (4.863) is then given by relations like (4.909), but with cosine and sine functions continued to the corresponding hyperbolic forms.

4.19 Higher Spin Fields

The construction of invariant actions can be generalized to fields of arbitrary spin. If we restrict ourselves to those representations which contain only one spin, the situation is very similar to the spin-1/2 case: There are two spinor fields of the Weyl-type ξ_α and $\eta^{\dot{\beta}}$, transforming according to the $D^{(s,0)}$ and $D^{(0,s)}$ -representations, respectively

$$\begin{aligned}\xi(x) &\xrightarrow{\Lambda} \xi'_{\alpha'}(x') = D^{(s,0)}(\Lambda)_{\alpha'}^{\alpha} \xi_{\alpha}(x), \\ \eta(x) &\xrightarrow{\Lambda} \eta'^{\dot{\beta}'}(x') = D^{(0,s)}(\Lambda)^{\dot{\beta}'}_{\dot{\beta}} \eta^{\dot{\beta}}(x).\end{aligned}\quad (4.912)$$

Now, according to the last section, the matrices $D^{(s,0)}(\Lambda)$ are just the symmetrized direct products of $2s$ representations $D^{(\frac{1}{2},0)}(\Lambda)$. They satisfy the same relation as $D^{(\frac{1}{2},0)}$ itself:

$$D^{(s,0)}(\Lambda) = D^{(0,s)}(\Lambda)^{-1}. \quad (4.913)$$

Hence

$$\xi^\dagger \eta \quad , \quad \eta^\dagger \xi \quad (4.914)$$

are the only Lorentz-invariant bilinear combinations of the spinor fields. What about invariants involving derivatives? For this we recall that in the spin- $\frac{1}{2}$ case, the expressions

$$\xi^\dagger i \tilde{\sigma}^\mu \partial_\mu \xi \quad , \quad \eta^\dagger i \sigma^\mu \partial_\mu \eta \quad (4.915)$$

were invariant due to the property (4.482). The invariance remains true for a product of $2s$ factors whose right and left indices are symmetrized. Therefore

$$\xi^\dagger (i^{2s} \tilde{\sigma}^{\mu_1} \times \dots \times \tilde{\sigma}^{\mu_{2s}} \partial_{\mu_1} \dots \partial_{\mu_{2s}}) \xi \equiv \xi^\dagger (\tilde{\sigma} i \partial)^{\{2s\}} \xi \quad (4.916)$$

and

$$\eta^\dagger (i^{2s} \sigma^{\mu_1} \times \dots \times \sigma^{\mu_{2s}} \partial_{\mu_1} \dots \partial_{\mu_{2s}}) \eta \equiv \eta^\dagger (\sigma i \partial)^{\{2s\}} \eta \quad (4.917)$$

are invariants, where the curly brackets indicate the symmetrization of the indices. We may therefore write the action as

$$\mathcal{A} = \int d^4x \left\{ \xi^\dagger (\tilde{\sigma} i \partial)^{\{2s\}} \xi + \eta^\dagger (\sigma i \partial)^{\{2s\}} \eta - M_1^{2s} \xi^\dagger \eta - M_2^{2s} \eta^\dagger \xi \right\}. \quad (4.918)$$

In the absence of mass terms, each of the derivative pieces gives by itself an invariant action which maximally violates parity. This fact is essential for accommodating maximal parity violation into the weak interactions discussed on p. 314. The equations of motion (4.487) and (4.488) become

$$(\tilde{\sigma} i \partial)^{\{2s\}} \xi(x) = M_1^{2s} \eta(x), \quad (4.919)$$

$$(\sigma i \partial)^{\{2s\}} \eta(x) = M_2^{2s} \xi(x). \quad (4.920)$$

They can be inserted into each other to give

$$(\tilde{\sigma} i \partial)^{\{2s\}} (\sigma i \partial)^{\{2s\}} \begin{Bmatrix} \xi(x) \\ \eta(x) \end{Bmatrix} = M_1^{2s} M_2^{2s} \begin{Bmatrix} \xi(x) \\ \eta(x) \end{Bmatrix}. \quad (4.921)$$

The left-hand side contains a product of two symmetrized products. Since each $2s$ factors of the product are symmetric under simultaneous exchange of left and right indices, we can omit the symmetrization in the contracted indices, and use in each of them relation (4.490) to derive

$$[(\tilde{\sigma} i \partial)(\sigma i \partial)]^{\{2s\}} = (-\partial^2 1)^{\{2s\}} = (-\partial^2)^{2s} (1)^{\{2s\}}, \quad (4.922)$$

with $(1)^{\{2s\}}$ being the unit matrix in the symmetrized subspace. In momentum space, this amounts to the mass shell relation

$$(p^2)^{2s} = M_1^{2s} M_2^{2s} = (M^2)^{2s}. \quad (4.923)$$

As in the spin-1/2 case, space inversion changes $\partial \rightarrow \tilde{\partial}$ and the representation matrices

$$D^{(s,0)}(\Lambda) \rightarrow D^{(0,s)}(\Lambda). \quad (4.924)$$

If one wants to have a representation space of the Lorentz group including space inversions, one must combine the two spinors $\xi(x)$ and $\eta(x)$ into a bispinor with $2 \times (2s + 1)$ components

$$\psi(x) = \begin{pmatrix} \xi(x) \\ \eta(x) \end{pmatrix}. \quad (4.925)$$

On this space, parity is represented as in (4.530) by

$$\psi(x) \xrightarrow{P} \psi'_P(x) = D(P)\psi(\tilde{x}), \quad (4.926)$$

with a representation matrix which looks like (4.531), but contains now four blocks of $(2s + 1) \times (2s + 1)$ -matrices:

$$D(P) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \eta_P \gamma_0. \quad (4.927)$$

It is obvious that this matrix changes the generators $\mathbf{L}$ and $\mathbf{M}$ of the Lorentz group in the spin- s representation as in Eqs. (4.529).

Invariance under space inversion requires

$$M_1 = M_2 = M^{2s}, \quad (4.928)$$

and thus the presence of both derivative terms in (4.918). The action (4.918) can now be reformulated in a Dirac-type form using generalized γ -matrices defined by

$$(\gamma_i \partial)^{\{2s\}} = \begin{pmatrix} 0 & (\sigma_i \partial)^{\{2s\}} \\ (\tilde{\sigma}_i \partial)^{\{2s\}} & 0 \end{pmatrix}. \quad (4.929)$$

With these we can write down a parity-invariant action for the bispinors $\psi(x)$ as

$$\mathcal{A} = \int d^4x \bar{\psi}(x) \left[(\gamma_i \partial)^{\{2s\}} - M^{2s} \right] \psi(x), \quad (4.930)$$

where the conjugate bispinor $\bar{\psi}(x)$ reads

$$\bar{\psi}(x) \equiv \begin{pmatrix} \eta^\dagger \\ \xi^\dagger \end{pmatrix} = \psi^\dagger(x) (\gamma^0)^{\{2s\}}. \quad (4.931)$$

The field equation is

$$\left[(\gamma_i \partial)^{\{2s\}} - M^{2s} \right] \psi(x) = 0. \quad (4.932)$$

4.19.1 Plane-Wave Solutions

One can easily write down plane wave solutions of the spin- s wave equation (4.932):

$$f_{\mathbf{p} s_3}(x) \equiv u(\mathbf{p}, s_3) \frac{e^{-ipx}}{\sqrt{Vp^0/M}}, \quad f_{\mathbf{p} s_3}^c(x) \equiv v(\mathbf{p}, s_3) \frac{e^{ipx}}{\sqrt{Vp^0/M}}, \quad (4.933)$$

where $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$ are the positive- and negative-energy solutions of momentum $\mathbf{p}$ and $-\mathbf{p}$, respectively, satisfying the generalized Dirac equations in momentum space

$$(\not{p}^{\{2s\}} - M)u(\mathbf{p}, s_3) = 0, \quad (\not{p}^{\{2s\}} + M)v(\mathbf{p}, s_3) = 0. \quad (4.934)$$

The second can be obtained from the first via a relation like (4.678):

$$v(\mathbf{p}, s_3) = C \bar{u}^T(\mathbf{p}, s_3). \quad (4.935)$$

Here C is the charge conjugation matrix for arbitrary spin:

$$C = \gamma^{\{2s\} 0} = \begin{pmatrix} c^{\{2s\}} & 0 \\ 0 & c^{\{2s\}} \end{pmatrix}. \quad (4.936)$$

The matrices $c^{\{2s\} 0}$ are equivalent to the matrices $c^{(s)}$ introduced in Eq. (4.900). They have the important property that

$$c^{\{2s\}} = (-1)^{2s}. \quad (4.937)$$

The rest spinors $\chi^{\{2s\}}(s_3)$ have symmetrized labels $1/2$ and $-1/2$. These are uniquely specified by the number n_1 of up-spins and n_2 of down-spins, which are the labels of the basis vectors $|n_1, n_2\rangle$ in Eq. (4.837). Thus we may write $\chi^{\{2s\}}(s_3)$ more explicitly as $\chi_{n_1, n_2}^{\{2s\}}(s_3)$. The label s_3 specifies the eigenvalues of the third component of angular momentum, and corresponds to the label m of the basis vectors (4.846). Hence

$$\chi_{n_1, n_2}^{\{2s\}}(s_3) = \delta_{s_3, (n_1 - n_2)/2}, \quad n_1 + n_2 = 2s. \quad (4.938)$$

These spinors satisfy the obvious completeness relation

$$\sum_{s_3} \chi_{n_1, n_2}^{\{2s\}}(s_3) \chi_{n'_1, n'_2}^{\{2s\}}(s_3)^* = \delta_{n_1, n'_1} \delta_{n_2, n'_2}. \quad (4.939)$$

Using this, we find that the spinors $u^{\{2s\}}(\mathbf{p}, s_3)$ have a polarization sum [compare (4.705)]

$$P(p) \equiv \sum_{s_3} u^{\{2s\}}(\mathbf{p}, s_3) u^{\{2s\}}(\mathbf{p}, s_3)^* = \left(\frac{M + p\sigma^{\{2s\}}}{2M} \right)^{\{2s\}}. \quad (4.940)$$

It is a straightforward generalization of the Dirac case. The polarization sums for the spinors $v^{\{2s\}}(\mathbf{p}, s_3)$ can be calculated similarly.

From the spinors $w^{2s}(\mathbf{p}, s_3)$ we form the mirror-reflected spinors $w^{2s}(-\mathbf{p}, s_3)$

$$w^{\{2s\}}(\tilde{\mathbf{p}}, s_3) = B_{\tilde{\mathbf{p}}}^{\{2s\}}(\zeta) \chi^{\{2s\}}(s_3) = \sqrt{\frac{\tilde{p}^0}{M}}^{\{2s\}}, \quad (4.941)$$

and after multiplication with the generalized charge-conjugation matrix c^{2s} , we combine both spinors to bispinors $u^{2s}(\mathbf{p}, s_3)$ and $v^{2s}(\mathbf{p}, s_3)$ of particle and antiparticles of spin s .

4.20 Vector Field as a Higher-Spin Field

Some remarks are useful concerning the field transformations under the representation $D^{(s_1, s_2)}(\Lambda)$, with both $s_1, s_2 \neq 0$. They were omitted in the above discussion, although the most prominent example is one of them. It is a spinor field with $s_1 = s_2 = \frac{1}{2}$, which we denote by $\xi_\alpha^{\dot{\beta}}(x)$. This field is equivalent to a vector field $A^\mu(x)$, which was discussed before in Section 4.6 for the massless case, and in Section 4.17 for a nonzero mass. To see this equivalence, we observe first of all that both representations have a spin content 0 and 1. For the spinor $\xi_\alpha^{\dot{\beta}}(x)$ this follows from the addition rule of angular momenta (4.861). In the vector field $A_\mu(x)$, the zeroth component transforms according to the spin-0 representation, the spatial components according to the spin-1 representation of the rotation group.

There exists a simple relation between the two fields. The spinor field transforms according to the $(\frac{1}{2}, \frac{1}{2})$ representation of the Lorentz group as follows:

$$\begin{aligned} \xi \xrightarrow{\Lambda} \xi'(x')_{\alpha'}^{\dot{\beta}'} &= D^{(\frac{1}{2}, 0)}(\Lambda)_{\alpha'}^\alpha D^{(0, \frac{1}{2})}(\Lambda)^{\dot{\beta}'}_{\dot{\beta}} \xi_\alpha^{\dot{\beta}}(x) \\ &= \left[D^{(\frac{1}{2}, 0)}(\Lambda) \xi(x) D^{(0, \frac{1}{2})T}(\Lambda) \right]_{\alpha'}^{\dot{\beta}'}. \end{aligned} \quad (4.942)$$

The 2×2 components of the spinor can be mapped into the four components of a vector by forming

$$\xi^\mu(x) \equiv c_{\dot{\beta}\dot{\beta}'} \tilde{\sigma}^{\mu\dot{\beta}'}_\alpha \xi_\alpha^{\dot{\beta}}(x) = \text{tr}[c\tilde{\sigma}^\mu \xi(x)]. \quad (4.943)$$

Using the Lorentz transformation rules of Section 4.16 it is easy to verify that $\xi^\mu(x)$ transforms indeed like the vector field $A^\mu(x)$ in Eq. (4.290):

$$\begin{aligned} \xi^\mu(x) \xrightarrow{\Lambda} \xi'^\mu(x') &= \text{tr} \left[c\tilde{\sigma}^\mu D^{(\frac{1}{2}, 0)}(\Lambda) \xi(x) D^{(0, \frac{1}{2})T}(\Lambda) \right] \\ &= \text{tr} \left[c(c^{-1} D^{(0, \frac{1}{2})T}(\Lambda) c) \tilde{\sigma}^\mu D^{(\frac{1}{2}, 0)}(\Lambda) \xi(x) \right]. \end{aligned} \quad (4.944)$$

Now we make use of the relation (4.683) to set

$$c^{-1} \sigma^{\mu T} c = -\sigma^\mu, \quad c^{-1} D^{(0, \frac{1}{2})T}(\Lambda) c = D^{(\frac{1}{2}, 0)\dagger}(\Lambda), \quad (4.945)$$

and to rewrite (4.944) as

$$\xi'^\mu(x') = \text{tr} \left[c D^{(\frac{1}{2}, 0)\dagger}(\Lambda) \tilde{\sigma}^\mu D^{(\frac{1}{2}, 0)}(\Lambda) \xi(x) \right]. \quad (4.946)$$

With the help of (4.482), we now obtain the vector property of the composite field $\xi^m(x)$:

$$\xi'^\mu(x') = \Lambda^\mu_\nu \text{tr} [c\tilde{\sigma}^\nu \xi(x)] = \Lambda^\mu_\nu \xi^\nu(x), \quad (4.947)$$

so that $\xi^\mu(x)$ transforms indeed like $A^\mu(x)$ in (4.290).

A special feature of all representations $D^{(s, s')}$ with $s = s'$ is that they are invariant under space inversions since this interchanges s and s' . Thus no doubling of fields is needed to accommodate space inversions. In the vector form of the $(\frac{1}{2}, \frac{1}{2})$ representation this was observed before in the transformation law (4.305).

4.21 Rarita-Schwinger Field for Spin 3/2

Another frequently-encountered form of higher spin fields which is not of the $(s, 0) + (0, s)$ type is due to Rarita and Schwinger and describes spin-3/2 particles [14]. It combines vector and bispinor properties and is written as $\psi_{\mu a}(x)$, thus transforming according to

$$\psi_{\mu a}(x) \xrightarrow{\Lambda} \psi'_{\mu a}(x') = \Lambda_{\mu}^{\nu} \begin{pmatrix} D^{(\frac{1}{2}, 0)}(\Lambda) & 0 \\ 0 & D^{(0, \frac{1}{2})}(\Lambda) \end{pmatrix}_{ab} \psi_{\nu b}(x). \quad (4.948)$$

Group-theoretically speaking, this is a direct product of the representations $(\frac{1}{2}, \frac{1}{2})$ (for the indices μ, ν) and $(\frac{1}{2}, 0) + (0, \frac{1}{2})$ (for the indices a, b).

We can employ the usual rules for the addition of angular momentum and apply them to $\mathbf{J}^{(1)}$ and $\mathbf{J}^{(2)}$ in (4.853). Then the direct product of two representations

$$D^{(s_1, s_2)} \times D^{(s'_1, s'_2)} \quad (4.949)$$

must have the following irreducible contents:

$$\begin{aligned} & D(|s_1 - s_2|, |s'_1 - s'_2|) + D(|s_1 - s_2|, |s'_1 - s'_2| + 1) + \dots + D(|s_1 - s_2|, s'_1 + s'_2) \\ & + D(|s_1 - s_2| + 1, |s'_1 - s'_2|) + D(|s_1 - s_2| + 1, |s'_1 - s'_2| + 1) + \dots + D(|s_1 - s_2| + 1, s'_1 + s'_2) \\ & + \dots \\ & + D(s_1 + s_2, |s'_1 - s'_2|) + D(s_1 + s_2, |s'_1 - s'_2| + 1) + \dots + D(s_1 + s_2, s'_1 + s'_2). \end{aligned}$$

In this expansion, the spins s_1 and s_2 of $\mathbf{J}^{1,2}$ combine to all spins from $|s_1 - s_2|$ to $s_1 + s_2$ [recall (4.861)]. Similarly, the spins s'_1 and s'_2 couple to all spins from $|s'_1 - s'_2|$ to $s'_1 + s'_2$. Therefore $\psi_{\mu a}$ is equivalent to a sum of $D^{(s_1, s_2)}$ representations:

$$\left(0, \frac{1}{2}\right) + \left(1, \frac{1}{2}\right) + \left(\frac{1}{2}, 0\right) + \left(\frac{1}{2}, 1\right). \quad (4.950)$$

Remember that the symmetry with respect to the interchange $s_1 \leftrightarrow s_2$ is necessary for a parity-invariant Lagrangian. Now, if we want to describe only a spin-3/2 particle, the representations $(0, \frac{1}{2})$ and $(\frac{1}{2}, 0)$ are superfluous and have to be projected out. This can be done by a constraint analogous to the Lorentz condition for the electromagnetic field:

$$\partial^{\mu} \psi_{\mu a}(x) = 0. \quad (4.951)$$

Obviously, this derivative transforms like $(0, \frac{1}{2}) + (\frac{1}{2}, 0)$ and has only a spin-1/2 content, which is therefore removed from (4.950). It remains to make sure that the representation $(1, \frac{1}{2}) + (\frac{1}{2}, 1)$ in $\psi_{\mu a}$ describes only a spin-3/2 particle. This is achieved by another condition imposed on the field:

$$\gamma^{\mu}_{ab} \psi_{\mu b} = 0. \quad (4.952)$$

The associated projection of the field transforms once more like $(0, \frac{1}{2}) + (\frac{1}{2}, 0)$, and setting it equal to zero eliminates one more spin- $\frac{1}{2}$ degree of freedom, thus ensuring the survival of only the spin-3/2 content in $\psi_{\mu a}$.

Finally we construct an invariant action with the property that the equations of motion automatically satisfy the constraints (4.951) and (4.952). There are now several possible invariants which can be used. If we allow at most a single derivative, we may combine

$$\bar{\psi}^\mu i\gamma^\nu \partial_\nu \psi_\mu, \quad \bar{\psi}_\mu \gamma^\mu \partial^\nu \psi_\nu, \quad \bar{\psi}_\mu \gamma^\nu \partial^\mu \psi_\nu, \quad \bar{\psi}_\mu \gamma^\mu \gamma^\nu \psi_\nu, \quad \bar{\psi}^\mu \psi_\mu. \quad (4.953)$$

The most general combination which leads to a Hermitian action of a pure spin-3/2 particle can be shown to be¹³

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \bar{\psi}_\mu(x) L^{\mu\nu} (i\partial) \psi_\nu(x). \quad (4.954)$$

Here $L^{\mu\nu}(i\partial)$ is the differential operator

$$\begin{aligned} L^{\mu\nu}(i\partial) &= (i\partial - M)g^{\mu\nu} + w \gamma^\mu i\partial^\nu + w^* \gamma^\nu \partial^\mu \\ &\quad + \frac{1}{2}(3ww^* + w + w^* + 1)\gamma^\mu i\partial \gamma^\nu \\ &\quad + M \left[3ww^* + \frac{3}{2}(w + w^*) + 1 \right] \gamma^\mu \gamma^\nu, \end{aligned} \quad (4.955)$$

and w is an arbitrary complex number. The equations of motion are given by

$$L^{\mu\nu}(i\partial) \psi_\nu(x) = 0. \quad (4.956)$$

It can easily be verified that a field $\psi_{\mu a}(x)$, which satisfies the constraints (4.951) and (4.952), solves (4.956) if and only if the Dirac equation is fulfilled separately for each vector index μ :

$$(i\partial - M)_a^{a'} \psi_{\mu a'}(x) = 0. \quad (4.957)$$

The particle has obviously a mass M . Some algebra is necessary to deduce that the constraints (4.951) and (4.952) follow from (4.956). For this we go to momentum space and contract $L^{\mu\nu}(p)\psi_\nu(p) = 0$ once with γ_μ and once with p_μ , using the relations $\gamma_\mu \not{p} = -\not{p} \gamma_\mu + 2p_\mu$ and $\gamma^\mu \gamma_\mu = 4$. The two contractions yield $\gamma^\mu \psi_\mu = 0$ and $p^\mu \psi_\mu = 0$, which are a direct consequence of the anticommutation rules (4.496).

Appendix 4A Derivation of Baker-Campbell-Hausdorff Formula

The standard Baker-Campbell-Hausdorff formula, from which our formula (4.74) can be derived, reads

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{C}}, \quad (4A.1)$$

where

$$\hat{C} = \hat{B} + \int_0^1 dt g(e^{\text{ad} \hat{A} t} e^{\text{ad} \hat{B}}) [\hat{A}]. \quad (4A.2)$$

¹³See Notes and References for literature.

Here $g(z)$ is the function

$$g(z) \equiv \frac{\log z}{z-1} = \sum_{n=0}^{\infty} \frac{(1-z)^n}{n+1} \quad (4A.3)$$

and $\text{ad}B$ is the operator associated with $\hat{B}$ in the so-called *adjoint representation*, which is defined by

$$\text{ad}B[\hat{A}] \equiv [\hat{B}, \hat{A}]. \quad (4A.4)$$

One also defines the trivial adjoint operator $(\text{ad}B)^0[\hat{A}] = 1[\hat{A}] \equiv \hat{A}$. By expanding the exponentials in Eq. (4A.2) and using the power series (2A.3), one finds the explicit formula

$$\begin{aligned} \hat{C} = \hat{B} + \hat{A} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n+1} \sum_{p_i, q_i; p_i+q_i \geq 1} \frac{1}{1 + \sum_{i=1}^n p_i} \\ \times \frac{(\text{ad}A)^{p_1}}{p_1!} \frac{(\text{ad}B)^{q_1}}{q_1!} \dots \frac{(\text{ad}A)^{p_n}}{p_n!} \frac{(\text{ad}B)^{q_n}}{q_n!} [\hat{A}]. \end{aligned} \quad (4A.5)$$

The lowest expansion terms are

$$\begin{aligned} \hat{C} &= \hat{B} + \hat{A} - \frac{1}{2} \left[\frac{1}{2} \text{ad}A + \text{ad}B + \frac{1}{6} (\text{ad}A)^2 + \frac{1}{2} \text{ad}A \text{ad}B + \frac{1}{2} (\text{ad}B)^2 + \dots \right] [\hat{A}] \\ &\quad + \frac{1}{3} \left[\frac{1}{3} (\text{ad}A)^2 + \frac{1}{2} \text{ad}A \text{ad}B + \frac{1}{2} \text{ad}B \text{ad}A + (\text{ad}B)^2 + \dots \right] [\hat{A}] \\ &= \hat{A} + \hat{B} - \frac{1}{2} [\hat{B}, \hat{A}] + \frac{1}{12} ([\hat{A}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{B}, \hat{A}]]) + \dots \end{aligned} \quad (4A.6)$$

To prove formula (4A.2) and thus the expansion (4A.5), we proceed in a way similar to the derivation of the interaction formula (1.303). We derive and solve a differential equation for the operator function

$$\hat{C}(t) = \log(e^{\hat{A}t} e^{\hat{B}}). \quad (4A.7)$$

This determines the function $\hat{C}(t)$ from its value $\hat{C}(1)$ at $t = 1$. The starting point is the observation that for any $\hat{M}$,

$$e^{\hat{C}(t)} \hat{M} e^{-\hat{C}(t)} = e^{\text{ad}C(t)} [\hat{M}], \quad (4A.8)$$

by the definition of $\text{ad}C$. The left-hand side can also be rewritten as

$$e^{\hat{A}t} e^{\hat{B}} \hat{M} e^{-\hat{B}} e^{-\hat{A}t} = e^{\text{ad}A t} e^{\text{ad}B} [\hat{M}], \quad (4A.9)$$

so that we have

$$e^{\text{ad}C(t)} = e^{\text{ad}A t} e^{\text{ad}B}. \quad (4A.10)$$

Differentiation of (4A.7) shows that

$$e^{\hat{C}(t)} \frac{d}{dt} e^{-\hat{C}(t)} = -\hat{A}. \quad (4A.11)$$

The left-hand side, on the other hand, can be rewritten in general as

$$e^{\hat{C}(t)} \frac{d}{dt} e^{-\hat{C}(t)} = -f(\text{ad}C(t)) [\dot{\hat{C}}(t)], \quad (4A.12)$$

where

$$f(z) \equiv \frac{e^z - 1}{z}. \quad (4A.13)$$

This will be verified below. It implies that

$$f(\text{ad}C(t)) [\dot{\hat{C}}(t)] = \hat{A}. \quad (4A.14)$$

We now define the function $g(z)$ as in (4A.3) and see that it satisfies

$$g(e^z)f(z) \equiv 1. \quad (4A.15)$$

We therefore have the trivial identity

$$\dot{\hat{C}}(t) = g(e^{\text{ad}C(t)})f(\text{ad}C(t))[\dot{\hat{C}}(t)]. \quad (4A.16)$$

Using (4A.14) and (4A.10), this turns into the differential equation

$$\dot{\hat{C}}(t) = g(e^{\text{ad}C(t)})[\hat{A}] = e^{\text{ad}A} e^{\text{ad}B}[\hat{A}], \quad (4A.17)$$

from which we find directly the result (4A.2).

To complete the proof we must verify (4A.12). For this consider the operator

$$\hat{O}(s, t) \equiv e^{\hat{C}(t)s} \frac{d}{dt} e^{-\hat{C}(t)s}. \quad (4A.18)$$

Differentiating this with respect to s gives

$$\begin{aligned} \partial_s \hat{O}(s, t) &= e^{\hat{C}(t)s} \hat{C}(t) \frac{d}{dt} \left(e^{-\hat{C}(t)s} \right) - e^{\hat{C}(t)s} \frac{d}{dt} \left(\hat{C}(t) e^{-\hat{C}(t)s} \right) \\ &= -e^{\hat{C}(t)s} \dot{\hat{C}}(t) e^{-\hat{C}(t)s} \\ &= -e^{\text{ad}C(t)s} [\dot{\hat{C}}(t)]. \end{aligned} \quad (4A.19)$$

Hence

$$\begin{aligned} \hat{O}(s, t) - \hat{O}(0, t) &= \int_0^s ds' \partial_{s'} \hat{O}(s', t) \\ &= - \sum_{n=0}^{\infty} \frac{s^{n+1}}{(n+1)!} (\text{ad}C(t))^n [\dot{\hat{C}}(t)], \end{aligned} \quad (4A.20)$$

from which we obtain

$$\hat{O}(1, t) = e^{\hat{C}(t)} \frac{d}{dt} e^{-\hat{C}(t)} = -f(\text{ad}C(t))[\dot{\hat{C}}(t)], \quad (4A.21)$$

which is what we wanted to prove.

Note that the final form of the series for $\hat{C}$ in (4A.6) can be rearranged in many different ways, using the Jacobi identity for the commutators. It is a nontrivial task to find a form involving the smallest number of terms.¹⁴

The derivation is an excerpt of the textbook cited in Ref. [1] on p. 80.

Appendix 4B Wigner Rotations and Thomas Precession

Here we calculate the full rate of Wigner rotations and the related Thomas precession.

Wigner Rotations

For brevity, we denote the small rotation (4.751) by

$$R(t) \equiv e^{-i d\alpha \cdot \sigma dt/2} = e^{\zeta(t+dt) \cdot \sigma/2} e^{-d\epsilon \cdot \sigma/2} e^{-\zeta \cdot \sigma/2} = B^{-1}(\zeta(t+dt))B(d\epsilon)B(\zeta). \quad (4B.1)$$

¹⁴For a discussion see J.A. Oteo, J. Math. Phys. 32, 419 (1991).

The pure rotation character of the product on the right-hand side is obvious, since a particle in its rest frame is transformed by three boost transformations back to the rest frame. Being a small rotation, the left-hand side has necessarily the form

$$R = 1 - i\mathbf{\Omega}_W \cdot \boldsymbol{\sigma} dt/2, \quad (4B.2)$$

where $\mathbf{\Omega}_W$ is an angular velocity describing the Wigner precession rate with a Heisenberg equation

$$\dot{\boldsymbol{\sigma}} = U(R)^{-1} \boldsymbol{\sigma} U(R)^{-1} = \mathbf{\Omega}_W \times \boldsymbol{\sigma}. \quad (4B.3)$$

The parameter $d\boldsymbol{\epsilon}$ of the infinitesimal Lorentz transformation in (4B.1) must be chosen such that the final laboratory rapidity is $\boldsymbol{\zeta} + d\boldsymbol{\zeta}$. As with every Lorentz transformation, the product

$$B^{-1}(\boldsymbol{\zeta})B(d\boldsymbol{\epsilon})B(\boldsymbol{\zeta}) \quad (4B.4)$$

can be decomposed into a product of a Lorentz transformation and rotation:

$$B^{-1}(\boldsymbol{\zeta})B(d\boldsymbol{\epsilon})B(\boldsymbol{\zeta}) \approx R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}'), \quad (4B.5)$$

where both parameters $d\boldsymbol{\alpha}'$ and $d\boldsymbol{\epsilon}'$ are small. Then we can expand (4B.1) up to first order in $d\boldsymbol{\zeta}$ as follows:

$$\begin{aligned} R &= B^{-1}(\boldsymbol{\zeta}(t+dt))B(\boldsymbol{\zeta})R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}') \\ &= 1 + \dot{B}(-\boldsymbol{\zeta})B(\boldsymbol{\zeta})dt + [R(d\boldsymbol{\alpha}') - 1] + [B(d\boldsymbol{\epsilon}') - 1]. \end{aligned} \quad (4B.6)$$

It is straightforward to calculate the second term in the notation (4.461), in natural units with $c = 1$, where

$$B(\boldsymbol{\zeta}) = \frac{1}{\sqrt{2(\gamma+1)}}(\gamma + 1 - \gamma \mathbf{v} \cdot \boldsymbol{\sigma}) \quad (4B.7)$$

and

$$\dot{B}(-\boldsymbol{\zeta}) = -\frac{\dot{\gamma}}{2(\gamma+1)}B(-\boldsymbol{\zeta}) + \frac{1}{\sqrt{2(\gamma+1)}}[\dot{\gamma}(1 + \mathbf{v} \cdot \boldsymbol{\sigma}) + \gamma \dot{\mathbf{v}} \cdot \boldsymbol{\sigma}]. \quad (4B.8)$$

After multiplying this with $\dot{B}(\boldsymbol{\zeta})$ we obtain

$$\dot{B}(-\boldsymbol{\zeta})B(\boldsymbol{\zeta}) = -\frac{\dot{\gamma}}{2(\gamma+1)} + \frac{1}{2(\gamma+1)}[\dot{\gamma}(1 + \mathbf{v} \cdot \boldsymbol{\sigma}) + \gamma \dot{\mathbf{v}} \cdot \boldsymbol{\sigma}](\gamma + 1 - \gamma \mathbf{v} \cdot \boldsymbol{\sigma}). \quad (4B.9)$$

The sum of all terms without any factor $\boldsymbol{\sigma}$ cancel each other since they are equal to

$$-\frac{\dot{\gamma}}{2(\gamma+1)} + \frac{\dot{\gamma}}{2} - \frac{1}{2(\gamma+1)}[\dot{\gamma}\gamma v^2 + \gamma^2 \mathbf{v} \cdot \dot{\mathbf{v}}], \quad (4B.10)$$

and this can be shown to vanish, being equal to

$$-\frac{\dot{\gamma}}{2(\gamma+1)} + \frac{\dot{\gamma}}{2} - \frac{\dot{\gamma}\gamma}{2(\gamma+1)}\gamma\gamma\left[v^2 + \frac{1}{\gamma^2}\right] = 0, \quad (4B.11)$$

after using the trivial identities

$$\dot{\gamma} = \mathbf{v} \cdot \dot{\mathbf{v}}\gamma^3, \quad v^2 = \frac{\gamma^2 - 1}{\gamma^2}. \quad (4B.12)$$

With the help of Eq. (4.753), the remaining terms can be decomposed as follows:

$$\dot{B}(-\boldsymbol{\zeta})B(\boldsymbol{\zeta}) = -i\dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma}/2 - \dot{\boldsymbol{\beta}} \cdot \boldsymbol{\sigma}/2, \quad (4B.13)$$

where the angular velocity $\dot{\boldsymbol{\alpha}}$ is

$$\dot{\boldsymbol{\alpha}} = -\frac{\gamma^2}{(\gamma+1)} \mathbf{v} \times \dot{\mathbf{v}}, \quad (4B.14)$$

whereas the acceleration parameter $\dot{\boldsymbol{\beta}}$ is found, via Eq. (4B.12), to be

$$\dot{\boldsymbol{\beta}} = \frac{1}{(\gamma+1)} [-\dot{\gamma} \mathbf{v} - \gamma(\gamma+1)\dot{\mathbf{v}}] = -\gamma^2 \dot{\mathbf{v}}_{\parallel} - \gamma \dot{\mathbf{v}}_{\perp}. \quad (4B.15)$$

The vectors $\dot{\mathbf{v}}_{\parallel}$ and $\dot{\mathbf{v}}_{\perp}$ denote the projections of $\dot{\mathbf{v}}$ parallel and orthogonal to $\mathbf{v}$, respectively. The second (Hermitian) term in (4B.13) corresponds in (4B.6) to a pure infinitesimal Lorentz transformation. Since the final result (4B.6) must be a pure rotation, this term must be canceled by the last term in (4B.6), which is also Hermitian. Thus we conclude that

$$B(d\boldsymbol{\epsilon}') = 1 - \frac{1}{2} (\gamma^2 \dot{\mathbf{v}}_{\parallel} + \gamma \dot{\mathbf{v}}_{\perp}) \cdot \boldsymbol{\sigma} dt. \quad (4B.16)$$

The remaining antihermitian term is of the type (4B.2). It gives a first contribution to the angular velocity of Wigner rotations (after reinserting here the omitted light velocity c):

$$\boldsymbol{\Omega}_{W_1} = -\frac{1}{c^2} \frac{\gamma^2}{\gamma+1} (\mathbf{v} \times \dot{\mathbf{v}}). \quad (4B.17)$$

In order to find the second contribution to the angular velocity we must calculate the term $R(d\boldsymbol{\alpha}') - 1$ in (4B.6). Thus we transform $B(d\boldsymbol{\epsilon}) = 1 - d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/2$ according to (4B.4) and (4B.5) and obtain:

$$\begin{aligned} R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}') &= e^{\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2} e^{-d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/2} e^{-\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}/2} = B^{-1}(\boldsymbol{\zeta})B(d\boldsymbol{\epsilon})B(\boldsymbol{\zeta}) \\ &= 1 - \frac{1}{\sqrt{2(\gamma+1)}} (\gamma+1 + \gamma \mathbf{v} \cdot \boldsymbol{\sigma}) \frac{d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}}{2} \frac{1}{\sqrt{2(\gamma+1)}} (\gamma+1 - \gamma \mathbf{v} \cdot \boldsymbol{\sigma}). \end{aligned} \quad (4B.18)$$

We now use the two rules

$$[\mathbf{a} \cdot \boldsymbol{\sigma}, \mathbf{b} \cdot \boldsymbol{\sigma}] = 2i(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}, \quad \mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma} \mathbf{c} \cdot \boldsymbol{\sigma} = \mathbf{a} \cdot \mathbf{b} \mathbf{c} \cdot \boldsymbol{\sigma} - \mathbf{a} \cdot \mathbf{c} \mathbf{b} \cdot \boldsymbol{\sigma} + \mathbf{b} \cdot \mathbf{c} \mathbf{a} \cdot \boldsymbol{\sigma} + i(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}, \quad (4B.19)$$

to calculate

$$R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}') - 1 = -\frac{1}{4(\gamma+1)} \{ [(\gamma+1)^2 + v^2 \gamma^2] d\boldsymbol{\epsilon} \cdot \boldsymbol{\sigma} - 2\gamma^2 \mathbf{v} \cdot d\boldsymbol{\epsilon} \mathbf{v} \cdot \boldsymbol{\sigma} + 2i\gamma(\mathbf{v} \times d\boldsymbol{\epsilon}) \cdot \boldsymbol{\sigma} \}. \quad (4B.20)$$

Expressing v^2 via (4B.12), the bracket simplifies to $2\gamma(\gamma+1)$. After separating $d\boldsymbol{\epsilon}$ into parallel and orthogonal projections with respect to $\mathbf{v}$, we obtain

$$R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}') - 1 = -\frac{1}{2} \left[\gamma d\boldsymbol{\epsilon}_{\parallel} \cdot \boldsymbol{\sigma} + d\boldsymbol{\epsilon}_{\perp} \cdot \boldsymbol{\sigma} + \frac{i\gamma}{\gamma+1} (\mathbf{v} \times d\boldsymbol{\epsilon}) \cdot \boldsymbol{\sigma} \right]. \quad (4B.21)$$

By comparison with (4B.16), we identify from the Hermitian terms

$$d\boldsymbol{\epsilon}_{\parallel} = \gamma \dot{\mathbf{v}}_{\parallel} dt, \quad d\boldsymbol{\epsilon}_{\perp} = \gamma \dot{\mathbf{v}}_{\perp} dt, \quad d\boldsymbol{\epsilon} = \gamma \dot{\mathbf{v}} dt, \quad (4B.22)$$

and find that the extra rotation $R(d\boldsymbol{\alpha}')$ in the decomposition (4B.6) is

$$R(d\boldsymbol{\alpha}') \approx 1 - i\boldsymbol{\Omega}_{W_2} \times \boldsymbol{\sigma}/2, \quad (4B.23)$$

with an angular velocity $\boldsymbol{\Omega}_{W_2}$ which is twice the negative of (4B.17):

$$\boldsymbol{\Omega}_{W_2} = \frac{2}{c^2} \frac{\gamma^2}{\gamma+1} (\mathbf{v} \times \dot{\mathbf{v}}). \quad (4B.24)$$

The total angular velocity of Wigner rotation is therefore

$$\boldsymbol{\Omega}_W = \boldsymbol{\Omega}_{W_1} + \boldsymbol{\Omega}_{W_2} = \frac{1}{c^2} \frac{\gamma^2}{\gamma+1} (\mathbf{v} \times \dot{\mathbf{v}}), \quad (4B.25)$$

which generalizes the small-velocity result in Eq. (4.758) to (4.766).

Thomas Precession

It is now easy to modify the calculation to obtain the corresponding generalization of the Thomas frequency (4.764). We simply replace the small Lorentz transformation $B(d\mathbf{e})$ in (4B.1) by the small Lorentz transformation (4.759) in the rest frame of the moving electron. As a consequence, the transformation (4B.5) is simply $\tilde{B}(d\mathbf{e})$ and the only difference with respect to the previous calculation is that the rotation $R(d\mathbf{\alpha}')$ is absent. For this reason the over-compensating rotation by $\mathbf{\Omega}_{W_2}$ is absent and we find again that the rate of Thomas precession $\mathbf{\Omega}_T$ is equal to the first contribution $\mathbf{\Omega}_{W_1}$ in Eq. (4B.17) to the Wigner precession, and thus precisely equal to the opposite of the total rate of Wigner rotation:

$$\mathbf{\Omega}_T = -\mathbf{\Omega}_W = -\frac{1}{c^2} \frac{\gamma^2}{\gamma + 1} (\mathbf{v} \times \dot{\mathbf{v}}). \quad (4B.26)$$

Appendix 4C Calculation in Four-Dimensional Representation

The above calculations can certainly also be performed in the 4×4 -representation of the Lorentz group. As an illustration, let us rederive the 4×4 -version of Eq. (4B.13). We denote the 4×4 -representation $\tilde{B}_{\hat{\zeta}}(-\zeta)B_{\hat{\zeta}}(\zeta)$ by $\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})$. Differentiating (4.18) with respect to time we see that

$$\dot{\Lambda}(-\mathbf{v}) = \left(\begin{array}{c|c} \dot{\gamma} & -\dot{\gamma} \frac{v^i}{c} - \gamma \frac{\dot{v}^i}{c} \\ \hline -\dot{\gamma} \frac{v^i}{c} - \gamma \frac{\dot{v}^i}{c} & \dot{\gamma} \frac{\gamma(\gamma+2)}{(\gamma+1)^2} \frac{v^i v^j}{c^2} + \frac{\gamma^2}{\gamma+1} \frac{\dot{v}^i v^j + v^i \dot{v}^j}{c^2} \end{array} \right). \quad (4C.1)$$

Multiplying this with $\Lambda(\mathbf{v})$ from the right yields a first row $[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0_i$ in the product:

$$\left[\dot{\gamma} \gamma \left(1 - \frac{v^2}{c^2} \right) - \gamma^2 \frac{\dot{\mathbf{v}} \mathbf{v}}{c^2}, \quad \dot{\gamma} \left(\gamma - 1 - \frac{\gamma^2}{\gamma+1} \frac{v^2}{c^2} \right) \frac{v^i}{c} - \gamma \frac{\dot{v}^i}{c} - \frac{\gamma^3}{\gamma+1} \frac{\dot{\mathbf{v}} \mathbf{v}}{c^2} \frac{v^i}{c} \right]. \quad (4C.2)$$

Using again the relations $\dot{\mathbf{v}} \mathbf{v}/c^2 = \dot{\gamma}/\gamma^3$, and $v^2/c^2 = (\gamma^2 - 1)/\gamma^2$ [compare (4B.12)], the first entry and the $\dot{\gamma}$ -terms in the second entry disappear, and we remain with

$$[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0_\mu = \left[0, -\gamma \frac{\dot{v}^i}{c} - \frac{\gamma^3}{\gamma+1} \frac{\dot{\mathbf{v}} \mathbf{v}}{c^2} \frac{v^i}{c} \right]. \quad (4C.3)$$

Introducing the components $\dot{\mathbf{v}}_\parallel$ and $\dot{\mathbf{v}}_\perp$ of the acceleration parallel and orthogonal to $\mathbf{v}$, such that $(\dot{\mathbf{v}} \mathbf{v}) = v^2 \dot{\mathbf{v}}_\parallel = (\gamma^2 - 1) \dot{\mathbf{v}}_\parallel / \gamma^2$, this can be expressed in terms of the 4×4 -matrices (4.60)–(4.62) generating pure Lorentz transformations. Their first rows are $(M_1)^0_i = i(0, 1, 0, 0)$, $(M_2)^0_i = i(0, 0, 1, 0)$, $(M_3)^0_i = i(0, 0, 0, 1)$, such that we can write with the vector notation $\mathbf{M} \equiv (M_1, M_2, M_3)$:

$$[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0_i = \frac{i}{c} (\gamma^2 \dot{\mathbf{v}}_\parallel + \gamma \dot{\mathbf{v}}_\perp) \cdot \mathbf{M}. \quad (4C.4)$$

If we replace the 4×4 -generators $\mathbf{M}$ in this equation by the 2×2 -generators $-i\boldsymbol{\sigma}/2$ of pure Lorentz transformations, we obtain

$$\frac{1}{2c} (\gamma^2 \dot{\mathbf{v}}_\parallel + \gamma \dot{\mathbf{v}}_\perp) \cdot \boldsymbol{\sigma}, \quad (4C.5)$$

which agrees with the previous result (4B.16), apart from the factor $1/c$ omitted there.

A third way of deriving this result makes use of the spin four-vector introduced in Eq. (4.767). Here the precession rate is calculated by comparing the spin at time t , where the velocity is $\mathbf{v}(t)$, with the spin at $t+dt$, where the velocity is $\mathbf{v}(t+dt)$. During this time interval, the spin four-vector

has changed from S^μ to $\bar{S}^\mu \equiv S^\mu + \dot{S}^\mu dt$. The initial spin is obtained by bringing the electron to its rest frame via a deboosting Lorentz transformation $\Lambda^\mu{}_\nu(-\mathbf{v})$. Using Eq. (4.18) and v^2 from (4B.12), we have

$$S_R^i = \Lambda^i{}_\mu(-\mathbf{v})S^\mu = -\gamma \frac{v^i}{c} S^0 + S^i + \frac{\gamma^2}{\gamma+1} \frac{v^i v^j}{c^2} S^j. \quad (4C.6)$$

The final spin is obtained by a similar Lorentz transformation with a slightly different velocity $\mathbf{v}(t+dt)$. The result is

$$\begin{aligned} S_R^i + dS_R^i &= \Lambda^i{}_\mu(-\mathbf{v}(t+dt))(S^\mu + \dot{S}^\mu dt) \\ &= \Lambda^i{}_\mu(-\mathbf{v})S^\mu + [\dot{\Lambda}^i{}_\mu(-\mathbf{v})S^\mu + \Lambda^i{}_\mu(-\mathbf{v})\dot{S}^\mu]dt. \end{aligned} \quad (4C.7)$$

We now use the fact that for an acceleration by a pure boost, which does not change the total angular momentum, the change of the spin four-vector $\dot{S}^\mu$ is parallel to the direction of $u^\mu = (\gamma, \gamma v^i)$. This will be shown in Eq. (6.59). Moreover, we can easily verify that $\Lambda^i{}_\mu(-\mathbf{v})u^\mu = 0$ by substituting u^μ for S^μ in (4C.6). Hence we obtain

$$\begin{aligned} \dot{S}_R^i &= \frac{dS_R^i}{dt} = \dot{\Lambda}^i{}_\mu(-\mathbf{v})S^\mu \\ &= -\left(\dot{\gamma} \frac{v^i}{c} + \gamma \frac{\dot{v}^i}{c}\right) S^0 + \dot{\gamma} \frac{\gamma(\gamma+2)}{(\gamma+1)^2} \frac{v^i v^j}{c^2} S^j + \frac{\gamma^2}{\gamma+1} \frac{\dot{v}^i v^j + v^i \dot{v}^j}{c^2} S^j. \end{aligned} \quad (4C.8)$$

Expressing S^i with the help of (4.779), and using $\dot{\mathbf{v}}\mathbf{v}/c^2 = \dot{\gamma}/\gamma^3$, the last term becomes

$$\frac{\gamma^2}{\gamma+1} \frac{v^i \dot{v}^j}{c^2} S^j = \frac{\gamma^2}{\gamma+1} \left(\frac{v^i \dot{v}^j}{c^2} S_R^j + \frac{\gamma^2}{\gamma+1} \frac{\mathbf{v}\dot{\mathbf{v}}}{c^2} \frac{v^i v^j}{c^2} S_R^j \right) = \frac{\gamma^2}{\gamma+1} \frac{v^i \dot{v}^j}{c^2} S_R^j + \dot{\gamma} \frac{\gamma}{(\gamma+1)^2} \frac{v^i v^j}{c^2} S_R^j.$$

We now use (4.779) to substitute $v^i S^i/c = \gamma v^i S_R^i/c$ and $S^0 = v^i S^i/c = \gamma v^i S_R^i/c$. Then all terms containing $\dot{\gamma}$ cancel each other and we arrive at the formula for the temporal change of the spin vector:

$$\dot{S}_R^i = \frac{1}{c^2} \frac{\gamma^2}{\gamma+1} (v^i \dot{v}^j - \dot{v}^i v^j) S_R^j = -\frac{1}{c^2} \frac{\gamma^2}{\gamma+1} [(\mathbf{v} \times \dot{\mathbf{v}}) \times \mathbf{S}_R]^i \equiv \boldsymbol{\Omega}_T \times \mathbf{S}_R, \quad (4C.9)$$

with the vector of angular velocity (4B.17). As a rate of change of a three-vector, it corresponds to a pure rotation. With the help of the generators $(L_i)_{jk} = -i\epsilon_{ijk}$ of the rotation group, we may also write

$$\dot{\mathbf{S}}_R = -i(\boldsymbol{\Omega}_T \cdot \mathbf{L})\mathbf{S}_R. \quad (4C.10)$$

Appendix 4D Hyperbolic Geometry

Such kinematic calculations can, incidentally, be done quite elegantly in a geometric approach, called here *Geometric Calculus*. One may exploit the fact that the four-velocities $u^\mu \equiv p^\mu/M$ can be written as

$$u^\mu = c(\cosh \zeta, \hat{\zeta} \sinh \zeta). \quad (4D.1)$$

This shows that up to a factor c they are vectors on a unit hyperbola. These are hyperbolic analogs of euclidean vectors on a unit sphere

$$u_E^\mu = c(\cos \alpha, \hat{\alpha} \sin \alpha). \quad (4D.2)$$

As such, relative rapidities follow the hyperbolic version of spherical trigonometry, called *Lobachevski geometry* [24]. The product of three pure Lorentz transformations $B(\zeta) = e^{-\zeta \sigma/2}$

with rapidities $\zeta_a, \zeta_b, \zeta_c$ can be represented as a triangle in hyperbolic space. The angles of the triangle $\gamma_a, \gamma_b, \gamma_c$ indicate the relative angles between the corresponding $\hat{\zeta}$ -vectors, i.e., $\cos \gamma_a = \hat{\zeta}_b \cdot \hat{\zeta}_c$, etc. (see Fig. 4.4). The angles and sides of the triangle are then related by the cosine and sine theorems

$$\cosh \zeta_a = \cosh \zeta_b \cosh \zeta_c - \sinh \zeta_a \sinh \zeta_b \cos \gamma_c, \quad (4D.3)$$

$$\cos \gamma_a = -\cos \gamma_b \cos \gamma_c + \sin \gamma_a \sin \gamma_b \cosh \zeta_c, \quad (4D.4)$$

and

$$\frac{\sinh \zeta_a}{\sin \gamma_a} = \frac{\sinh \zeta_b}{\sin \gamma_b} = \frac{\sinh \zeta_c}{\sin \gamma_c}, \quad (4D.5)$$

respectively.

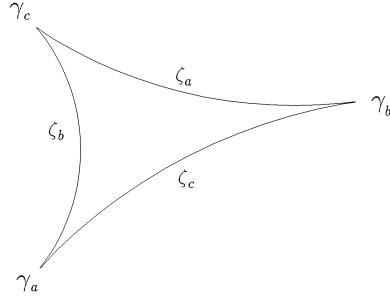


FIGURE 4.4 Triangle formed by rapidities in a hyperbolic space. The sum of angles is smaller than 180° . The angular defect yields the angle of the Thomas precession.

Given two sides plus one of the three angles, say $\zeta_a, \zeta_b, \gamma_c$, we can use the *Napier analogies*,

$$\begin{aligned} \frac{\sinh \frac{1}{2}(\zeta_a - \zeta_b)}{\sin \frac{1}{2}(\zeta_a + \zeta_b)} &= \frac{\tan \frac{1}{2}(\gamma_a - \gamma_b)}{\cot \frac{1}{2}\gamma_c}, \\ \frac{\cosh \frac{1}{2}(\zeta_a - \zeta_b)}{\cosh \frac{1}{2}(\zeta_a + \zeta_b)} &= \frac{\tan \frac{1}{2}(\gamma_a + \gamma_b)}{\cot \frac{1}{2}\gamma_c} \end{aligned} \quad (4D.6)$$

to calculate the other two angles γ_a, γ_b . After that, either one of the two analogous formulas

$$\begin{aligned} \frac{\sin \frac{1}{2}(\gamma_a - \gamma_b)}{\sin \frac{1}{2}(\gamma_b + \gamma_c)} &= \frac{\tanh \frac{1}{2}(\zeta_a - \zeta_b)}{\tanh \frac{1}{2}\zeta_c}, \\ \frac{\cos \frac{1}{2}(\gamma_a - \gamma_b)}{\cos \frac{1}{2}(\gamma_a + \gamma_b)} &= \frac{\tanh \frac{1}{2}(\zeta_a + \zeta_b)}{\tanh \frac{1}{2}\zeta_c} \end{aligned} \quad (4D.7)$$

serves to calculate the third side ζ_c .

Since the hyperboloid has a negative unit radius, the sum of the angles is less than π . The angular defect, also called *excess*,

$$E = \pi - \gamma_a - \gamma_b - \gamma_c, \quad (4D.8)$$

determines the area A of the triangle. For a hyperbola of radius R , the area is

$$A = R^2 E. \quad (4D.9)$$

In spherical geometry this formula is known as *Girard's theorem*. The angular defect is given in terms of the three sides by the hyperbolic version of the *L'Huilier's formula* in spherical trigonometry [22]

$$\tan \frac{E}{4} = \sqrt{\tanh \frac{s}{2} \tanh \frac{s - \zeta_a}{2} \tanh \frac{s - \zeta_b}{2} \tanh \frac{s - \zeta_c}{2}}, \quad (4D.10)$$

where

$$s = (\zeta_a + \zeta_b + \zeta_c)/2. \quad (4D.11)$$

For $R \rightarrow \infty$ it reduces to *Heron's formula* [23]

$$A = \sqrt{s(s-a)(s-b)(s-c)}, \quad s = (a+b+c)/2 = \text{semiparameter}. \quad (4D.12)$$

Another formula is

$$\cos \frac{E}{2} = \frac{1 + \cosh \zeta_a + \cosh \zeta_b + \cosh \zeta_c}{4 \cosh^2(\zeta_a/2) \cosh^2(\zeta_b/2) \cosh^2(\zeta_c/2)}. \quad (4D.13)$$

A pure Lorentz transformation of a particle is a parallel transport along one side of a triangle. When doing three successive parallel transports around a triangle, a particle which was initially at rest comes again to rest. Its spin, however, changes the direction by the angular defect which is determined by the area integral. Since the radius is here equal to -1 , formula (4D.13) determines directly the total angle of the Thomas precession.

The reader is encouraged to derive the rate of the Thomas precession once more using the Geometric Calculus [24].

Appendix 4E Clebsch-Gordan Coefficients

A direct product of irreducible representation states $|s_1, m_1\rangle$ and $|s_2, m_2\rangle$ can be decomposed into a sum of irreducible representation states $|sm\rangle$ with total angular momentum $s = |s_1 - s_2|, \dots, (s_1 + s_2)$. This is done with the help of Clebsch-Gordan coefficients. For this we multiply any product state with the *completeness relation* of all irreducible representation states

$$\sum_s \sum_{m=-s}^s |s, m\rangle \langle s, m| = 1, \quad (4E.1)$$

and obtain

$$|s_1, m_1; s_2, m_2\rangle = \sum_{s=|s_1-s_2|}^{s_1+s_2} \sum_{m=-s}^s |s, m\rangle \langle s, m|s_1, m_1; s_2, m_2\rangle. \quad (4E.2)$$

The expansion coefficients on the right-hand side are the desired Clebsch-Gordan coefficients.

The expansion (4E.2) can be inverted by means of a similar completeness relation in the product space:

$$\sum_{m_1=-s_1}^{s_1} \sum_{m_2=-s_2}^{s_2} |s_1, m_1; s_2, m_2\rangle \langle s_1, m_1; s_2, m_2| = 1, \quad (4E.3)$$

yielding the expansion

$$|s, m\rangle = \sum_{m_1=-s_1}^{s_1} \sum_{m_2=-s_2}^{s_2} |s_1, m_1; s_2, m_2\rangle \langle s_1, m_1; s_2, m_2|s, m\rangle. \quad (4E.4)$$

By subjecting these relations to an arbitrary rotation (4.863), and using (4.865), we find the transformation behavior of the Clebsch-Gordan coefficients:

$$D_{m, m'}^s \langle s, m'|s_1, m'_1; s_2, m'_2\rangle (D^s)_{m'_1, m_1}^{-1} (D^s)_{m'_2, m_2}^{-1} = \langle s, m|s_1, m_1; s_2, m_2\rangle, \quad (4E.5)$$

or, because of unitarity of the representation matrices,

$$D_{m,m'}^s (D_{m_1,m_1'}^s)^* (D_{m_2,m_2'}^s)^* \langle s, m' | s_1, m_1'; s_2, m_2' \rangle = \langle s, m | s_1, m_1; s_2, m_2 \rangle. \quad (4E.6)$$

Since the Clebsch-Gordan coefficients are real following the Condon-Shortley convention we also have

$$(D_{m,m'}^s)^* D_{m_1,m_1'}^s D_{m_2,m_2'}^s \langle s, m' | s_1, m_1'; s_2, m_2' \rangle = \langle s, m | s_1, m_1; s_2, m_2 \rangle. \quad (4E.7)$$

The Clebsch-Gordan coefficients are related in a simple way to the more symmetric *Wigner 3j-symbols* defined as follows:

$$\langle s_3, -m_3 | s_1, m_1; s_2, m_2 \rangle = (-1)^{s_1-s_2-m_3} (2s_3+1)^{1/2} \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (4E.8)$$

As a consequence of relation (4.901), this has the invariance property

$$D_{m_1,m_1'}^s D_{m_2,m_2'}^s D_{m_3,m_3'}^s \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1' & m_2' & m_3' \end{pmatrix} = \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (4E.9)$$

The Levi-Civita symbol ϵ_{ijk} is a cartesian version of the Wigner 3j-symbol for $s_1 = s_2 = s_3 = 1$. It exhibits the invariance (4E.9) with respect to the 3×3 defining representation matrices of the rotation group:

$$R_{i_1 i_1'} R_{i_2 i_2'} R_{i_3 i_3'} \epsilon_{i_1' i_2' i_3'} = \epsilon_{i_1 i_2 i_3}. \quad (4E.10)$$

Under even permutations of columns, the 3j-symbols are invariant, whereas under odd permutations, they pick up a phase factor $(-1)^{s_1+s_2+s_3}$. Note also the property

$$\begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{s_1+s_2+s_3} \begin{pmatrix} s_1 & s_2 & s_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \quad (4E.11)$$

In Eq. (4.906) we introduced a contravariant notation for spin- j objects. This is also done in relation (4E.8), writing it as

$$\langle s_3, m_3 | s_1, m_1; s_2, m_2 \rangle \equiv (-1)^{s_1-s_2-s_3} (2s_3+1)^{1/2} \begin{pmatrix} s_1 & s_2 & m_3 \\ m_1 & m_2 & s_3 \end{pmatrix}. \quad (4E.12)$$

The simplest 3j-symbol is

$$\begin{pmatrix} j & j & 0 \\ m & m' & 0 \end{pmatrix} = (-1)^{j-m} (2j+1)^{-1/2} \delta_{m,-m'}, \quad (4E.13)$$

this being also equal to $(-1)^{2j} c_{m,m'}^{(j)}$. In the contravariant notation, one has

$$\begin{pmatrix} j & m' & 0 \\ m & j & 0 \end{pmatrix} = (-1)^{2j} (2j+1)^{-1/2} \delta_m^{m'}. \quad (4E.14)$$

In order to calculate the Clebsch-Gordan coefficients we observe that the state of maximal quantum numbers $|s_1, s_1; s_2, s_2\rangle$ is a state $|s, m\rangle$ of the irreducible representation with the maximal angular momentum $s = m = s_1 + s_2$. By repeatedly applying the lowering operator of angular momentum to it, following the general relation (4.849), we obtain the matrix elements (compare Fig. 4.3)

$$\begin{aligned} L_- |s, s\rangle &= \sqrt{(2s) \cdot 1} |s, s-1\rangle, \\ L_- |s, s-1\rangle &= \sqrt{(2s-1) \cdot 2} |s, s-2\rangle, \\ &\vdots \\ L_- |s, -s+2\rangle &= \sqrt{(2s-1) \cdot 2} |s, -s+1\rangle, \\ L_- |s, -s+1\rangle &= \sqrt{(2s) \cdot 1} |s, -s\rangle. \end{aligned} \quad (4E.15)$$

Figure 1 displays 18 diagrams representing the decomposition of tensor products of irreducible representations of the Lie algebra $\mathfrak{so}(2, 1)$. Each diagram is a Young diagram with boxes containing numerical coefficients. The diagrams are labeled with tensor products of irreducible representations, such as $1/2 \times 1/2$, $2 \times 1/2$, $3/2 \times 1/2$, etc. The coefficients are integers or fractions. The diagrams are arranged in a grid-like fashion, with some overlapping. The labels are placed to the left of each diagram. The coefficients are placed inside the boxes of the Young diagrams.

Notation:

s	s	$\dots$
m_1	m_2	$\dots$

Coefficients

$\langle s_1, m_1; s_2, m_2 | s, m \rangle$

$$\begin{aligned} & \langle s_1, m_1; s_2, m_2 | s, m \rangle \\ &= (-1)^{s-s_1-s_2} \langle s_2, -m_2; s_1, -m_1 | s, -m \rangle \\ &= (-1)^{s-s_1-s_2} \langle s_2, m_2; s_1, m_1 | s, m \rangle \end{aligned}$$

In the direct-product space, an application of the lowering operator $L_- \times 1 + 1 \times L_-$ to the state $|s_1, s_1; s_2, s_2\rangle$ yields, with the same rules as in (4E.15),

$$\begin{aligned} (L_- \times 1 + 1 \times L_-)|s_1, s_1; s_2, s_2\rangle &= \sqrt{(2s_1) \cdot 1}|s_1, s_1 - 1; s_2, s_2\rangle \\ &+ \sqrt{(2s_2) \cdot 1}|s_1, s_1; s_2, s_2 - 1\rangle. \end{aligned} \quad (4E.16)$$

Continuing this with the help of the general relation

$$\begin{aligned} (L_- \times 1 + 1 \times L_-)|s_1, m_1; s_2, m_2\rangle &= \sqrt{(s_1 + m_1)(s_1 - m_1 + 1)}|s_1, m_1 - 1; s_2, m_2\rangle \\ &+ \sqrt{(s_2 + m_2)(s_2 - m_2 + 1)}|s_1, m_1; s_2, m_2 - 1\rangle, \end{aligned} \quad (4E.17)$$

we find all other states $|s, m\rangle$ of the irreducible representation with $s = s_1 + s_2$.

The state of the lower total angular momentum $s_1 + s_2 - 1$ with a maximal magnetic quantum number $m = s$ is obtained from the orthogonal combination of (4E.17):

$$|s_1 + s_2 - 1, s_1 + s_2 - 1\rangle = \sqrt{(2s_1) \cdot 1}|s_1, s_1 - 1; s_2, s_2\rangle - \sqrt{(2s_2) \cdot 1}|s_1, s_1; s_2, s_2 - 1\rangle. \quad (4E.18)$$

This can be verified by applying to it the raising operator $(L_+ \times 1 + 1 \times L_+)$, generalizing (4.849) to the direct-product space:

$$\begin{aligned} (L_+ \times 1 + 1 \times L_+)|s_1, m_1; s_2, m_2\rangle &= \sqrt{(s_1 - m_1)(s_1 + m_1 + 1)}|s_1, m_1 + 1; s_2, m_2\rangle \\ &+ \sqrt{(s_2 - m_2)(s_2 + m_2 + 1)}|s_1, m_1; s_2, m_2 + 1\rangle, \end{aligned} \quad (4E.19)$$

and finding that it is annihilated if m_1 or m_2 reach their highest possible values s_1 or s_2 , respectively.

By applying the lowering operator to the state (4E.18), we generate all states of the irreducible representation $|s_1 + s_2 - 1, m\rangle$ with $m = -s_1 - s_2 + 1, \dots, s_1 + s_2 - 1$.

Multiplying (4E.17) from the left by $\langle s, m|$ and using the Hermitian adjoint of relation (4.849), we obtain the recursion relation

$$\begin{aligned} \sqrt{(s + m)(s - m + 1)}\langle s_1, m_1; s_2, m_2|s, m\rangle &= \sqrt{(s_1 - m_1 + 1)(s_1 + m_1)}\langle s_1, m_1 - 1; s_2, m_2|s, m - 1\rangle \\ &+ \sqrt{(s_2 - m_2 + 1)(s_2 + m_2)}\langle s_1, m_1; s_2, m_2 - 1|s, m - 1\rangle. \end{aligned} \quad (4E.20)$$

Similarly we can take the raising operator relation (4E.19) in the direct-product space, go over to the adjoint, and multiply it by $\langle s, m|$ from the left to find

$$\begin{aligned} \sqrt{(s - m)(s + m + 1)}\langle s_1, m_1; s_2, m_2|s, m\rangle &= \sqrt{(s_1 + m_1 + 1)(s_1 - m_1)}\langle s_1, m_1 + 1; s_2, m_2|s, m + 1\rangle \\ &+ \sqrt{(s_2 + m_2 + 1)(s_2 - m_2)}\langle s_1, m_1; s_2, m_2 + 1|s, m + 1\rangle. \end{aligned} \quad (4E.21)$$

The Clebsch-Gordan coefficients have the following important symmetry properties:

$$\begin{aligned} \langle s, m|s_1, m_1; s_2, m_2\rangle &= (-1)^{j-s_1-s_2}\langle s, m|s_2, m_2; s_1, m_1\rangle \\ &= \langle s, -m|s_2, -m_2; s_1, -m_1\rangle \\ &= (-1)^{j-s_1-s_2}\langle s, -m|s_1, -m_1; s_2, -m_2\rangle \\ &= (-1)^{s_1-m_1}\sqrt{\frac{2s+1}{2s_2+1}}\langle s_2, -m_2|s_1, m_1; s, -m\rangle \\ &= (-1)^{s_2+m_2}\sqrt{\frac{2s+1}{2s_1+1}}\langle s_1, -m_1|s, -m; s_2, -m_3\rangle. \end{aligned} \quad (4E.22)$$

Some frequently-needed values are listed in Table 4.2.

Appendix 4F Spherical Harmonics

The spherical harmonics are defined as

$$Y_{lm}(\theta, \varphi) \equiv (-1)^m \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\varphi}, \quad (4F.1)$$

where $P_l^m(z)$ are the *associated Legendre polynomials*

$$P_l^m(z) = \frac{1}{2^l l!} (1-z^2)^{m/2} \frac{d^{l+m}}{dz^{l+m}} (z^2-1)^l. \quad (4F.2)$$

The spherical harmonics are orthonormal with respect to the rotation-invariant scalar product

$$\int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi Y_{lm}^*(\theta, \varphi) Y_{l'm'}(\theta, \varphi) = \delta_{ll'} \delta_{mm'}. \quad (4F.3)$$

Explicitly, they read for the lowest few angular momenta:

$$\begin{aligned} Y_{00}(\theta, \phi) &= \frac{1}{2\sqrt{\pi}}, \\ Y_{11}(\theta, \phi) &= -\sqrt{\frac{3}{4\pi}} \sin \theta \frac{1}{\sqrt{2}} e^{i\phi}, \\ Y_{10}(\theta, \phi) &= \sqrt{\frac{3}{4\pi}} \cos \theta, \\ Y_{22}(\theta, \phi) &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{2i\phi}, \\ Y_{21}(\theta, \phi) &= -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi}, \\ Y_{20}(\theta, \phi) &= \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right), \\ Y_{33}(\theta, \phi) &= -\frac{1}{4} \sqrt{\frac{35}{4\pi}} \sin^3 \theta e^{3i\phi}, \\ Y_{32}(\theta, \phi) &= \frac{1}{4} \sqrt{\frac{105}{2\pi}} \sin^2 \theta \cos \theta e^{2i\phi}, \\ Y_{31}(\theta, \phi) &= -\frac{1}{4} \sqrt{\frac{21}{4\pi}} \sin \theta (5 \cos^2 \theta - 1) e^{i\phi}, \\ Y_{30}(\theta, \phi) &= \sqrt{\frac{7}{4\pi}} \left(\frac{5}{2} \cos^3 \theta - \frac{3}{2} \cos \theta \right). \end{aligned} \quad (4F.4)$$

The spherical harmonics with a negative magnetic quantum number m are obtained from the relation

$$Y_{lm}(\theta, \phi) = (-1)^m Y_{l,-m}^*(\theta, -\phi). \quad (4F.5)$$

For $m = 0$, the spherical harmonics reduce to

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta), \quad (4F.6)$$

where

$$P_l(z) \equiv P_l^0(z) = \frac{1}{2^l l!} \frac{d^l}{dz^l} (z^2-1)^l \quad (4F.7)$$

are the *Legendre polynomials*.

For integer $j = l$, the rotation functions $d_{m,m'}^j(\beta)$ can be derived recursively from $d_{m,0}^l(\beta) = P_l(\cos \theta)$ with the help of the recursion relation

$$\begin{aligned} 2\sqrt{(j+m')(j+m'-1)}d_{m,m'}^j(\beta) &= \sqrt{(j+m)(j+m-1)}(1+\cos\theta)d_{m-1,m'-1}^{j-1}(\beta) \\ &+ 2\sqrt{j^2-m^2}\sin\theta d_{m,m'-1}^{j-1}(\beta) + \sqrt{(j-m)(j-m-1)}(1-\cos\theta)d_{m+1,m'-1}^{j-1}(\beta). \end{aligned} \quad (4F.8)$$

For an iterative determination of the rotation functions $d_{m,m'}^j(\beta)$ with half-integer j we use the recursion relation

$$d_{m',m}^j(\beta) = \sqrt{\frac{j-m'}{j-m}}d_{m'+1/2,m+1/2}^{j-1/2}\cos\frac{\beta}{2} + \sqrt{\frac{j+m'}{j-m}}d_{m'-1/2,m+1/2}^{j-1/2}\sin\frac{\beta}{2}. \quad (4F.9)$$

Inserting $m = -1/2$ and using (4.876), we deduce

$$d_{m+1/2}^j(\beta) = \sqrt{\frac{j+m}{j+1/2}}d_{m-1/2,0}^{j-1/2}\cos\frac{\beta}{2} - \sqrt{\frac{j-m}{j+1/2}}d_{m+1/2,0}^{j-1/2}\sin\frac{\beta}{2}. \quad (4F.10)$$

For $j = l + 1/2$, the right-hand side contains only Legendre polynomials. Starting from $d_{m,1/2}^j(\beta)$, we find all other rotation functions with half-integer j from the recursion relation (4F.8).

For $j = 1/2$ and $j = 1$, the explicit results were given in Eqs. (4.881) and (4.882). For $j = 3/2$ we obtain

$$\begin{aligned} d_{3/2,3/2}^{3/2}(\beta) &= \frac{1}{2}(1+\cos\beta)\cos\frac{\beta}{2}, \\ d_{3/2,1/2}^{3/2}(\beta) &= -\frac{\sqrt{3}}{2}(1+\cos\beta)\sin\frac{\beta}{2}, \\ d_{3/2,-1/2}^{3/2}(\beta) &= \frac{\sqrt{3}}{2}(1-\cos\beta)\cos\frac{\beta}{2}, \\ d_{3/2,-3/2}^{3/2}(\beta) &= -\frac{1}{2}(1-\cos\beta)\sin\frac{\beta}{2}, \\ d_{1/2,1/2}^{3/2}(\beta) &= \frac{1}{2}(3\cos\beta-1)\cos\frac{\beta}{2}, \\ d_{1/2,-1/2}^{3/2}(\beta) &= \frac{1}{2}(3\cos\beta+1)\sin\frac{\beta}{2}. \end{aligned} \quad (4F.11)$$

The remaining matrix elements are obtained via the relation (4.876). Similarly we have for $j = 2$ the matrix elements:

$$\begin{aligned} d_{2,2}^2(\beta) &= \frac{1}{4}(1+\cos\beta)^2, \\ d_{2,1}^2(\beta) &= -\frac{1}{2}(1+\cos\beta)\sin\beta, \\ d_{2,0}^2(\beta) &= \frac{\sqrt{6}}{4}\sin^2\beta, \\ d_{2,-1}^2(\beta) &= -\frac{1}{2}(1-\cos\beta)\sin\beta, \\ d_{2,-2}^2(\beta) &= \frac{1}{4}(1-\cos\beta)^2, \\ d_{1,1}^2(\beta) &= \frac{1}{2}(1+\cos\beta)(2\cos\beta-1), \\ d_{1,0}^2(\beta) &= -\sqrt{\frac{3}{2}}\sin\beta\cos\beta, \end{aligned}$$

$$\begin{aligned}
d_{1,-1}^2(\beta) &= \frac{1}{2}(1 - \cos \beta)(2 \cos \beta + 1), \\
d_{0,0}^2(\beta) &= \frac{1}{2}(3 \cos^2 \beta - 1).
\end{aligned} \tag{4F.12}$$

Appendix 4G Projection Matrices for Symmetric Tensor Fields in D Dimension

These projection matrices can all be constructed from appropriate combinations of the longitudinal and transversal projection matrices whose $D = 3$ -dimensional versions were stated in Eqs. (4.336) and (4.334):

$$P_{\mu\nu}^l(k) = \hat{k}_\mu \hat{k}_\nu \quad \text{and} \quad P_{\mu\nu}^t(k) = \eta_{\mu\nu} - P_{\mu\nu}^l(k). \tag{4G.1}$$

Recall that due to the identity

$$P_{\mu\nu}^l(k) + P_{\mu\nu}^t(k) = \eta_{\mu\nu}, \tag{4G.2}$$

these permit decomposing any vector field into its longitudinal and transversal parts:

$$A_\mu = A_\mu^l + A_\mu^t \equiv P_{\mu\nu}^l A^\nu + P_{\mu\nu}^t A^\nu. \tag{4G.3}$$

Here $\eta_{\mu\nu}$ is the D -dimensional generalization of the Minkowski metric (4.27), and $\hat{k}^\mu \equiv k^\mu / \sqrt{k^2}$. The spin-2 projection matrix reads

$$P_{\mu\nu,\lambda\kappa}^{(2)}(k) = \frac{1}{2} [P_{\mu\lambda}^t(k) P_{\nu\kappa}^t(k) + P_{\mu\kappa}^t(k) P_{\nu\lambda}^t(k)] - \frac{1}{D-1} P_{\mu\nu}^t(k) P_{\lambda\kappa}^t(k), \tag{4G.4}$$

which for $D = 3$ reduces to (4.428). The spin-1 projection matrix reads

$$\begin{aligned}
P_{\mu\nu,\lambda\kappa}^{(1)}(k) &= \frac{1}{2} [P_{\mu\lambda}^t(k) P_{\nu\kappa}^l(k) + P_{\mu\kappa}^t(k) P_{\nu\lambda}^l(k) + P_{\nu\kappa}^t(k) P_{\mu\lambda}^l(k) + P_{\nu\lambda}^t(k) P_{\mu\kappa}^l(k)] \\
&= \frac{1}{2} (\hat{k}_\mu \hat{k}_\lambda \eta_{\nu\kappa} + \hat{k}_\mu \hat{k}_\kappa \eta_{\nu\lambda} + \hat{k}_\nu \hat{k}_\lambda \eta_{\mu\kappa} + \hat{k}_\nu \hat{k}_\kappa \eta_{\mu\lambda}) - 2 \hat{k}_\mu \hat{k}_\nu \hat{k}_\lambda \hat{k}_\kappa.
\end{aligned} \tag{4G.5}$$

There are four further projections

$$\begin{aligned}
P_{\mu\nu,\lambda\kappa}^{(0_s)}(k) &= \frac{1}{D-1} P_{\mu\nu}^t(k) P_{\lambda\kappa}^t(k), \\
P_{\mu\nu,\lambda\kappa}^{(0_w)}(k) &= \frac{1}{D-1} P_{\mu\nu}^l(k) P_{\lambda\kappa}^l(k), \\
P_{\mu\nu,\lambda\kappa}^{(0_{sw})}(k) &= P_{\mu\nu}^t(k) P_{\lambda\kappa}^l(k), \\
P_{\mu\nu,\lambda\kappa}^{(0_{ws})}(k) &= P_{\mu\nu}^l(k) P_{\lambda\kappa}^t(k).
\end{aligned} \tag{4G.6}$$

The first two are commonly collected into a single spin-0 projection:

$$P_{\mu\nu,\lambda\kappa}^{(0)}(k) \equiv P_{\mu\nu,\lambda\kappa}^{(0_w)}(k) + P_{\mu\nu,\lambda\kappa}^{(0_s)}(k) = \frac{1}{D-1} (\eta_{\mu\nu} \eta_{\lambda\kappa} - \hat{k}_\mu \hat{k}_\nu \eta_{\lambda\kappa} - \eta_{\mu\nu} \hat{k}_\lambda \hat{k}_\kappa + \hat{k}_\mu \hat{k}_\nu \hat{k}_\lambda \hat{k}_\kappa). \tag{4G.7}$$

The projections satisfy the completeness relation

$$P_{\mu\nu,\lambda\kappa}^{(2)}(k) + P_{\mu\nu,\lambda\kappa}^{(1)}(k) + P_{\mu\nu,\lambda\kappa}^{(0)}(k) = \frac{1}{2} [\eta_{\mu\lambda} \eta_{\nu\kappa} + \eta_{\mu\kappa} \eta_{\nu\lambda}] = \mathbf{1}_{\mu\nu,\lambda\kappa}. \tag{4G.8}$$

By analogy with (31.15), the gravitational field can be decomposed into the three associated components

$$h_{\mu\nu}(k) = h_{\mu\nu}^{(2)}(k) + h_{\mu\nu}^{(1)}(k) + h_{\mu\nu}^{(0)}(k), \tag{4G.9}$$

where

$$h_{\mu\nu}^{(2)} \equiv P_{\mu\nu,\lambda\kappa}^{(2)} h^{\lambda\kappa} \equiv (P_{\mu\lambda}^t P_{\nu\kappa}^t - \frac{1}{D-1} P_{\mu\nu}^t P_{\lambda\kappa}^t) h^{\lambda\kappa}, \quad (4G.10)$$

$$h_{\mu\nu}^{(1)} \equiv P_{\mu\nu,\lambda\kappa}^{(1)} h^{\lambda\kappa} = h_{\mu\nu} - P_{\mu\nu}^t P_{\lambda\kappa}^t h^{\lambda\kappa} - \frac{1}{D-1} P_{\mu\nu}^l P_{\lambda\kappa}^l h^{\lambda\kappa}, \quad (4G.11)$$

and

$$h_{\mu\nu}^{(0)} \equiv P_{\mu\nu,\lambda\kappa}^{(0)} h^{\lambda\kappa} = \frac{1}{D-1} P_{\mu\nu}^t P_{\lambda\kappa}^t h^{\lambda\kappa}. \quad (4G.12)$$

Alternatively we may decompose the field $h_{\lambda\kappa}$ into

$$h_{\mu\nu}(k) = h_{\mu\nu}^{(2)}(k) + h_{\mu\nu}^l(k) + h_{\mu\nu}^s(k), \quad (4G.13)$$

where

$$h_{\mu\nu}^{(2)} \equiv P_{\mu\nu,\lambda\kappa}^{(2)} h^{\lambda\kappa} \equiv (P_{\mu\lambda}^t P_{\nu\kappa}^t h^{\nu\kappa} - \frac{1}{D-1} P_{\mu\nu}^t P_{\lambda\kappa}^t) h^{\lambda\kappa}, \quad (4G.14)$$

$$h_{\mu\nu}^l \equiv P_{\mu\nu,\lambda\kappa}^l h^{\lambda\kappa} \equiv h_{\mu\nu} - P_{\mu\lambda}^t P_{\nu\kappa}^t h^{\nu\kappa} \quad (4G.15)$$

and

$$h_{\mu\nu}^s \equiv P_{\mu\nu,\lambda\kappa}^s h^{\lambda\kappa} \equiv P_{\mu\nu,\lambda\kappa}^{0s} h^{\lambda\kappa} \equiv \frac{1}{D-1} P_{\mu\nu}^t P_{\lambda\kappa}^t h^{\lambda\kappa} \quad (4G.16)$$

is the scalar part. The three projections together satisfy the completeness relation

$$P_{\mu\nu,\lambda\kappa}^{(2)} + P_{\mu\nu,\lambda\kappa}^l + P_{\mu\nu,\lambda\kappa}^s = \mathbf{1}_{\mu\nu,\lambda\kappa}. \quad (4G.17)$$

Notes and References

For other introductions to the theory of fields can be found in the textbooks by

S. Schweber, *An Introduction to Relativistic Quantum Field Theory*, Harper and Row, New York, 1962;

C. Itzykson and J.-B. Zuber, *Quantum Field Theory*, McGraw-Hill, New York, 1985;

S. Weinberg, *The Quantum Theory of Fields*, Cambridge Univ. Press, London, 1996;

M.E. Peskin and D.V. Schroeder, *An Introduction to Quantum Field Theory*, Sarat Book House, Kolkata, 2005.

The particular citations in this chapter refer to:

- [1] The Lorenz condition is named after the Dutch physicist Ludvig Lorenz, *On the Identity of the Vibrations of Light with Electrical Currents*, Philos. Mag. **34**, 287 (1867). It is a Lorentz-invariant gauge condition and often falsely called "Lorentz condition", confusing the author with Hendrik Lorentz [H.A. Lorentz, *Theory of Electrons*, 2nd edition, (1915), Dover. N.Y. (1966)].
- [2] B.W. Petley, Nature **303**, 373 (1983).
Note that the light velocity c has, *by definition*, the value stated in Eq. (4.2). This has been so since 1983, when the previous meter has been redefined in the *Conférence Générale des Poids et Mesures* in Paris to make this value exact.

- [3] Experimentally, the best upper limit for the mass term M_γ in the electromagnetic field equations can be deduced under terrestrial conditions from the shape of the Earth's magnetic field. The limit is $M_\gamma < 4 \cdot 10^{-48} \text{g}$. This corresponds to a Compton wavelength $\lambda_\gamma = \hbar/M_\gamma c > 10^{10} \text{cm}$, which is larger than the diameter of the sun. Astrophysical considerations ("wisps" in the crab nebula) give $\lambda_\gamma > 10^{16} \text{cm}$. If metagalactic magnetic fields would be discovered, the Compton wavelength would be larger than $10^{24} - 10^{25} \text{cm}$, quite close to the ultimate limit set by the horizon of the universe $= c \times \text{age of the universe} \sim 10^{28} \text{cm}$. See G.V. Chibisov, *Sov. Phys. Usp.* **19**, 624 (1976).
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5

Classical Radiation

Changes in the local or temporal charge distribution lead to changes in the electromagnetic field created by them. If the change is sufficiently rapid, the electromagnetic field will start propagating with light-velocity through spacetime. The standard example is the radiation emitted by an antenna, or the ultraviolet light emitted by an electron synchrotron. These and related phenomena will now be discussed.

5.1 Classical Electromagnetic Waves

In the presence of a classical source $j^\mu(x)$, the electromagnetic action (4.237) contains an extra term

$$\mathcal{A}^j = -\frac{1}{c} \int d^4x A^\mu(x) j_\mu(x), \quad (5.1)$$

so that the Euler-Lagrange equation for the electromagnetic field becomes

$$\partial_\nu F^{\mu\nu} = -\partial^2 A^\mu + \partial^\mu \partial_\nu A^\nu = -\frac{1}{c} j^\mu. \quad (5.2)$$

Note that this equation is consistent with current conservation. Indeed, both sides vanish if multiplied by the derivative ∂_μ . The right-hand side vanishes due to the conservation law (4.172), the left-hand side due to the antisymmetry of $F^{\mu\nu}$ which guarantees the validity of the so-called Bianchi identity

$$\partial_\mu \partial_\nu F^{\mu\nu} \equiv 0. \quad (5.3)$$

In order to solve the field equation (5.2), we have to choose a specific gauge. The Lorenz gauge is most convenient:

$$\partial_\mu A^\mu(x) = 0. \quad (5.4)$$

Then the equation reduces to the Klein-Gordon form (4.170) for each vector component [compare (4.253) and the related discussion of gauge transformations]:

$$\partial^2 A^\mu = \frac{1}{c} j^\mu. \quad (5.5)$$

5.1.1 Electromagnetic Field of a Moving Charge

A point charge moving along the trajectory $\bar{\mathbf{x}}(s)$ gives rise to a current

$$j^\mu(x) = ec \int ds \dot{\bar{x}}^\mu(s) \delta^{(4)}(x - \bar{x}(s)) = ec \frac{\dot{\bar{x}}^\mu(s)}{d\bar{x}^0/ds} \delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}(s)), \quad (5.6)$$

where s is an invariant length parameter, such that

$$\frac{d\bar{x}^0}{ds} = \sqrt{1 - \frac{\bar{\mathbf{v}}^2(t)}{c^2}} = \gamma(t). \quad (5.7)$$

Here $\bar{\mathbf{v}}(t)$ is the velocity along the trajectory $\bar{\mathbf{x}}(t)$:

$$\bar{\mathbf{v}}(t) \equiv \dot{\bar{\mathbf{x}}}(t). \quad (5.8)$$

The current components are

$$j^0(x) = ec\delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}(t)), \quad \mathbf{j}(x) = e\bar{\mathbf{v}}(t)\delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}(t)). \quad (5.9)$$

To find the electromagnetic field emerging from this current we solve the field equation (5.5) by

$$A^\mu(x) = \frac{i}{c} \int d^4y G_R(x - y) j^\mu(y), \quad (5.10)$$

where $G^R(x)$ is the retarded Green function

$$G_R(x) = -i\Theta(x^0)\delta(x^2) = -i\Theta(x^0)\frac{1}{4\pi R} [\delta(x^0 - R) + \delta(x^0 + R)], \quad (5.11)$$

which satisfies the differential equation

$$-\partial^2 G_R(x) = i\delta(x). \quad (5.12)$$

In momentum space, Eq. (5.5) can be solved by

$$A^\mu(k) = -\frac{1}{ck^2} j^\mu(k). \quad (5.13)$$

Inserting (5.10) into the electromagnetic action consisting of a free part (4.237) plus a source term (5.1), we obtain the total action

$$\mathcal{A}_{\text{BS}} = -\frac{1}{4} \int d^4x F_{\mu\nu} F^{\mu\nu} - \frac{1}{c} \int d^4x A^\mu j_\mu = -\frac{1}{2c^2} \int d^4x d^4y j_\mu^*(x) G_R(x-y) j^\mu(y). \quad (5.14)$$

This was first found in the nonrelativistic setting by Biot and Savart (see the textbook [1]). A similar action was found for fluctuating vortex lines in superfluids [2]. In energy-momentum space, the last term can be written as

$$\mathcal{A}_{\text{BS}} = \frac{1}{2c^2} \int \frac{d^4k}{(2\pi)^4} j_\mu^*(k) \frac{1}{k^2} j^\mu(k). \quad (5.15)$$

This is composed of a charge-charge and a current-current term

$$\mathcal{A}_{\text{BS}} = \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \left[\rho^*(k) \frac{1}{k^2} \rho(k) - \mathbf{j}^*(k) \frac{1}{k^2} \mathbf{j}(k) \right] \equiv \mathcal{A}_{\rho\rho} + \mathcal{A}_{\mathbf{j}\mathbf{j}}. \quad (5.16)$$

The current-current term may be decomposed further into a longitudinal and a transversal part. By inserting the projection matrices (4.334) and (4.336) between the currents, we find

$$\mathcal{A}_{\mathbf{j}\mathbf{j}} = -\frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \mathbf{j}^*(k) \frac{1}{k^2} \mathbf{j}(k) = -\frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \left[j_i^*(k) \frac{\hat{k}_i \hat{k}_j}{k^2} j_j(k) + j_i^*(k) \frac{\delta_{ij} - \hat{k}_i \hat{k}_j}{k^2} j_j(k) \right], \quad (5.17)$$

where $\hat{k}_i \equiv k_i/|\mathbf{k}|$ is the unit vector pointing into the direction of the momentum. Now we make use of current conservation in momentum space $k_\mu j^\mu(k) = 0$ to equate

$$\hat{k}_i j_i(k) = (k_0/|\mathbf{k}|) j_0(k), \quad (5.18)$$

and the interaction (5.17) becomes

$$\mathcal{A}_{\mathbf{j}\mathbf{j}} = -\frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \left[\frac{k_0^2}{\mathbf{k}^2} j_0^*(k) \frac{1}{k^2} j_0(k) + j_i^*(k) \frac{\delta_{ij} - \hat{k}_i \hat{k}_j}{k^2} j_j(k) \right]. \quad (5.19)$$

Adding this to $\mathcal{A}_{\rho\rho}$, we obtain the total interaction

$$\mathcal{A}_{\text{BS}} = \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \left[-\rho^*(k) \frac{1}{\mathbf{k}^2} \rho(k) - \mathbf{j}_T^*(k) \frac{1}{k^2} \mathbf{j}_T(k) \right] = \mathcal{A}_{\text{Coul}} + \mathcal{A}_{\mathbf{j}_T \mathbf{j}_T}. \quad (5.20)$$

The first term is the instantaneous Coulomb interaction between the charges, the second is due to the transverse electromagnetic radiation between the currents.

Let us write the vector potential (5.13) of the emitted radiation as

$$A^\mu(x) = \frac{1}{4\pi c} \int d^3 x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} j^\mu(x') \Big|_{t'=t-|\mathbf{x}'-\mathbf{x}|/c}. \quad (5.21)$$

The Lorenz gauge may be exhibited more explicitly by multiplying Eq. (5.13) with the transverse projection operator for this gauge [see Eq. (4G.1)]:

$$P_{\mu\nu}^t(i\partial) = \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right). \quad (5.22)$$

Then (5.13) becomes

$$A_\mu^t(k) = -\frac{1}{ck^2} \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) j^\nu(k) = -\frac{1}{ck^2} P_{\mu\nu}^t(k) j^\nu(k), \quad (5.23)$$

which fulfills explicitly the Lorenz gauge $k_\mu A^\mu(k) = 0$. In x -space it reads

$$A_\mu^t(x) = \frac{1}{4\pi c} \int d^3 x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} P_{\mu\nu}^t(i\partial) j^\nu(x') \Big|_{t'=t-|\mathbf{x}'-\mathbf{x}|/c}. \quad (5.24)$$

Introducing the distance vector $\mathbf{R}(t) \equiv \mathbf{x} - \bar{\mathbf{x}}(t)$ from the charge, the spacetime components $(A^0(x), \mathbf{A}(x))$ of the four-vector $A^\mu(x)$ are the famous Liénard-Wiechert potentials:

$$A^0(x) = ec \int dt' \Theta(t - t') \frac{1}{4\pi R} \delta(t - t' - R(t')), \quad (5.25)$$

$$\mathbf{A}(x) = e \int dt' \Theta(t - t') \frac{1}{4\pi R} \bar{\mathbf{v}}(t') \delta(t - t' - R(t')). \quad (5.26)$$

We now simplify the δ -functions as follows:

$$\delta(t - t' - R(t')) = \frac{1}{|d[t' + R(t')]/dt'|_{t'=t_R}} \delta(t' - t_R) = \frac{1}{1 - \mathbf{n}(t_R) \cdot \bar{\mathbf{v}}(t_R)} \delta(t' - t_R), \quad (5.27)$$

where

$$t_R \equiv t - R(t_R)/c \quad (5.28)$$

is the earlier time at which the field has to be emitted in order to arrive at time t at the observation point $\mathbf{x}$. The unit vector $\mathbf{n}(t)$ denotes the direction of the emission:

$$\mathbf{n}(t) \equiv \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|}. \quad (5.29)$$

Inserting $\mathbf{R}(t)$ into (5.25) and (5.26), we find the vector potential

$$A^0(x) = \frac{1}{4\pi} \left[\frac{e}{(1 - \mathbf{n} \cdot \bar{\mathbf{v}}/c)R} \right]_{\text{ret}}, \quad \mathbf{A}(x) = \frac{1}{4\pi} \left[\frac{e\bar{\mathbf{v}}/c}{(1 - \mathbf{n} \cdot \bar{\mathbf{v}}/c)R} \right]_{\text{ret}}. \quad (5.30)$$

The brackets with the subscript “ret” indicate that the time argument t inside the brackets is equal to the earlier time t_R of emission as determined by (5.28). By forming the gauge-invariant combinations of derivatives of the vector potential we find the field strengths

$$\mathbf{E}(x) = -\frac{1}{c} \dot{\mathbf{A}}(x) - \nabla A^0(x), \quad (5.31)$$

$$\mathbf{B}(x) = \nabla \times \mathbf{A}(x), \quad (5.32)$$

which, for the Liénard-Wiechert potentials (5.30), have the values

$$\mathbf{E}(\mathbf{x}, t) = \frac{e}{4\pi} \left[\frac{(\mathbf{n} - \bar{\mathbf{v}}/c)}{(1 - \mathbf{n} \cdot \bar{\mathbf{v}}/c)^2} \frac{1}{R^2} + \frac{\mathbf{n} \times [(\mathbf{n} - \bar{\mathbf{v}}/c) \times \dot{\bar{\mathbf{v}}}]}{(1 - \mathbf{n} \cdot \bar{\mathbf{v}}/c)^3} \frac{1}{R} \right]_{\text{ret}}, \quad (5.33)$$

$$\mathbf{B}(\mathbf{x}, t) = [\mathbf{n} \times \mathbf{E}]_{\text{ret}}. \quad (5.34)$$

The two terms in $\mathbf{E}(\mathbf{x}, t)$ have different falloff-behaviors as functions of the distance R from the source. The first is a *velocity field* which falls off like $1/R^2$. It is essentially the moving static field around the particle. The second term is an *acceleration field*, which has a slower fall-off proportional to $1/R$. For this reason it can carry off radiation energy to infinity. Indeed, the energy flux through a solid

angle $d\Omega$ is given by the scalar product of the Poynting vector¹ $\mathbf{E} \times \mathbf{B}$ with the area element $d\mathbf{S} = r^2 d\Omega$:

$$\dot{\mathcal{E}} = d\mathbf{S} \cdot (\mathbf{E} \times \mathbf{B}) = r^2 d\Omega r^2 (\mathbf{E} \times \mathbf{B}) \cdot \hat{\mathbf{k}} = \frac{1}{8\pi c^3} |\hat{\mathbf{k}} \times (\hat{\mathbf{k}} \times \ddot{\mathbf{x}})|^2 = r^2 d\Omega c \mathbf{E}^2. \quad (5.35)$$

For a radiating electron at small velocities near the coordinate origin, the acceleration field simplifies to

$$\mathbf{E}(\mathbf{x}, t) = \frac{e}{4\pi r c^2} [\hat{\mathbf{x}} \times (\hat{\mathbf{x}} \times \ddot{\mathbf{x}})], \quad \mathbf{B}(\mathbf{x}, t) = \frac{e}{4\pi r c^2} (\hat{\mathbf{x}} \times \ddot{\mathbf{x}}), \quad (5.36)$$

with $r = |\mathbf{x}|$. The radiated power per solid angle is then

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{e^2}{(4\pi)^2 c^3} (\hat{\mathbf{x}} \times \ddot{\mathbf{x}})^2 = \frac{e^2}{(4\pi)^2 c^3} \ddot{\mathbf{x}}^2 \sin^2 \beta, \quad (5.37)$$

where β is the angle between the oscillating dipole ends and the direction of emission. By integrating over all solid angles, we obtain the total radiated power

$$\dot{\mathcal{E}} = \frac{e^2}{(4\pi)^2 c^3} \int d\Omega (\hat{\mathbf{x}} \times \ddot{\mathbf{x}})^2 = \frac{2}{3c^3} \frac{e^2}{4\pi} \ddot{\mathbf{x}}^2. \quad (5.38)$$

This is the famous *Larmor formula* of classical electrodynamics.

For a harmonically oscillating charge at position

$$x(t) = x_0 e^{-i\omega t} + x_0^* e^{i\omega t} = 2|x_0| \cos(\omega t + \delta), \quad (5.39)$$

equation (5.37) yields the temporal average power

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{e^2}{8\pi^2} \frac{\omega^4}{c^4} |\hat{\mathbf{x}} \times \mathbf{x}_0|^2 = \frac{e^2}{8\pi^2} \frac{\omega^4}{c^4} |\mathbf{x}_0|^2 \sin^2 \beta, \quad (5.40)$$

and the total radiated power is given by the *antenna formula*

$$\dot{\mathcal{E}} = \frac{e^2}{4\pi} \frac{4}{3} \frac{\omega^4}{c^4} |\mathbf{x}_0|^2. \quad (5.41)$$

Note that, in comparison with standard textbooks on classical electrodynamics such as the one in Ref. [1] where the electromagnetic Lagrangian carries a prefactor $1/4\pi$, the square of the charge carries here an extra factor $1/4\pi$. Thus the factor e^2 in (5.41) is related to the fine-structure constant α by $e^2 = 4\pi\alpha\hbar c$.

Inserting (5.28) into (5.21) we obtain, for the radiated vector potential, the formula

$$A^\mu(x) = \frac{1}{4\pi c} \int d^3x' \frac{e^{i\omega|\mathbf{x}-\mathbf{x}'|/c}}{|\mathbf{x}-\mathbf{x}'|} \int \frac{d\omega}{2\pi} j^\mu(\mathbf{x}', \omega) e^{-i\omega t}, \quad (5.42)$$

¹Note that the Poynting vector coincides with the components $T^{0i} = (\mathbf{E} \times \mathbf{B})^i$ of the energy-momentum tensor $T^{\mu\nu}$ of the electromagnetic field, whose component $T^{00} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)$ is the energy density. For more details see the textbook in Ref. [1].

where

$$j^\mu(\mathbf{x}', \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} j^\mu(\mathbf{x}', t) \quad (5.43)$$

are the temporal Fourier components of the current density. For large $r = |\mathbf{x}|$, we may approximate

$$\frac{e^{i\omega|\mathbf{x}-\mathbf{x}'|/c}}{|\mathbf{x}-\mathbf{x}'|} \approx \frac{e^{i\omega r/c}}{r} e^{-i\omega\mathbf{n}\mathbf{x}'/c}, \quad (5.44)$$

leaving an $\mathbf{x}'$ -dependence only in the sensitive phase factor. This allows an exact splitting of (5.33) into a velocity and an acceleration field to carry off energy to infinity.

At a point $\mathbf{x}$ far away from the source, the spherically radiated field (5.42) looks like a passing plane wave with $e^{i\omega r/c} \approx e^{i\mathbf{k}\mathbf{x}}$. Thus (5.42) becomes

$$A^\mu(\mathbf{x}, t) = \frac{1}{4\pi c} \frac{1}{r} \int \frac{d\omega}{2\pi} e^{-i\omega t_R} j^\mu(\mathbf{k}, \omega), \quad (5.45)$$

where the time accounting for the retardation is

$$t_R = t - r/ct, \quad (5.46)$$

and $j^\mu(\mathbf{k}, \omega)$ is the momentum-space version of (5.43):

$$j^\mu(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt \int d^3x e^{i\omega t - i\mathbf{k}\mathbf{x}} j^\mu(\mathbf{x}, t). \quad (5.47)$$

At a fixed $\mathbf{k}$ of the outgoing wave, we can thus write

$$A^\mu(\mathbf{x}, t) = \frac{1}{4\pi c} \frac{1}{r} j^\mu(\mathbf{k}, t_R). \quad (5.48)$$

We now calculate the energy flux from formula (5.35). On the right-hand side of this equation, we express the electric field $\mathbf{E}(\mathbf{x})$ in terms of the vector potential via (5.31) and find

$$\frac{d^2\mathcal{E}}{d\Omega} = r^2 c \left[\frac{1}{c} \dot{\mathbf{A}} + \nabla A^0 \right]^2. \quad (5.49)$$

In momentum space, the Lorenz gauge (5.4) implies that

$$A^0(\mathbf{k}, t) = \hat{\mathbf{k}} \cdot \mathbf{A}(\mathbf{k}, t), \quad (5.50)$$

so that we can rewrite

$$\frac{1}{c} \dot{\mathbf{A}}(\mathbf{k}, t) + i\mathbf{k}A^0(\mathbf{k}, t) = \frac{1}{c} \partial_t [\mathbf{A}(\mathbf{k}, t) - \hat{\mathbf{k}}A^0(\mathbf{k}, t)] = \frac{1}{c} \partial_t \mathbf{A}_T(\mathbf{k}, t), \quad (5.51)$$

where

$$\mathbf{A}_T(\mathbf{k}, t) \equiv P_T(\hat{\mathbf{k}}) \mathbf{A}(\mathbf{k}, t) \quad (5.52)$$

is the transverse part of the vector field $\mathbf{A}(\mathbf{k}, t)$ defined by the projection matrix (4.334):

$$P_T^{ij}(\hat{\mathbf{k}}) \equiv \delta^{ij} - \hat{k}^i \hat{k}^j. \quad (5.53)$$

We now express $\mathbf{A}_T$ in terms of $\mathbf{j}_T \equiv P_T \mathbf{j}$ using Eqs. (5.48) and (5.49), to find the radiated energy per unit time and solid angle:

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{1}{16\pi^2 c^3} [\partial_t \mathbf{j}_T(\mathbf{k}, t_R)]^* \cdot [\partial_t \mathbf{j}_T(\mathbf{k}, t_R)]. \quad (5.54)$$

If the emission is from a periodically oscillating source with frequency $\omega = ck_0$, so that $\mathbf{j}(\mathbf{k}, t) = \mathbf{j}(k)e^{-i\omega t}$, we can replace this by

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{\omega^2}{16\pi^2 c^3} |\mathbf{j}_T(k)|^2. \quad (5.55)$$

Note that this radiated power was encountered before in the transverse part of the Biot-Savart interaction energy (5.20).

An equivalent expression can be obtained by using current conservation in momentum space (5.18) to write

$$|\mathbf{j}_T(k)|^2 = j^l(k)^* (\delta_{lm} - \hat{k}_l \hat{k}_m) j^m(k) = |\mathbf{j}(k)|^2 - \frac{k_0^2}{k^2} |j^0(k)|^2 = -j_\mu(k)^* j^\mu(k) - \frac{k^2}{k^2} |j^0(k)|^2. \quad (5.56)$$

The momenta of the outgoing waves are real on-shell photons with $k^2 = 0$, implying that (5.55) can be rewritten in the completely covariant form

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = -\frac{\omega^2}{16\pi^2 c^3} j_\mu(k)^* j^\mu(k). \quad (5.57)$$

5.1.2 Dipole Moment

For long wavelengths, the spatial components of current density have a negligible dependence on $\mathbf{k}$: $j^i(\mathbf{k}, t) \approx j^i(\mathbf{k} = \mathbf{0}, t) = \int d^3x j^i(\mathbf{x}, t)$. With the help of an integration by parts, the right-hand side can further be rewritten as $-\int d^3x x^i \partial_k j^k(\mathbf{x}, t)$, so that we have the approximate relation

$$\mathbf{j}(\mathbf{k}, t) \approx -\int d^3x \mathbf{x} \nabla \mathbf{j}(\mathbf{x}, t). \quad (5.58)$$

We can now use the current conservation law (4.172) and find

$$\mathbf{j}(\mathbf{k}, t) \approx \partial_0 \int d^3x \mathbf{x} j^0(\mathbf{x}, t) = \partial_t \int d^3x \mathbf{x} \rho(\mathbf{x}, t) = \dot{\mathbf{d}}(t), \quad (5.59)$$

where

$$\mathbf{d}(t) \equiv \int d^3x \mathbf{x} \rho(\mathbf{x}, t) \quad (5.60)$$

is the dipole of the charge distribution.

Let us perform the integral over all angles in (5.54). For this we use (5.56) and the angular averages

$$\langle \hat{k}_i \hat{k}_j \rangle = \frac{1}{3} \delta_{ij}, \quad \langle P_{ij}^T(\hat{\mathbf{k}}) \rangle = \frac{2}{3} \delta_{ij}, \quad (5.61)$$

to obtain, for long wavelengths,

$$\dot{\mathcal{E}} \approx \frac{1}{4\pi c^3} \frac{2}{3} \left[\partial_t \int d^3x \mathbf{j}(\mathbf{x}, t) \right]^2. \quad (5.62)$$

Inserting here Eq. (5.59), we find the famous dipole formula for the total radiated power

$$\dot{\mathcal{E}} = \frac{2}{3c^4} \frac{1}{4\pi} [\ddot{\mathbf{d}}(t)]^2. \quad (5.63)$$

For a single nonrelativistic point particle moving along the orbit $\bar{x}(t)$, the spatial current density is

$$\mathbf{j}(\mathbf{x}, t) = e \dot{\bar{\mathbf{x}}}(t) \delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}(t)), \quad (5.64)$$

and Eq. (5.64) becomes

$$\dot{\mathcal{E}} = \frac{2}{3c^3} \frac{e^2}{4\pi} [\ddot{\bar{\mathbf{x}}}(t)]^2, \quad (5.65)$$

in agreement with the Larmor formula (5.38).

5.2 Classical Gravitational Waves

By analogy with the generation of electromagnetic waves, changes in mass distributions lead to changes of the gravitational field. Since the adjustment to a new field configuration can propagate with the speed of light, the universe must be filled with gravitational waves. The collapse of stars, explosion of supernovas, birth of neutron stars, and similar dramatic events in the universe must all be accompanied by bursts of such waves whose general properties will now be studied.

5.2.1 Gravitational Field of Matter Source

The gravitational field is determined by Einstein's equation. That is derived by extending the Einstein-Hilbert action (4.352) for the gravitational field by the action of all matter. Its action will be denoted by $\overset{\text{m}}{\mathcal{A}}$ and consists of a sum of the actions of various matter fields plus those of worldlines of massive point particles. If we vary the metric $g_{\mu\nu}$ in $\overset{\text{m}}{\mathcal{A}}$, we find the energy-momentum tensor $\overset{\text{m}}{T}^{\mu\nu}(x)$ of all matter from the resulting variation

$$\delta \overset{\text{m}}{\mathcal{A}} = -\frac{1}{2} \int d^4x \sqrt{-g} \delta g_{\mu\nu}(x) \overset{\text{m}}{T}^{\mu\nu}(x). \quad (5.66)$$

A corresponding variation of the field action (4.352) yields

$$\begin{aligned}\delta^f \mathcal{A} &= -\frac{1}{2} \int d^4x \sqrt{-g} \left\{ -\frac{1}{2} g_{\mu\nu} \delta g^{\mu\nu} R + \delta g^{\mu\nu} R_{\mu\nu} + g^{\mu\nu} \delta R_{\mu\nu} \right\} \\ &= -\frac{1}{2} \int d^4x \sqrt{-g} \left[\delta g^{\mu\nu} (R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R) + g^{\mu\nu} \delta R_{\mu\nu} \right],\end{aligned}\quad (5.67)$$

where we have used the relation

$$\delta \sqrt{-g} = \frac{1}{2} \sqrt{-g} g^{\mu\nu} \delta g_{\mu\nu} = -\frac{1}{2} g_{\mu\nu} \delta g^{\mu\nu}. \quad (5.68)$$

The last term in (5.67) vanishes in spaces without torsion², so that we can express $\delta^f \mathcal{A}$ in terms of the Einstein tensor $G^{\mu\nu}(x)$ of Eq. (4.375) as

$$\delta^f \mathcal{A} = -\frac{1}{2} \int d^4x \sqrt{-g} \delta g^{\mu\nu}(x) G_{\mu\nu}(x) = \frac{1}{2} \int d^4x \sqrt{-g} \delta g_{\mu\nu}(x) G^{\mu\nu}(x). \quad (5.69)$$

If we finally extremize the total gravitational action

$$\mathcal{A}^{\text{grav}} = \mathcal{A}^f + \mathcal{A}^m \quad (5.70)$$

with respect to $\delta g_{\mu\nu}$, we obtain the Einstein equation for the gravitational field in the presence of matter:

$$G^{\mu\nu} = \kappa \overset{m}{T}{}^{\mu\nu}. \quad (5.71)$$

This corresponds to

$$-G_\mu{}^\mu = R_\mu{}^\mu = R = -\kappa \overset{m}{T}_\mu{}^\mu(x). \quad (5.72)$$

We have seen in Eq. (4.408) that, in the weak-field limit, the free gravitational field equation is simplest if written down in terms of the field $\phi^{\mu\nu} = h^{\mu\nu} - \frac{1}{2} \eta^{\mu\nu} h$. Since the Einstein tensor is given by (4.376), the linearized Einstein equation (5.71) has the somewhat involved differential form

$$G^{\mu\nu} = -\frac{1}{2} (\partial^2 h^{\mu\nu} - \partial^\mu \partial_\lambda h^{\lambda\nu} - \partial^\nu \partial_\lambda h^{\lambda\mu} + \partial^\mu \partial^\nu h) + \frac{1}{2} \eta^{\mu\nu} (\partial^2 h - \partial_\nu \partial_\lambda h^{\nu\lambda}) = \kappa \overset{m}{T}{}^{\mu\nu}. \quad (5.73)$$

Similar to the electromagnetic field equation (31.15) in the presence of sources, the sources on the right-hand side are consistent with the Bianchi identity of the free gravitational field (4.379). In the electromagnetic case, this is due to the current conservation law (2.226), whose relativistic formulation is $\partial_\mu j^\mu = 0$. Here the Bianchi identity for $G^{\mu\nu}$ is a consequence of the conservation law of the symmetric energy-momentum tensor:

$$\partial_\nu \overset{m}{T}{}^{\mu\nu} = 0. \quad (5.74)$$

²See Section 15.2 in the textbook Ref. [17].

The symmetry basis of this conservation law will be discussed in Chapter 8 [see in particular Eq. (8.319)].

To solve the field equation (5.73) it is convenient to express the differential operator on the left-hand side in an easily invertible form. For this purpose we introduce the combination of products of transverse projection operators (4.276) [compare (4G.4)]:

$$P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial) \equiv \frac{1}{2}[P_{\mu\lambda}^t(i\partial)P_{\nu\kappa}^t(i\partial) + P_{\mu\kappa}^t(i\partial)P_{\nu\lambda}^t(i\partial)] - \frac{1}{3}P_{\mu\nu}^t(i\partial)P_{\lambda\kappa}^t(i\partial). \quad (5.75)$$

This projects the symmetric tensor field $h_{\mu\nu}(x)$ into the irreducible spin-2 subspace. We further introduce the spin-0 projection operator [compare (4G.6)]:

$$P_{\mu\nu,\lambda\kappa}^s \equiv \frac{1}{3}P_{\mu\nu}^t P_{\lambda\kappa}^t. \quad (5.76)$$

The two operators (5.75) and (5.76) can be used to express the left-hand side of (5.73) as follows:

$$\begin{aligned} G_{\mu\nu} &= -\frac{1}{2}[\partial^2 h_{\mu\nu} - \partial_\mu \partial^\lambda h_{\lambda\nu} - \partial_\nu \partial^\lambda h_{\lambda\mu} + \partial_\mu \partial_\nu \hat{\partial}^\lambda \hat{\partial}^\kappa h_{\lambda\kappa} + (\hat{\partial}_\mu \hat{\partial}_\nu - \eta_{\mu\nu})\partial^2 h_s] \\ &= -\frac{1}{2}P_{\mu\nu,\lambda\kappa}^{(2)}\partial^2 h^{\lambda\kappa} + \frac{1}{3}P_{\mu\nu}^t P_{\lambda\kappa}^t \partial^2 h^{\lambda\kappa} \\ &= -\frac{1}{2}P_{\mu\nu,\lambda\kappa}^{(2)}\partial^2 h^{\lambda\kappa} + P_{\mu\nu,\lambda\kappa}^s \partial^2 h^{\lambda\kappa}. \end{aligned} \quad (5.77)$$

Using the decomposition (4.436) of the symmetric tensor field $h_{\mu\nu}$, this equation can be written as

$$G_{\mu\nu}(x) = -\frac{1}{2}\partial^2 h_{\mu\nu}^{(2)}(x) + h_{\mu\nu}^s(x), \quad (5.78)$$

and the field equation (5.73) takes the form

$$-\frac{1}{2}\partial^2 h_{\mu\nu}^{(2)}(x) + \partial^2 h_{\mu\nu}^s(x) = \kappa \overset{\text{m}}{T}^{\mu\nu}(x). \quad (5.79)$$

Multiplying this successively by $P_{\mu\nu,\lambda\kappa}^{(2)}$ and by $P_{\mu\nu,\lambda\kappa}^s$, we find the two projected equations:

$$-\frac{1}{2}\partial^2 h_{\mu\nu}^{(2)}(x) = \kappa P_{\mu\nu,\lambda\kappa}^{(2)} \overset{\text{m}}{T}^{\lambda\kappa}(x) \equiv \kappa \overset{\text{m}}{T}_{\mu\nu}^{(2)}(x), \quad (5.80)$$

$$\partial^2 h_{\mu\nu}^s(x) = \kappa P_{\mu\nu,\lambda\kappa}^s \overset{\text{m}}{T}^{\lambda\kappa}(x) \equiv \kappa \overset{\text{m}}{T}_{\mu\nu}^s(x). \quad (5.81)$$

The second equation determines the scalar part of the field $h^s \equiv h_\lambda{}^\lambda - \hat{\partial}_\mu \hat{\partial}_\nu h^{\mu\nu}$ from

$$\partial^2 h^s(x) = \kappa P_{\lambda\kappa}^t \overset{\text{m}}{T}^{\lambda\kappa}(x). \quad (5.82)$$

Combining (5.80) and (5.81) we find

$$\begin{aligned} h_{\mu\nu}^{(2)} + h_{\mu\nu}^s &= -\frac{2\kappa}{\partial^2} \left(P_{\mu\nu,\lambda\kappa}^{(2)} - \frac{1}{2}P_{\mu\nu,\lambda\kappa}^s \right) \overset{\text{m}}{T}^{\lambda\kappa} \\ &= -\frac{\kappa}{\partial^2} \left(P_t^{\mu\lambda} P_t^{\nu\kappa} + P_t^{\mu\kappa} P_t^{\nu\lambda} - P_t^{\mu\nu} P_t^{\lambda\kappa} \right) \overset{\text{m}}{T}_{\lambda\kappa}. \end{aligned} \quad (5.83)$$

At this place we can make use of the energy-momentum conservation law (5.74) on the right-hand side to rewrite this as

$$h_{\mu\nu}^{(2)}(x) + h_{\mu\nu}^s(x) = -\frac{2\kappa}{\partial^2} \left(\overset{\text{m}}{T}_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu} \overset{\text{m}}{T}_{\lambda}{}^{\lambda} \right) (x). \quad (5.84)$$

Here it is useful to introduce the combination of energy-momentum tensors on the right-hand side as

$$\overset{\text{m}}{T}_{\mu\nu}(x) \equiv \overset{\text{m}}{T}_{\mu\nu}(x) - \frac{1}{2}\eta_{\mu\nu} \overset{\text{m}}{T}_{\lambda}{}^{\lambda}(x). \quad (5.85)$$

The corresponding field combination of the fields on the left-hand side is

$$\bar{h}_{\mu\nu}(x) \equiv h_{\mu\nu}^{(2)}(x) + h_{\mu\nu}^s(x). \quad (5.86)$$

This has (5.85) as its source, i.e.:

$$\bar{h}_{\mu\nu}(x) = -\frac{2\kappa}{\partial^2} \overset{\text{m}}{T}_{\mu\nu}(x). \quad (5.87)$$

This satisfies the Hilbert gauge condition (4.399).

For the field $\phi_{\mu\nu}(x) = h_{\mu\nu}(x) - \frac{1}{2}g_{\mu\nu}h(x)$, this equation implies that

$$\phi_{\mu\nu}(x) = -\frac{2\kappa}{\partial^2} \overset{\text{m}}{T}_{\mu\nu}(x), \quad (5.88)$$

and the energy-momentum conservation law (5.74) ensures that $\partial^\nu \phi_{\mu\nu} = 0$, thus guaranteeing the Hilbert gauge [see (4.406)]. These are direct analogs of the electrodynamic field equation (5.4).

Using (5.77), the quadratic part of the field action (4.378) takes the form

$$\overset{\text{f}}{\mathcal{A}} = \frac{1}{4\kappa} \int d^4x h_{\mu\nu} G^{\mu\nu} = -\frac{1}{8\kappa} \int d^4x h_{\mu\nu} \left(P_{\mu\nu,\lambda\kappa}^{(2)} - 2P_{\mu\nu,\lambda\kappa}^s \right) \partial^2 h^{\lambda\kappa}, \quad (5.89)$$

which can also be written as

$$\overset{\text{f}}{\mathcal{A}} = -\frac{1}{8\kappa} \int d^4x \left[h^{(2)\mu\nu} \partial^2 h_{\lambda\kappa}^{(2)} - 2h^{s\lambda\kappa} \partial^2 h_{\lambda\kappa}^s \right]. \quad (5.90)$$

To this we have to add the coupling of matter $\overset{\text{m}}{\mathcal{A}}$ coming from the linearized interaction

$$\overset{\text{m}}{\mathcal{A}} = \mathcal{A}^{\text{int}} = -\frac{1}{2} \int d^4x h_{\mu\nu}(x) \overset{\text{m}}{T}^{\mu\nu}(x). \quad (5.91)$$

This can be decomposed into spin-2 and scalar parts as

$$\overset{\text{m}}{\mathcal{A}} = \mathcal{A}^{\text{int}} = -\frac{1}{2} \int d^4x h^{\mu\nu}(x) \left(P_{\mu\nu,\lambda\kappa}^{(2)} + P_{\mu\nu,\lambda\kappa}^s \right) \overset{\text{m}}{T}^{\mu\nu}(x), \quad (5.92)$$

or

$$\overset{\text{m}}{\mathcal{A}} = \mathcal{A}^{\text{int}} = -\frac{1}{2} \int d^4x \left[h_{\mu\nu}^{(2)}(x) + h_{\mu\nu}^s(x) \right] \overset{\text{m}}{T}^{\mu\nu}(x). \quad (5.93)$$

The extremum of the sum of the gravitational actions (5.90) and (5.91)

$$\overset{\text{grav}}{\mathcal{A}} = \overset{\text{f}}{\mathcal{A}} + \overset{\text{m}}{\mathcal{A}} \quad (5.94)$$

lies at the field (5.86). This equation can be solved by analogy with (5.5) and (5.95), yielding

$$h_{\mu\nu}(x) = -\frac{2\kappa}{4\pi c} \int d^3x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \overset{\text{m}}{T}_{\mu\nu}(x') \Big|_{t'=t-|\mathbf{x}'-\mathbf{x}|/c}. \quad (5.95)$$

A similar equation holds for $\phi^{\mu\nu}$ expressed in terms of $\overset{\text{m}}{T}^{\mu\nu}(x')$.

Reinserting (5.86) into (5.94) yields the gravitational analog of the Biot-Savart law (5.20) in momentum space:

$$\overset{\text{grav}}{\mathcal{A}}_{\text{BS}} = -\frac{\kappa}{2} \int d^4k \overset{\text{m}}{T}^{\mu\nu}(k) \frac{1}{k^2} \overset{\text{m}}{T}_{\mu\nu}(k)^*, \quad (5.96)$$

where

$$\begin{aligned} \overset{\text{m}}{T}^{\mu\nu}(k) \overset{\text{m}}{T}_{\mu\nu}(k)^* &= \overset{\text{m}}{T}^{\mu\nu}(k) \overset{\text{m}}{T}_{\mu\nu}(k)^* - \frac{1}{2} \overset{\text{m}}{T}_{\mu}^{\mu}(k) \overset{\text{m}}{T}_{\nu}^{\nu}(k)^* \\ &= \overset{\text{m}}{T}^{(2)\mu\nu}(k) \overset{\text{m}}{T}_{\mu\nu}^{(2)}(k)^* - \frac{1}{2} \overset{\text{m}}{T}^{s\mu\nu}(k) \overset{\text{m}}{T}_{\mu\nu}^s(k)^*. \end{aligned} \quad (5.97)$$

The latter form follows directly from extremizing the sum of (5.90) and (5.93). It is a consequence of the propagator of the field $h_{\mu\nu}$ obtained from the free-field action (5.90):

$$\langle h_{\mu\nu}(k) h_{\lambda\kappa}^*(k) \rangle = 4\kappa \left[\frac{P_{\mu\nu,\lambda\kappa}^{(2)}(k)}{k^2} - \frac{1}{2} \frac{P_{\mu\nu,\lambda\kappa}^s(k)}{k^2} \right], \quad (5.98)$$

after coupling it to the source via (5.93).

For two static point charges of masses M and M' at the origin and $\mathbf{x}$ with the energy-momentum densities $\overset{\text{m}}{T}^{00}(\mathbf{x}') = Mc^2\delta^3(\mathbf{x})$ and $\overset{\text{m}}{T}^{00}(\mathbf{x}') = M'c^2\delta^3(\mathbf{x}' - \mathbf{x})$, this amounts to an interaction energy

$$\mathcal{E}^{\text{int}} = -\frac{\kappa c^4 M M'}{4\pi r} = -\frac{G_N M M'}{2r}. \quad (5.99)$$

From this we derive the famous attractive *Newton force* between the mass points

$$F = -\frac{G_N M M'}{r^2}. \quad (5.100)$$

Evaluating the integral in Eq. (5.95) for $\mathbf{x}$ far away from the source, in the radiation zone, we may approximate $1/|\mathbf{x} - \mathbf{x}'| \approx 1/|\mathbf{x}| \equiv 1/r$. Then $\phi^{\mu\nu}(\mathbf{x}, t)$ behaves locally like an outgoing plane wave. Thus it must be purely transverse, i.e., it is some linear combination of the polarization tensors $\epsilon_{H+}^{\mu\nu}$ and $\epsilon_{H\times}^{\mu\nu}$ of Eqs. (4.425) and (4.426). These have no 00-component and are traceless [recall (4.418)]. Thus only the spatially traceless part of $\phi^{\mu\nu}$ will contribute and we can approximate:

$$\phi^{ij} \approx \varphi^{ij} \equiv -\frac{2\kappa}{4\pi r} \int d^3x' [\overset{\text{m}}{T}{}^{ij}(\mathbf{x}', t - |\mathbf{x} - \mathbf{x}'|/c) - \frac{1}{3}\delta^{ij} \overset{\text{m}}{T}{}^k{}_k(\mathbf{x}', t - |\mathbf{x} - \mathbf{x}'|/c)]. \quad (5.101)$$

In a linear approximation, the energy-momentum term of the source is conserved à la (5.74):

$$\partial_\nu \overset{\text{m}}{T}{}^{\mu\nu} = 0 + \dots \quad (5.102)$$

The neglected terms come from the contribution of the gravitational field to the energy-momentum tensor. These are of order $\mathcal{O}(\kappa)$. Neglecting them we have

$$\partial_0 \overset{\text{m}}{T}{}^{i0}(\mathbf{x}, t) = -\partial_j \overset{\text{m}}{T}{}^{ij}(\mathbf{x}, t), \quad (5.103)$$

$$\partial_0 \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) = -\partial_j \overset{\text{m}}{T}{}^{0j}(\mathbf{x}, t). \quad (5.104)$$

From these equations we find that

$$\begin{aligned} \int d^3x' \overset{\text{m}}{T}{}^{0j}(\mathbf{x}', t) &= \int d^3x' x'^i \partial_k \overset{\text{m}}{T}{}^{0k}(\mathbf{x}', t) \\ &= \partial_0 \int d^3x' x'^i \overset{\text{m}}{T}{}^{00}(\mathbf{x}', t). \end{aligned} \quad (5.105)$$

We see further that

$$\begin{aligned} \int d^3x' \overset{\text{m}}{T}{}^{ij}(\mathbf{x}', t) &= -\int d^3x' x'^j \partial_k \overset{\text{m}}{T}{}^{ik}(\mathbf{x}', t) = \int d^3x' x'^j \partial_0 \overset{\text{m}}{T}{}^{i0}(\mathbf{x}', t) \\ &= -\int d^3x' x'^i \partial_k \overset{\text{m}}{T}{}^{jk}(\mathbf{x}', t) = \int d^3x' x'^i \partial_0 \overset{\text{m}}{T}{}^{j0}(\mathbf{x}', t) \\ &= \frac{1}{2} \partial_0 \int d^3x' [x'^i \overset{\text{m}}{T}{}^{j0}(\mathbf{x}', t) + x'^j \overset{\text{m}}{T}{}^{i0}(\mathbf{x}', t)] \end{aligned} \quad (5.106)$$

and that

$$\begin{aligned} \int d^3x' [x'^j \overset{\text{m}}{T}{}^{i0}(\mathbf{x}', t) + x'^i \overset{\text{m}}{T}{}^{j0}(\mathbf{x}', t)] &= -\int d^3x' x'^i x'^j \partial_k \overset{\text{m}}{T}{}^{k0}(\mathbf{x}', t) \\ &= \partial_0 \int d^3x' x'^i x'^j \overset{\text{m}}{T}{}^{00}(\mathbf{x}', t). \end{aligned} \quad (5.107)$$

Hence

$$\int d^3x' \overset{\text{m}}{T}{}^{ij}(\mathbf{x}', t) = \frac{1}{2} \partial_0^2 \int d^3x' x'^i x'^j \overset{\text{m}}{T}{}^{00}(\mathbf{x}', t). \quad (5.108)$$

Note the analogy with the electromagnetic equation (5.59).

5.2.2 Quadrupole Moment

The equality (5.108) permits us to express the right-hand side of (5.101) in terms of the quadrupole moment

$$Q^{ij}(t) \equiv \frac{1}{c} \int d^3x' \left(x'^i x'^j - \frac{1}{3} r'^2 \delta^{ij} \right) \ddot{T}^{m00}(\mathbf{x}', t). \quad (5.109)$$

For the field emitted by a moving gravitational source we obtain therefore the simple equation

$$\varphi^{ij}(\mathbf{x}, t) = \frac{\kappa}{4\pi r} \frac{1}{c} \ddot{Q}^{ij}(t_R), \quad (5.110)$$

where the retarded time is given by (5.46). Note the analogy with the electromagnetic formula (5.48).

The field components $\phi^{\mu\nu}(\mathbf{x}, t)$ determine the energy carried away by the wave. To quantify this, we need the analog of the Poynting vector for linearized gravity. This is supplied by the symmetric energy-momentum tensor. For weak fields, it can be derived from the quadratic action (4.372) by techniques to be developed later in Section 8. Anticipating the result we shall find, in Eq. (8.262), the symmetric energy-momentum tensor in the Hilbert gauge $\partial_\mu \phi^{\mu\nu} = 0$:

$$\overset{f}{T}^{\mu\nu} = \frac{1}{8\kappa} \left[2\partial^\mu \phi^{\lambda\kappa} \partial^\nu \phi_{\lambda\kappa} - \partial^\mu \phi \partial^\nu \phi - \eta^{\mu\nu} \left(\partial_\lambda \phi^{\sigma\kappa} \partial^\lambda \phi_{\sigma\kappa} - \frac{1}{2} \partial_\lambda \phi \partial^\lambda \phi \right) \right]. \quad (5.111)$$

If the components $\overset{f}{T}^{0i}$ are multiplied with the unit vector of the outgoing wave $\hat{\mathbf{k}}$ to form

$$c^2 \overset{f}{T}^{0i} \hat{k}^i = \frac{c^2}{8\kappa} \left[2\partial^0 \phi^{\lambda\kappa} \partial^i \phi_{\lambda\kappa} - \partial^0 \phi \partial^i \phi \right] \hat{k}^i, \quad (5.112)$$

we obtain the energy current density along the $\hat{\mathbf{k}}$ -direction. Separating $\phi^{\mu\nu}$ into space and time parts, we can write

$$\begin{aligned} \frac{d\dot{\mathcal{E}}}{r^2 d\Omega} = c^2 \overset{f}{T}^{0i} \hat{k}^i &= \frac{c^2}{8\kappa} \left[2\partial^0 \phi^{kl} \partial^i \phi_{kl} - 4\partial^0 \phi^{k0} \partial^i \phi_{k0} + \partial^0 \phi^{00} \partial^i \phi^{00} \right. \\ &\quad \left. + \partial^0 \phi^{kk} \partial^i \phi^{00} + \partial^0 \phi^{00} \partial^i \phi^{kk} - \partial^0 \phi^{kk} \partial^i \phi^{kk} \right] \hat{k}^i. \end{aligned} \quad (5.113)$$

This has to be integrated over the surface of a large sphere with infinite radius. Before doing so we note that at large r we can forget all space derivatives of the prefactor $1/r$ since they give nonleading $1/r^2, 1/r^3, \dots$ contributions. We have to keep, however, derivatives with respect to r arising from the retarded time argument [recall the approximation (5.44)]. Hence we can approximate, to leading order in $1/r$,

$$\partial^i \phi^{\mu\nu} \approx -\partial^0 \phi^{\mu\nu} \partial^i r = \partial^0 \phi^{\mu\nu} \hat{k}^i. \quad (5.114)$$

Applying this to the components ϕ^{kl} brings the first term in (5.113) to the form $2\dot{\phi}^{kl^2}$, while $\partial^i \phi^{00}$ becomes $\partial_0 \phi^{00} \hat{k}^i$. It is furthermore possible to express the time

derivatives on the right-hand side of (5.113) in terms of time derivatives of the purely spatial field components of Eq. (5.88) in the Hilbert gauge (4.406):

$$\partial_0 \phi^{k0} = -\partial_i \phi^{ki} = \partial^0 \phi^{ki} \hat{k}^i, \quad (5.115)$$

implying that

$$\partial_0 \phi^{00} = -\partial_i \phi^{i0} = \partial_0 \phi^{i0} \hat{k}_i = -\partial_j \phi^{ij} \hat{k}_j = \phi^{ij} \hat{k}_i \hat{k}_j. \quad (5.116)$$

Inserting on the right-hand side the asymptotic traceless expressions ϕ^{ij} of Eq. (5.101), we finally obtain the radiated energy current, which becomes, to leading order in $1/r$,

$$\frac{d\dot{\mathcal{E}}}{r^2 d\Omega} = c^2 \frac{f}{T} {}^{0i} \hat{k}^i = \frac{1}{4\kappa} \left[\dot{\varphi}_{kl}^2 - 2\dot{\varphi}_{kl} \dot{\varphi}_{km} \hat{k}^l \hat{k}^m + \frac{1}{2} \dot{\varphi}^{kl} \dot{\varphi}^{mn} \hat{k}_k \hat{k}_l \hat{k}_m \hat{k}_n \right]. \quad (5.117)$$

The terms in brackets contain the transverse projection matrix (4.434). They can therefore be written as contractions with the polarization tensors (4.425), (4.426), and thus because of (4.427), as

$$|\epsilon_+^{kl}(\hat{\mathbf{k}}) \dot{\varphi}_{kl}|^2 + |\epsilon_\times^{kl}(\hat{\mathbf{k}}) \dot{\varphi}_{kl}|^2 = \dot{\varphi}_{kl} P_{TT}^{kl,mn}(\hat{\mathbf{k}}) \dot{\varphi}_{mn}. \quad (5.118)$$

Inserting here the field (5.110), we obtain the rate of energy emitted per unit solid angle $d\Omega$:

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = r^2 c \frac{f}{T} {}^{0i} \hat{k}^i = \frac{1}{4} \frac{\kappa}{(4\pi)^2} \frac{1}{c^2} \ddot{Q}_{kl} P_{TT}^{kl,mn}(\hat{\mathbf{k}}) \ddot{Q}_{mn}. \quad (5.119)$$

This has a complicated angular dependence. However, the integral over all directions is easily found using the angular averages of products of all direction vectors

$$\langle \hat{k}_i \hat{k}_j \rangle = \frac{1}{3} \delta_{ij}, \quad \langle \hat{k}_i \hat{k}_j \hat{k}_k \hat{k}_m \rangle = \frac{1}{15} (\delta^{ij} \delta^{kl} + \delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}). \quad (5.120)$$

The tensor structure on the right-hand side follows directly from the rotational symmetry. The normalizations are found by contracting the indices, using $n_i n_i = 1$. Inserting (5.120) into (4.428) yields

$$\langle P_{TT}^{ij,kl}(\hat{\mathbf{k}}) \rangle = \frac{2}{5} \left[\frac{1}{2} (\delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}) - \frac{1}{3} \delta^{ij} \delta^{kl} \right]. \quad (5.121)$$

Now the angular integral is straightforward, and we find, recalling κ from (4.357),

$$\dot{\mathcal{E}} = \frac{1}{4} \frac{\kappa}{4\pi} \frac{1}{c^2} \frac{2}{5} (\ddot{Q}^{kl})^2 = \frac{G}{5c^5} (\ddot{Q}^{kl})^2, \quad \frac{G}{c^5} \approx \frac{1}{3.6 \times 10^{52} \text{ W}}. \quad (5.122)$$

For comparison, recall the analogous electromagnetic radiation formula (5.35), where the direction-dependent energy loss due to dipole radiation is

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{1}{8\pi c^3} |\hat{\mathbf{k}} \times (\hat{\mathbf{k}} \times \ddot{\mathbf{d}})|^2, \quad (5.123)$$

with the total radiated power:

$$\dot{\mathcal{E}} = \frac{1}{3c^3} \ddot{\mathbf{d}}^2. \quad (5.124)$$

Since a quadrupole moment possesses a reference point, the reader may wonder about the translational invariance of the gravitational radiation formulas (5.122). Consider the second moment of the energy-momentum tensor after a translation

$$\begin{aligned} \int d^3x (x_i - a_i)(x_j - a_j) \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) &= \int d^3x x_i x_j \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) \\ &\quad - a_i \int d^3x x_j \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) - a_j \int d^3x x_i \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) + a_i a_j \int d^3x \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t). \end{aligned} \quad (5.125)$$

We now observe that the last term is time-independent because of energy conservation. The other two terms in the second line may be rewritten using the conservation law $\partial_\mu T^{\mu\nu}(\mathbf{x}, t)$ and a partial integration:

$$\begin{aligned} \partial_0^2 \int d^3x x_j \overset{\text{m}}{T}{}^{00}(\mathbf{x}, t) &= -\partial_0 \int d^3x x_j \partial_i \overset{\text{m}}{T}{}^{i0}(\mathbf{x}, t) = \int d^3x x_j \partial_i \partial_k \overset{\text{m}}{T}{}^{ik}(\mathbf{x}, t) \\ &= -\int d^3x \partial_k \overset{\text{m}}{T}{}^{jk}(\mathbf{x}, t) = -\partial_0 \int d^3x \overset{\text{m}}{T}{}^{j0}(\mathbf{x}, t) = 0. \end{aligned} \quad (5.126)$$

The last zero on the right-hand side follows from momentum conservation. Thus $Q_{ij}(t)$ changes at most by a linear function of t , and formula (5.124) is indeed independent of the choice of the reference point when calculating the quadrupole moment.³

There exists another way of stating the radiation formula (5.119) that is more similar to the electromagnetic formula (5.55). We employ the relation (5.88) and the transverse traceless projection matrix (4.431) to replace (5.119) by

$$\frac{d^2 \dot{\mathcal{E}}}{d\Omega} = \frac{\kappa}{16\pi^2} \left\{ \left[\partial_t \overset{\text{m}}{T}{}_{kl}(\mathbf{k}, t) \right]^* P_{TT}^{kl, mn}(\mathbf{k}) \partial_t \overset{\text{m}}{T}{}_{mn}(\mathbf{k}, t) \right\}. \quad (5.127)$$

Now we make use of the energy-momentum conservation law (5.103) in Fourier space $\hat{k}_i \overset{\text{m}}{T}{}^{i\mu}(\mathbf{k}, \omega) = \overset{\text{m}}{T}{}^{0\mu}(\mathbf{k}, \omega)$, $\hat{k}_i \hat{k}_j \overset{\text{m}}{T}{}^{ij}(\mathbf{k}, \omega) = \overset{\text{m}}{T}{}^{00}(\mathbf{k}, \omega)$, and rewrite this in a fully covariant form analogous to (5.57) as

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{\kappa}{16\pi^2} \left\{ \left| \partial_t \overset{\text{m}}{T}{}_{\mu}{}^{\nu}(\mathbf{k}, t) \right|^2 - \frac{1}{2} \left| \partial_t \overset{\text{m}}{T}{}_{\lambda}{}^{\lambda}(\mathbf{k}, t) \right|^2 \right\}. \quad (5.128)$$

For long wavelengths, the spatial components of the energy-momentum tensor have a negligible dependence on $\mathbf{k}$: $\overset{\text{m}}{T}{}^{ij}(\mathbf{k}, t) \approx \overset{\text{m}}{T}{}^{ij}(\mathbf{k} = \mathbf{0}, t) = \int d^3x \overset{\text{m}}{T}{}^{ij}(\mathbf{x}, t)$. Then we can perform the integral over all angles in (5.128) using the angular averages (5.120), yielding

$$\dot{\mathcal{E}} = \frac{\kappa}{4\pi} \frac{2}{5} \left\{ \left[\partial_t \int d^3x \overset{\text{m}}{T}{}_{ij}(\mathbf{x}, t) \right]^2 - \frac{1}{3} \left[\partial_t \int d^3x \overset{\text{m}}{T}{}_{ii}(\mathbf{x}, t) \right]^2 \right\}. \quad (5.129)$$

³For more subtle aspects of gravitational radiation see F.I. Cooperstock and P.H. Lim, Phys. Rev. Lett. **55**, 265 (1985).

The right-hand side can be rewritten as

$$\dot{\mathcal{E}} = \frac{\kappa}{4\pi} \frac{2}{5} \left\{ \int d^3x \partial_t \left[\overset{m}{T}_i{}^j(\mathbf{x}, t) - \frac{1}{3} \delta_i^j \overset{m}{T}_k{}^k(\mathbf{x}, t) \right] \partial_t \left[\overset{m}{T}_j{}^i(\mathbf{x}, t) - \frac{1}{3} \delta_j^i \overset{m}{T}_k{}^k(\mathbf{x}, t) \right] \right\}. \quad (5.130)$$

As before we use (5.108) and (5.110) to replace

$$\int d^3x \left[\overset{m}{T}{}^{ij}(\mathbf{x}, t) - \frac{1}{3} \delta^{ij} \overset{m}{T}_k{}^k(\mathbf{x}, t) \right] = \frac{1}{2c} \ddot{Q}^{ij}, \quad (5.131)$$

and obtain once more the flux equations (5.122).

5.2.3 Average Radiated Energy

If we express the time-dependent energy-momentum tensors in Eq. (5.128) in terms of their Fourier integrals, we obtain the radiated power per solid angle

$$\begin{aligned} \frac{d\dot{\mathcal{E}}}{d\Omega} &= \frac{\kappa}{16\pi^2} \int d\omega d\omega' \omega \omega' e^{-i(\omega-\omega')t} \\ &\times \left\{ \left[\overset{m}{T}_\mu{}^\nu(\mathbf{k}, \omega) - \frac{1}{2} \delta_\mu^\nu \overset{m}{T}_\lambda{}^\lambda(\mathbf{k}, \omega) \right]^* \left[\overset{m}{T}_\nu{}^\mu(\mathbf{k}, \omega') - \frac{1}{2} \delta_\nu^\mu \overset{m}{T}_\lambda{}^\lambda(\mathbf{k}, \omega') \right] \right\}. \end{aligned} \quad (5.132)$$

To understand the averaging process, consider the double frequency integral

$$f(t) \equiv \int d\omega d\omega' \omega \omega' e^{-i(\omega-\omega')t} A(\omega) B(\omega), \quad (5.133)$$

with smooth functions $A(\omega)$ and $B(\omega)$. Over a long time, the oscillation of the frequency difference $\Delta\omega = \omega - \omega'$ cancel each other, and only the average rate of the integral

$$\int_{t_1}^{t_2} dt e^{i(\omega-\omega')t} \rightarrow 2\pi \delta(\omega - \omega') \quad (5.134)$$

survives, implying that

$$\dot{f}(t) \approx \frac{2\pi}{t_2 - t_1} \int d\omega \omega^2 A(\omega) B(\omega). \quad (5.135)$$

Integrating this over all times from t_1 to t_2 gives therefore the total radiated energy per unit solid angle:

$$\frac{d\mathcal{E}}{d\Omega} = \frac{\kappa}{8\pi} \int d\omega \omega^2 \left\{ \left[\overset{m}{T}_\mu{}^\nu(\mathbf{k}, \omega) - \frac{1}{2} \delta_\mu^\nu \overset{m}{T}_\lambda{}^\lambda(\mathbf{k}, \omega) \right]^* \left[\overset{m}{T}_\nu{}^\mu(\mathbf{k}, \omega) - \frac{1}{2} \delta_\nu^\mu \overset{m}{T}_\lambda{}^\lambda(\mathbf{k}, \omega) \right] \right\}. \quad (5.136)$$

5.3 Simple Models for Sources of Gravitational Radiation

Let us calculate the radiated power for a few typical radiating systems. Following the textbook [3] we distinguish between *oscillating* and *bursting systems*.

Consider a single nonrelativistic point particle moving along the orbit $\bar{x}(t)$. Its energy-momentum tensor has the spatial components

$$T^{ij}(\mathbf{x}, t) = \frac{M}{c} \dot{\bar{x}}^i(t) \dot{\bar{x}}^j(t) \delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}(t)). \quad (5.137)$$

Then Eq. (5.129) becomes

$$\dot{\mathcal{E}} = \frac{\kappa'}{4\pi} \frac{2}{5} \frac{M^2}{c^2} \left[\partial_t \left(\dot{\bar{x}}^i \dot{\bar{x}}^j - \frac{1}{3} \delta^{ij} \dot{\bar{x}}^k \dot{\bar{x}}_k \right) \right]^2. \quad (5.138)$$

The radiated energy decreases in time, and so does the total angular momentum of the gravitational system

$$L_i(t) = \epsilon_{ijk} \int d^3x x^j T^{0k}(\mathbf{x}, t). \quad (5.139)$$

This happens at a rate

$$\dot{L}_k = \frac{2\kappa'}{8\pi} \frac{1}{5c^2} \epsilon_{klm} \ddot{Q}^{il}(t) \ddot{Q}^{im}(t) = \frac{2G}{5c^5} \epsilon_{klm} \ddot{Q}^{il}(t) \ddot{Q}^{im}(t). \quad (5.140)$$

For checking the dimensions of the above equations the following list of dimensions is useful:

$$\begin{aligned} [\mathcal{A}] &= \hbar, & [T^{\mu\nu}] &= \frac{\hbar}{\text{cm}^4}, & [E] &= \frac{\hbar}{\text{sec}}, & [p] &= \frac{\hbar}{\text{cm}}, & [Q^{ij}] &= \hbar \text{ sec}, & [\ddot{Q}^{ij}] &= \frac{\hbar}{\text{sec}^2}, \\ [\kappa] &= \frac{\text{cm}^2}{\hbar}, & [G] &= \frac{\text{cm}^5}{\hbar \text{ sec}^3}, & [c^5/G] &= \frac{\hbar}{\text{sec}^2} \approx 3.6 \times 10^{52} \text{ W}. \end{aligned} \quad (5.141)$$

Note that $\ddot{Q}^{ij}$ has the dimension of a power.

5.3.1 Vibrating Quadrupole

Imagine two equal masses M oscillating at the ends of a spring (see Fig. 5.1). Their time-dependent distance is

$$z = \pm \left(\frac{d}{2} + a \sin \omega t \right). \quad (5.142)$$

Assuming that $a \ll d$, we may approximate

$$z^2 \sim \frac{d^2}{4} + ad \sin \omega t. \quad (5.143)$$

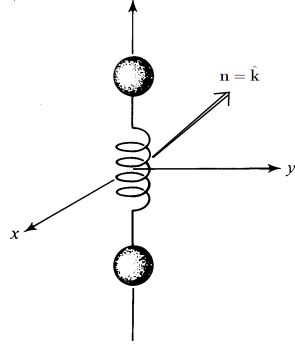


FIGURE 5.1 Two equal masses M oscillating at the ends of a spring as a source of gravitational radiation.

The quadrupole moment is therefore

$$Q_{ij}(t) = \left(1 + \frac{4a}{d} \sin \omega t\right) Q_{ij} \quad (5.144)$$

where

$$Q_{ij}(0) = \frac{Md^2}{6} \begin{pmatrix} -1 & & \\ & -1 & \\ & & 2 \end{pmatrix}, \quad (5.145)$$

so that

$$\ddot{Q}_{11}(t) = \ddot{Q}_{22}(t) = -\frac{1}{2} \ddot{Q}_{22}(t) = -\frac{2Mad}{3} \omega^3 \sin \omega t. \quad (5.146)$$

According to Eq. (5.119), the angular distribution of the quadrupole radiation in the direction $\mathbf{n} = \hat{\mathbf{k}}$ is (see Fig. 5.1)

$$\begin{aligned} \frac{d\dot{\mathcal{E}}}{d\Omega} = & \frac{1}{4} \frac{\kappa}{(4\pi)^2 c^2} \left\{ \ddot{Q}_{11}^2 + \ddot{Q}_{22}^2 + \ddot{Q}_{33}^2 - 2 \left[(\ddot{Q}_{11}n_1)^2 + (\ddot{Q}_{22}n_2)^2 + (\ddot{Q}_{33}n_3)^2 \right] \right. \\ & \left. + \frac{1}{2} (\ddot{Q}_{11}n_1n_1 + \ddot{Q}_{22}n_2n_2 + \ddot{Q}_{33}n_3n_3)^2 \right\}. \end{aligned} \quad (5.147)$$

Introducing spherical angles

$$n_1 = \sin \theta \cos \phi, \quad n_2 = \sin \theta \sin \phi, \quad n_3 = \cos \theta \quad (5.148)$$

for the direction $\mathbf{n}$, and assuming that $Q_{11} = Q_{22}$, the curly brackets in (5.147) become

$$\left\{ 2\ddot{Q}_{11}^2 + \ddot{Q}_{33}^2 - 2(\ddot{Q}_{11}^2 \sin^2 \theta + \ddot{Q}_{33}^2 \cos^2 \theta) + \frac{1}{2} [\ddot{Q}_{11} \sin^2 \theta + \ddot{Q}_{33} \cos^2 \theta]^2 \right\}. \quad (5.149)$$

For $Q_{33} = -2Q_{11}$, this reduces to

$$\ddot{Q}_{11}^2 \frac{9}{2} \sin^4 \theta. \quad (5.150)$$

The rate of energy radiation per solid angle $d\Omega$ is then

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{1}{2c^2} \frac{\kappa}{(4\pi)^2} M^2 [\omega^3 a d \sin \omega t]^2. \quad (5.151)$$

The radiation is maximal in the direction of the equator, and vanishes in the pole directions of the oscillator.

Integrating (5.151) over all angles gives the total emitted power

$$\begin{aligned} \dot{\mathcal{E}} &= \frac{1}{2c^2} \frac{\kappa}{(4\pi)^2} M^2 [\omega^3 a d \sin \omega t]^2 \frac{32}{15} \pi \\ &= \frac{8G}{15c^5} M^2 [\omega^3 a d \sin \omega t]^2, \end{aligned} \quad (5.152)$$

whose temporal average is

$$\dot{\mathcal{E}} = \frac{8G}{15c^5} M^2 \omega^6 a^2 d^2. \quad (5.153)$$

The rate of radiation damping is defined as

$$\gamma_{\text{rad}} \equiv \frac{1}{t_{\text{rad}}} \equiv \frac{1}{E} \frac{dE}{dt}, \quad (5.154)$$

where t_{rad} is the damping time. Since the kinetic energy of each mass is $M\omega^2 a^2/2$, we obtain

$$\gamma_{\text{rad}} = \frac{46}{15c^5} M d^2 \omega^4. \quad (5.155)$$

The formula estimates the damping rate of any linearly oscillating system of two masses. The linear character of the oscillation is important since there is no gravitational radiation at all for a spherically symmetric pulsating star.

Vibrational radiation may emerge from nova explosions at an early stage. These arise if a star circles around a white dwarf and transfers matter to him. After some time, the matter becomes large enough to explode.

This explosion causes vibrations in the white dwarf with frequencies 0.01 to 1 Hz. The energy released in a nova explosion is typically 10^{45} erg, of which 10% could be deposited in vibrations, which send out gravitational radiation.

5.3.2 Two Rotating Masses

If the two masses in the previous example rotate around the z -axis (see Fig. 5.2) the quadrupole moment (5.145) in the xy -plane becomes

$$Q_{ij}(t) = \frac{Md^2}{4} \begin{pmatrix} 1 - 3 \cos 2\omega t & -3 \sin 2\omega t \\ -3 \sin 2\omega t & 1 + 3 \cos 2\omega t \end{pmatrix}, \quad (5.156)$$

where M is the reduced mass

$$M \equiv \frac{M_1 M_2}{M_1 + M_2}, \quad (5.157)$$

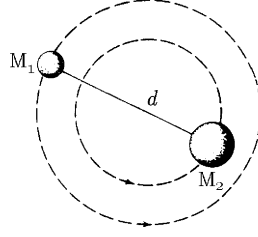


FIGURE 5.2 Two spherical masses in circular orbits around their center of mass.

and ω is given by the third Kepler law:

$$\omega = \sqrt{\frac{G(M_1 + M_2)}{r^3}}. \quad (5.158)$$

The third time derivatives of the quadrupole moments are therefore

$$\ddot{Q}_{ij}(t) = -6Md^2\omega^3 \begin{pmatrix} -\sin 2\omega t & -\cos 2\omega t \\ 0 & 0 \\ -\cos 2\omega t & \sin 2\omega t \end{pmatrix}. \quad (5.159)$$

Inserting these into (5.147), integrating over all angles, and averaging over all times yields the total emitted power

$$\dot{\mathcal{E}} = \frac{8G}{5c^5} M^2 d^4 \omega^6. \quad (5.160)$$

Using ω of Eq. (5.158), this becomes

$$\dot{\mathcal{E}} = \frac{32G^4}{5c^5 d^5} (M_1 M_2)^2 (M_1 + M_2). \quad (5.161)$$

The total energy of the binary system is

$$\mathcal{E} = \frac{1}{2} \frac{M_1 M_2}{M_1 + M_2} d^2 \omega^2 = \frac{1}{2} \frac{G M_1 M_2}{d}, \quad (5.162)$$

implying a rate of radiation loss

$$\gamma = \frac{64G^4}{5c^5 d^4} M_1 M_2 (M_1 + M_2). \quad (5.163)$$

Since E is inversely proportional to the distance d in (5.162), the relative decrease of the distance between the masses is

$$\frac{\dot{d}}{d} = -\frac{64G^3}{5c^5 d^4} M_1 M_2 (M_1 + M_2). \quad (5.164)$$

By Eq. (5.158) this implies that the frequency increases at a rate

$$\frac{\dot{\omega}}{\omega} = -\frac{3}{2} \frac{\dot{d}}{d}. \quad (5.165)$$

Due to the smallness of the gravitational constant, the power radiated by planetary systems is extremely small. The Earth orbiting around the sun emits only 200 W, the Jupiter emits 5300 W. For neighboring double stars, the power can increase to 10^{30} W and more. For double neutron stars, d can be quite small, and the radiated power can easily reach values of 10^{45} W.

Table 5.1 shows various astronomical objects and the gravitational amplitudes that can arrive from them here on Earth. See also the illustration on Fig. 5.3.

TABLE 5.1 Binary systems as sources of gravitational radiation [4]. The binary PSR 1913+16 emits radiation at multiples of 70×10^{-6} Hz due to the large eccentricity of the orbit.

System	Masses ($M_{\odot}$)	Dist. (pc)	Wave frequ. (10^{-6} Hz)	Luminosity at Earth (10^{30} erg/s)	Flux at Earth (10^{-22})	Amplitude at Earth
<i>Eclipsing binaries</i>						
ι Boo	1.0, 0.5	11.7	86	1.1	68.0	51
μ Sco	12, 12	109	16	51	38.0	210
V Pup	16.5, 9.7	520	16	59	1.9	46
<i>Cataclysmic binaries (novas)</i>						
AM CVn	1.0, 0.041	100	1900	300	240	5
WZ Sge	1.5, 0.12	75	410	24	37	8
SS Cyg	0.97, 0.83	30	84	2	20	30
<i>Binary X-ray sources (black holes or neutron stars)</i>						
Cyg X ₁	30, 6	2500	4.1	1.0	1	4
PSR 1913+16	1.4, 1.4	5000	70	0.6	0.2	0.12
			140	2.9	1.1	0.14
			210	5.8	2.1	0.12

Formula (5.165) has been used as an indirect evidence for the existence of gravitational radiation. In 1974, Hulse and Taylor searched for pulsars (rotating neutron stars emitting radio pulses) with the Arecibo telescope and found an object whose emitted radio frequency is periodically modulated. The modulation is attributed to the Doppler shift caused by the orbital motion around an undetected companion. A careful analysis of the modulation allowed them to derive the eccentricity and the rate of the perihelion precession of the binary object (see Table 5.2 for details).

The observed shift of the time of periastron passage is plotted in Fig. 5.4. The values of the masses were deduced from the perihel precession and the time delay of the signal passing the companion. They depend only on $M_1 + M_2$, M_1 , and M_2 in different combinations. From the data, one deduces

$$M_1 \sim (1.4414 \pm 0.0002) M_{\odot} \quad \text{for pulsar,} \quad (5.166)$$

$$M_2 \sim (1.3867 \pm 0.0002) M_{\odot} \quad \text{for companion.} \quad (5.167)$$

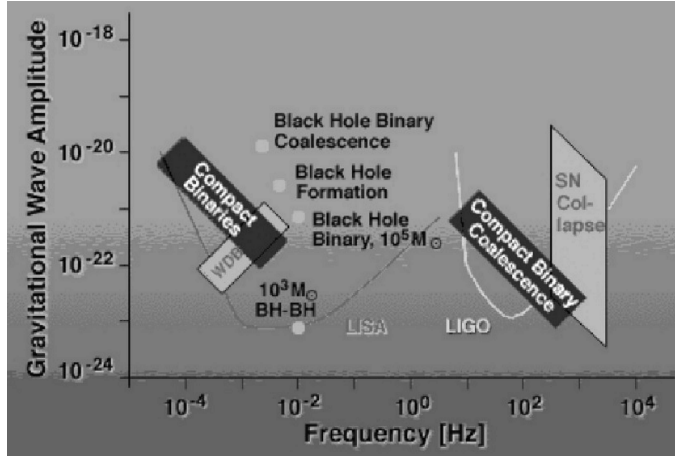


FIGURE 5.3 Gravitational amplitudes arriving on Earth from two possible sources. They are measured by LISA, which is a **L**aser **I**nterferometer **S**pace **A**ntenna built by a joint three-spacecraft mission of ESA and NASA (see http://www.esa.int/esaSC/120376_index_0_m.html). The other is measured by LIGO, a **L**aser **I**nterferometer **G**ravitational **W**ave **O**bservatory (see <http://www.ligo.caltech.edu>). Correlations must be monitored for distances between two objects lying 5×10^6 km apart. The letters WDB in the box near $(10^{-3}, 10^{-22})$ denotes **W**hite **D**warf **B**inaries.

The properties of binary objects containing a pulsar can be studied so well that the approximation (5.161) is sensitive to several corrections [6]. Consider two masses orbiting around the common center-of-mass (see Figs. 5.5 and 5.6). If d denotes the distance of the two masses, the distances from the center-of-mass are $d_1 = M_2 d / (M_1 + M_2)$, $d_2 = M_1 d / (M_1 + M_2)$. Denoting the reduced mass $M_1 M_2 / (M_1 + M_2)$ as before by M , the components of the quadrupole moment are

$$Q_{ij}(t) = M d^2 \begin{pmatrix} \cos^2 \varphi & \sin \varphi \cos \varphi \\ \sin \varphi \cos \varphi & \sin^2 \varphi \end{pmatrix}. \quad (5.168)$$

The orbit of a Kepler ellipse has the general form

$$d = \frac{a(1 - e^2)}{1 + e \cos \varphi}, \quad (5.169)$$

where a is the semi-major axis of the ellipse, $e \equiv \sqrt{1 - b^2/a^2}$ is the eccentricity (b denotes the semi-minor axis), and the angular velocity is given by

$$\dot{\varphi}(t) = d^{-2}(t) \sqrt{(M_1 + M_2) a (1 - e^2)}. \quad (5.170)$$

From this we derive immediately

$$\ddot{Q}_{11} = P(1 + e \cos \varphi)^2 (2 \sin 2\varphi + 3e \sin \varphi \cos^2 \varphi), \quad (5.171)$$

$$\ddot{Q}_{22} = P(1 + e \cos \varphi)^2 [2 \sin 2\varphi + e \sin \varphi (1 + 3 \cos^2 \varphi)], \quad (5.172)$$

$$\ddot{Q}_{12} = -P(1 + e \cos \varphi)^2 [2 \sin 2\varphi - e \sin \varphi (1 - 3 \cos^2 \varphi)] = \ddot{Q}_{21}, \quad (5.173)$$

TABLE 5.2 Some observed parameters of PSR 1913+16 (Table taken from Ref. [5]).

Distance	21 000 ly
Pulsar period (nominal)	59.02999792988 ms
Semi-major axis	1 950 100 km
Eccentricity	0.617131 ± 0.000003
Orbital period	27907 ± 0.00002 s
Rate of precession of the periastron	$(4.22263 \pm 0.0003)^\circ/\text{y}$
Amplitude of time-dilation factor	0.0044 ± 0.0001
Rate of decrease of orbital period	$2.4184(9) \times 10^{-12} \text{ s/s} = 0.0000765 \text{ s/y}$
Rate of decrease of semimajor axis	3.5 m/y
Calculated lifetime (to final inspiral)	300 000 000 y
Diameter of each neutron star	20 km
Periastron separation	746 600 km
Apoastron separation	3 153 600 km
Velocity of stars at periastron in CM frame	450 km/sec
Velocity of stars at apoastron in CM frame	110 km/sec
Rate of precession of spin axis	??

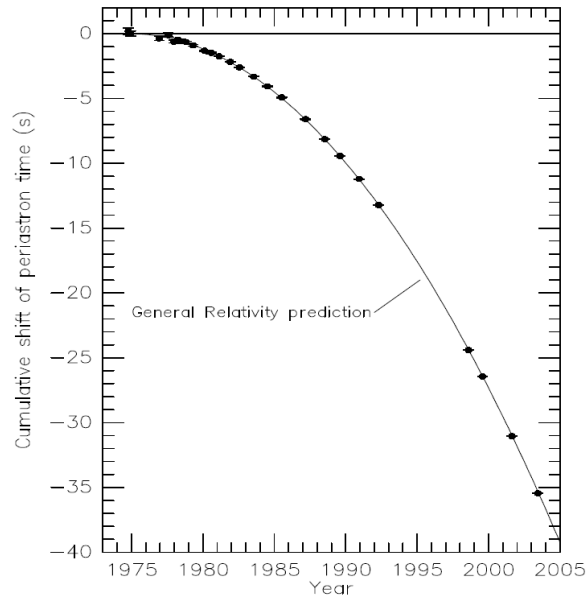


FIGURE 5.4 Shift of time of the periastron passage of PSR 1913+16 for each orbit caused by the shrinking of the Kepler orbits as a consequence of formula (5.179). Curve is from Einstein theory {see Eq. (5.179) and Ref. [5]}.

where P is a power factor

$$P \equiv 2 \sqrt{\frac{G^3 M_1^2 M_2^2 (M_1 + M_2)}{a^5 (1 - e^2)^5}}. \quad (5.174)$$

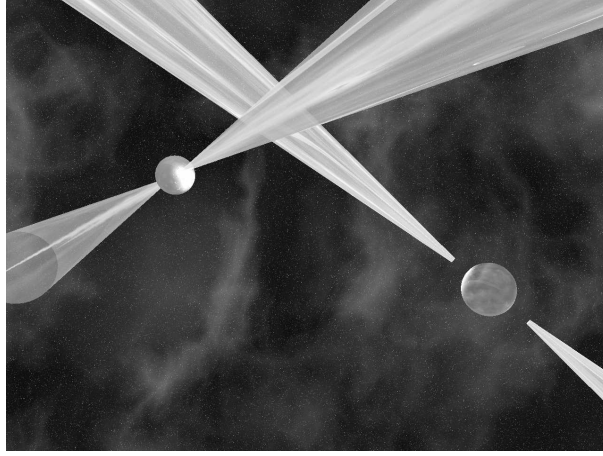


FIGURE 5.5 Two pulsars orbiting around each other.

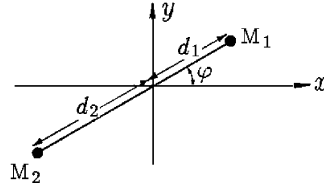


FIGURE 5.6 Two masses in a Keplerian orbit around the common center-of-mass.

Inserting (5.171)–(5.173) into the radiation power formula (5.147), and integrating over all emission angles $d\Omega$ yields the total emitted power as a function of time t :

$$\dot{\mathcal{E}} = \frac{8G^4}{15c^5} \frac{M_1^2 M_2^2 (M_1 + M_2)}{a^5 (1 - e^2)^5} [1 + e \cos \varphi(t)]^4 \{12[1 + e \cos \varphi(t)]^2 + e^2 \sin^2 \varphi(t)\}. \quad (5.175)$$

The time dependence of the semi-major axis $a(t)$ follows the differential equation

$$\frac{\dot{a}}{a} = -\frac{64G^3}{5c^5} \frac{M_1 M_2 (M_1 + M_2)}{a^4 (1 - e^2)^{7/2}} \left(1 + \frac{73}{24}e^2 + \frac{37}{964}e^4\right). \quad (5.176)$$

The excentricity $e(t)$ changes in time according to

$$\frac{\dot{e}}{e} = -\frac{304G^3}{15c^5} \frac{M_1 M_2 (M_1 + M_2)}{a^4 (1 - e^2)^{5/2}} \left(1 + \frac{121}{304}e^2\right). \quad (5.177)$$

An arbitrary Kepler orbit will shrink to zero in the *coalescence time* τ_{coales} . For a circular orbit of semi-major axis $a_0 = a(0)$ and $e_0 = e(0) = 0$, this is

$$\frac{1}{\tau_{\text{coales}}} = -\frac{4 \cdot 64G^3}{5c^5} \frac{M_1 M_2 (M_1 + M_2)}{a_0^4}. \quad (5.178)$$

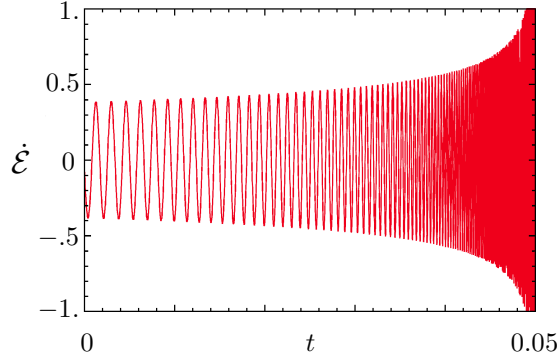


FIGURE 5.7 Energy emitted by two point-masses on a circular orbit around each other.

For a circular orbit, the time dependence is shown in Fig. 5.7. Averaging over one period of the elliptical orbit yields

$$\langle \dot{\mathcal{E}} \rangle = \frac{32G^4}{5c^5} \frac{M_1^2 M_2^2 (M_1 + M_2)}{a^5 (1 - e^2)^{7/2}} \left(1 + \frac{73}{24}e^2 + \frac{37}{96}e^4 \right). \quad (5.179)$$

With respect to a circular orbit of equal total energy, the power is enhanced by a factor

$$f = \frac{1 + \frac{73}{24}e^2 + \frac{37}{96}e^4}{(1 - e^2)^{7/2}}, \quad (5.180)$$

which grows rapidly from $f(e) = 1$ at $e = 0$ to infinity at $e = 1$. For a full multipole analysis of the radiation see [6].

Due to the shrinking of the Kepler orbits implied by formula (5.179), the orbital time shrinks according to the elliptic generalization of Eq. (5.165), implying that the periastron is reached a few seconds earlier for each orbit. The time shift was plotted in Fig. 5.4.

The radiation properties of binary objects can be studied especially well if both stars are pulsars (recall Fig. 5.5). Such astronomical objects have recently been found. One of the two pulsars rotates with a period of 23 milliseconds (PSR J0737-3039A) around its axis, the other with a period of 2.8 seconds (PSR J0737-3039B) [7].

5.3.3 Particle Falling into Star

Among the bursting sources of gravitational radiation the simplest one consists of a mass falling into a star (see Fig. 5.8) emitting a spectrum shown in Fig. 5.9.

If the mass starts at $z = \infty$, its velocity is

$$\frac{1}{2}m\dot{z}^2 = \frac{GmM}{z}, \quad (5.181)$$

so that

$$\dot{z} = -\frac{1}{z^{1/2}}(2GM)^{1/2}, \quad \ddot{z} = -\frac{GM}{z^2}, \quad \dot{\ddot{z}} = -\frac{(2GM)^{3/2}}{z^{7/2}}. \quad (5.182)$$

The triple time derivative of the quadrupole moment

$$Q_{ij} = m \begin{pmatrix} -z^2 & 0 & 0 \\ 0 & -z^2 & 0 \\ 0 & 0 & 2z^2 \end{pmatrix} \quad (5.183)$$

is

$$\ddot{Q}_{ij} = m(6\dot{z}\ddot{z} + 2z\dot{\ddot{z}}) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad (5.184)$$

and thus, because of (5.182),

$$\ddot{Q}_{ij} = m \frac{(2GM)^{3/2}}{z^{5/2}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \quad (5.185)$$

Inserted into (5.122), this leads to an energy loss per second

$$\dot{\mathcal{E}} = \frac{2Gm^2}{15c^5}(6\dot{z}\ddot{z} + 2z\dot{\ddot{z}})^2. \quad (5.186)$$

Combining this with (5.182) implies

$$\frac{d\mathcal{E}}{dz} = \frac{1}{z^{9/2}} \frac{2Gm^2}{15c^2} (2GM)^{5/2}. \quad (5.187)$$

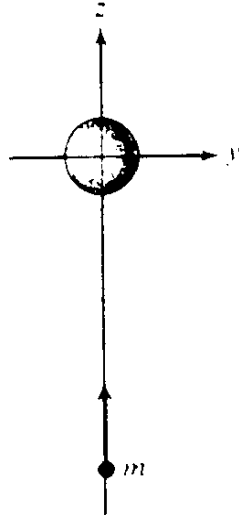


FIGURE 5.8 Particle falling radially towards a large mass.

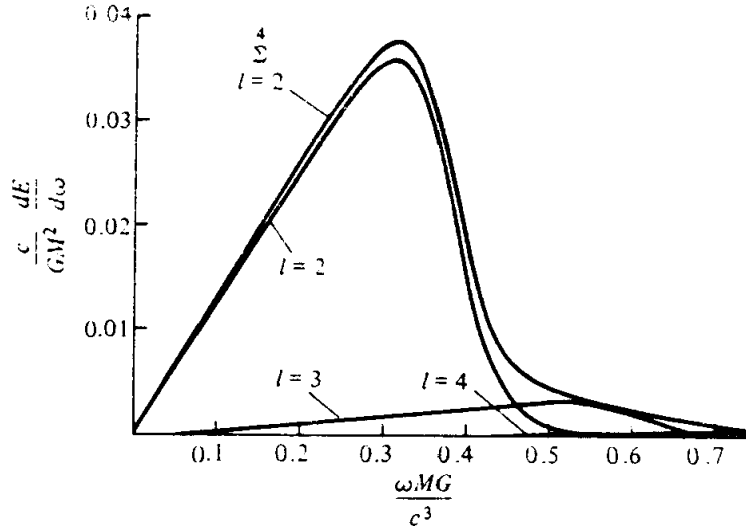


FIGURE 5.9 Spectrum of the gravitational radiation emitted by a particle of mass m falling radially into a black hole of mass M . The quantity $dE/d\omega$ gives the amount of energy radiated per unit frequency interval. The curve marked $l = 2$ corresponds to quadrupole radiation; the other curves ($l = 3, l = 4$) correspond to multipole radiation of higher order. Note that most of the radiation is emitted with frequencies below $\omega \simeq 0.5c^3/GM$ [8].

The radiated energy from $z = \infty$ to $z = R$ is

$$\mathcal{E} = \frac{1}{R^{7/2}} \frac{4Gm^2}{105c^5} (2GM)^{5/2}. \quad (5.188)$$

Obviously, the radiated energy increases with decreasing R . Suppose the large object is a black hole. If we let the mass m fall down to the Schwarzschild radius:

$$R_s = 2 \frac{GM}{c^2}, \quad (5.189)$$

we obtain

$$\mathcal{E} = \frac{2}{105} mc^2 \frac{m}{M} \approx 0.019 mc^2 \frac{m}{M}. \quad (5.190)$$

If one takes relativistic effects into account which are due to the deviations of the Schwarzschild metric from flat space as the particle approaches R_s , the number 0.019 changes to 0.0104.

For a black hole of mass $M \sim 10M_\odot$ with Schwarzschild $R_s \sim 30$ km, the total radiated energy is

$$\mathcal{E} \sim 2 \times 10^{51} \text{ erg}. \quad (5.191)$$

The radiated energy is mostly emitted near the end of the process. See also Table 5.3 for a list of possible sources of astrophysical gravitational radiation.

TABLE 5.3 Typical astrophysical sources of gravitational radiation. Distances have been selected large enough to yield approximately three events per year [9].

Source	Frequency	Distance	Amplitude (κA)
<i>Periodic sources</i>			
Binaries	10^{-4} Hz	10 pc	10^{-20}
Nova	10^{-2} to 1	500 pc	10^{-22}
Spinning neutron star (Crab)	60	2 kpc	$< 10^{-24}$
<i>Bursting sources</i>			
Coalescence of binary	10 to 10^3	100 MPC	10^{-21}
Infall of star into $10M_{\odot}$ b.h.	10^{-4}	10 Mpc	10^{-21}
Supernova	10^3	10 kpc	10^{-18}
Gravitational collapse of $10^4M_{\odot}$ star	10^{-1}	3 Gpc	10^{-19}

5.3.4 Cloud of Colliding Stars

Let us treat the stars in a cloud approximately as point-like objects moving with velocities $\mathbf{v}_n$, where they have an energy-momentum tensor

$$T^{\mu\nu} = \sum_n \frac{p_n^\mu p_n^\nu}{E_n} \delta^{(3)}(\mathbf{x} - \mathbf{x}(t)). \quad (5.192)$$

Suppose the stars all collide at the origin at $t = 0$ and run away with changed velocities $\bar{\mathbf{v}}_n$. Then the time-dependent energy-momentum tensor is

$$T^{\mu\nu}(\mathbf{x}, t) = \sum_n \frac{p_n^\mu p_n^\nu}{E_n} \delta^{(3)}(\mathbf{x} - \mathbf{v}_n t) \Theta(-t) - \sum_n \frac{\bar{p}_n^\mu \bar{p}_n^\nu}{\bar{E}_n} \delta^{(3)}(\mathbf{x} - \bar{\mathbf{v}}_n t) \Theta(t), \quad (5.193)$$

where $\Theta(t)$ is the Heaviside function defined in Eq. (1.311). Representing this as a Fourier integral

$$\Theta(t) = -i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{i\omega t}}{\omega - i\eta}, \quad (5.194)$$

and the δ -function similarly as

$$\delta^{(3)}(\mathbf{x} - \mathbf{v}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (5.195)$$

we see that the energy momentum tensor (5.193) has the Fourier components

$$T^{\mu\nu}(\mathbf{k}, \omega) = - \sum_n \left(\frac{p_n^\mu p_n^\nu}{E_n} \frac{i}{\omega - \mathbf{v}_n \cdot \mathbf{k} - i\eta} - \frac{\bar{p}_n^\mu \bar{p}_n^\nu}{\bar{E}_n} \frac{i}{\omega - \mathbf{v}_n \cdot \mathbf{k} + i\eta} \right). \quad (5.196)$$

Now we observe that

$$E_n \times (\mathbf{v}_n \cdot \mathbf{k} - \omega) = p_n k, \quad (5.197)$$

where k is the four-momentum of the emerging gravitational wave. Since the stars are nonrelativistic objects, we can further drop the $i\eta$'s. Thus

$$T^{\mu\nu}(\mathbf{k}, \omega) = -i \sum_n \left(\frac{p_n^\mu p_n^\nu}{p_n k} - \frac{\bar{p}_n^\mu \bar{p}_n^\nu}{\bar{p}_n k} \right). \quad (5.198)$$

This energy-momentum tensor satisfies $k_\mu T^{\mu\nu} = \sum_n (p_n - \bar{p}_n) = 0$, as it should by momentum conservation. Inserting (5.198) into (5.132) yields the total radiated energy per solid angle and frequency interval $d\omega$:

$$\frac{d\mathcal{E}}{d\Omega d\omega} = \frac{\kappa}{16\pi^2} \omega^2 \sum_{nn'} \frac{\sigma_n \sigma_{n'}}{(p_n k)(p_{n'} k)} \left[(p_n p_{n'})^2 - \frac{1}{2} M_n^2 M_{n'}^2 \right], \quad (5.199)$$

where the index n runs over the particles before and σ_n is equal to 1 before the collisions, and -1 afterwards. Integrating over all directions of $\mathbf{k}_n$ yields

$$\frac{d\mathcal{E}}{d\Omega d\omega} = \frac{\kappa}{16\pi^2} \omega^2 \sum_{nn'} \sigma_n \sigma_{n'} M_n M_{n'} \frac{1 + \beta_{nn'}^2}{(1 - \beta_{nn'}^2)^{1/2}} \frac{1}{\beta_{nn'}} \log \left(\frac{1 + \beta_{nn'}}{1 - \beta_{nn'}} \right), \quad (5.200)$$

where $\beta_{nn'}$ is the relative velocity divided by c :

$$\beta_{nn'} \equiv \left[1 - \frac{M_n M_{n'}}{(p_n p_{n'})^2} \right]^{1/2}. \quad (5.201)$$

The integral over all frequencies diverges. This is due to the fact that we have assumed an instantaneous change of momenta during the collisions. In actual collisions, the change takes place over some finite collision time Δt and the integral contains frequencies up to $1/\Delta t$. For nonrelativistic two-body scattering, the radiated energy is

$$\frac{d\mathcal{E}}{d\Omega} = \frac{2\kappa}{5\pi} \mu^2 \int \frac{d\omega}{2\pi} v^4 \sin^2 \theta, \quad (5.202)$$

where μ is the reduced mass, v are the relative velocities, and θ the scattering angles in the center-of-mass frame.

5.4 Orders of Magnitude of Different Radiation Sources

In order to have an idea of the amounts of energy that can be radiated in various processes, consider a massive steel rod of radius 1m, length $d=20\text{m}$, mass $M \sim 4.9 \times 10^8 g$ ($=490$ tons, using the steel density 7.89g/cm^3). If the maximal quadrupole radiation can be obtained by rotating it around an axis orthogonal to the rod with an angular velocity ω , then formula (5.122) yields the total emitted power

$$\dot{\mathcal{E}} = \frac{2}{45c^5} M^2 l^4 \omega^6. \quad (5.203)$$

The angular velocity is limited by the tensile strength, which is $t \approx 3 \times 10^9 \text{ dyn/cm}^2$. Thus one can maximally use an angular velocity

$$\omega = \left(\frac{8t}{\rho l^2} \right)^{1/2} \approx 28 \frac{1}{\text{sec}}. \quad (5.204)$$

This gives a radiated power

$$\dot{\mathcal{E}} \approx 10^{-23} \text{ erg/sec}. \quad (5.205)$$

In order to have an idea how small this is we note that a single photon in the visible range has an energy

$$\hbar c \frac{2\pi}{4000 \text{ \AA}} \approx 10^{-27} 10^{10} \frac{2\pi}{4 \times 10^{-5}} \text{ erg} \approx 1.5 \times 10^{-12} \text{ erg}. \quad (5.206)$$

Thus the radiated power corresponds to the emission of one visible photon in $\approx 10^{11}$ seconds or ≈ 3000 years.

If one wants to have any observable effects it is therefore necessary to look for radiation emitted by large stellar objects. Consider a bunch of stars of total mass M distributed over a region of size R . Their velocity is of the order R/T where T is the time it takes for the masses to move from one side to the diametrically opposite one. Their quadrupole moment is of the order of

$$Q \sim R^2 M. \quad (5.207)$$

Hence we can estimate

$$\ddot{Q} \sim \frac{R^2 M}{T^3} \sim M \left(\frac{R}{T} \right)^2 \frac{1}{T}. \quad (5.208)$$

The right-hand side has the dimension energy per time. It gives an estimate for the internal power flow in the system. The radiated power is equal to

$$\dot{\mathcal{E}} \sim \frac{1}{c^5/G} \left(\frac{R^2 M}{T^3} \right)^2. \quad (5.209)$$

For the Sun-Jupiter system, this time is $\approx 2.5 \times 10^{23}$ years. But for the binary system PSR 1913+16, the spiral time shrinks to 3×10^8 years, as shown in Table 5.2. This makes it observable, as we have seen in Fig. 5.4. For Kepler orbits of planets, on the other hand, the radiation damping is too small to be observed.

For neutron stars a few thousand kilometers apart, the spiral times could shrink to the order of years or days, so it could be observed, at least in principle. Here the problem lies in the identification of the source.

5.5 Detection of Gravitational Waves

In order to observe more details of the gravitational waves, consider a test particle whose equation of motion reads

$$\frac{du^\mu}{d\tau} = - \left(\partial_b h^\mu_\lambda - \frac{1}{2} \partial^\mu h_{bc} \right) u^\nu u^\lambda. \quad (5.210)$$

If it is initially at rest or moving very slowly, the right-hand side reduces to

$$- \left(\partial_0 h^\mu_0 - \frac{1}{2} \partial^\mu h_{00} \right) c^2. \quad (5.211)$$

Since the two physical polarization tensors have neither 00 nor 0i components, this vanishes. Thus two particles retain their relative positions as seen from the background Minkowski frame.

This does not mean that their physical distance remains unchanged. This distance is evaluated not via the Minkowski metric η_{ab} , but via the proper slightly distorted metric $g_{ab} = \eta_{ab} + h_{ab}$. If a wave with a linear polarization $\epsilon_+(\mathbf{k})$ runs along the z -axis

$$h_{ab} = \frac{1}{\sqrt{2}} [\epsilon_\mu(1)\epsilon_b(1) - \epsilon_\mu(2)\epsilon_b(2)] a_+ e^{i(kz - \omega t)} + \text{c.c.} \quad (5.212)$$

and hits two particles at $(0, d_0/2, 0, 0)$ and $(0, -d_0/2, 0, 0)$, which initially do not move due to the vanishing of $du^\mu/d\tau$, their spatial distance changes as follows:

$$\begin{aligned} d^2 &= -(0, d_0, 0, 0)^a (\eta_{ab} + h_{ab}) \begin{pmatrix} 0 \\ d_0 \\ 0 \\ 0 \end{pmatrix}^b \\ &= d_0^2 \left[1 - \frac{a_+}{\sqrt{2}} \cos(\omega t - \delta) \right], \end{aligned} \quad (5.213)$$

where δ is the phase of the wave amplitude a_+ .

We can best picture the change in the metric by imagining a circular necklace of mass points placed in the gravitational beam. If the momentum points into the orthogonal direction of the paper plane, the circle distorts into vertical and horizontal ellipses, as shown in Fig. 5.10. The distortions are of quadrupole character, and the area within the necklace remains invariant, due to the tracelessness of $\epsilon_+^{\mu\nu}(\mathbf{k})$ (giving $g_{ab} = \eta_{ab} + h_{ab}$ a determinant $\sqrt{-g} = 1 + \mathcal{O}(a^2)$ leading to an invariant volume element $d^3x' = \sqrt{g}d^3x$ to lowest order in a). For a wave with polarization tensor $\epsilon_\times(k_{zab}) = [\epsilon_\mu(1)\epsilon_b(2) + (a \leftrightarrow b)]/\sqrt{2}$, the distance changes with time as follows:

$$d_\times^2 = d_0^2 \left[1 - \frac{a}{\sqrt{2}} \sin(2\phi) \cos(\omega t - \delta) \right]. \quad (5.214)$$

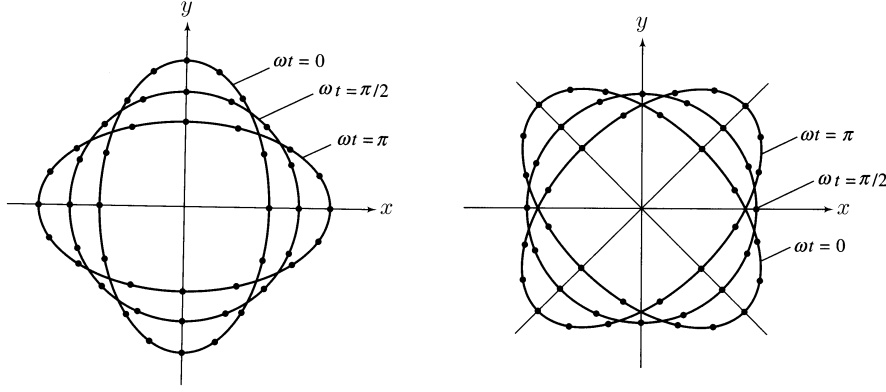


FIGURE 5.10 Distortions of a circular array of mass points caused by the passage of a gravitational quadrupole wave. The left is caused by a polarization tensor $\epsilon_{+}^{\mu\nu}$, the second by $\epsilon_{\times}^{\mu\nu}$.

The situation is the same as before, except for a rotation $\phi \rightarrow \phi - \pi/4$. Thus the necklace undergoes the same quadrupole distortions, except that the principal axes of the ellipses lie along the diagonals as indicated by the subscript $\times$ of the polarization tensor. The rotation by 45° can also be displayed more directly by writing the polarization tensor $\epsilon_{H\times}^{\mu\nu}$ of Eq. (4.426) as a combination:

$$\epsilon_{H\times}^{\mu\nu} = \frac{1}{\sqrt{2}}[\epsilon^\mu(1)\epsilon^\nu(2) + (a \leftrightarrow b)] = \frac{1}{\sqrt{2}}[\epsilon^\mu(\nearrow)\epsilon^\nu(\nearrow) - \epsilon^\mu(\nwarrow)\epsilon^\nu(\nwarrow)], \quad (5.215)$$

where

$$\epsilon^\mu(\nearrow) = \frac{1}{\sqrt{2}}[\epsilon^\mu(1) + \epsilon^\mu(2)], \quad \epsilon^\mu(\nwarrow) = \frac{1}{\sqrt{2}}[\epsilon^\mu(1) - \epsilon^\mu(2)] \quad (5.216)$$

are the diagonal polarization vectors. Similarly we rewrite $\epsilon_{H+}^{\mu\nu}(k_z)$ of (4.425) as

$$\epsilon_{H+}^{\mu\nu}(k_z) = \frac{1}{\sqrt{2}}[\epsilon_\mu(1)\epsilon_b(1) - \epsilon_\mu(2)\epsilon_b(2)] = \frac{1}{\sqrt{2}}[\epsilon^\mu(\nearrow)\epsilon^\nu(\nwarrow) + \epsilon^\mu(\nwarrow)\epsilon^\nu(\nearrow)]. \quad (5.217)$$

The right-hand sides of (5.215) and (5.217) have the same forms as $\epsilon_{H+}^{\mu\nu}$ and $\epsilon_{H\times}^{\mu\nu}$ expressed in terms of $\epsilon_\mu(1)$ and $\epsilon_b(2)$, but with $\epsilon_\mu(1)$ and $\epsilon_b(2)$ exchanged by the 45° -rotated diagonal polarization vectors $\epsilon^\mu(\nearrow)$ and $\epsilon^\mu(\nwarrow)$.

The acceleration of the distance

$$\frac{d^2 d}{dt^2} = \frac{1}{d} d_0 \frac{a}{\sqrt{2}} \omega^2 \begin{Bmatrix} \cos 2\phi \\ \sin 2\phi \end{Bmatrix} \cos(\omega t - \delta) \quad (5.218)$$

implies the presence of tidal forces acting upon the necklace. Their field lines are shown in Fig. 5.11. If gravitational waves of helicity ± 2 hit the necklace, it is

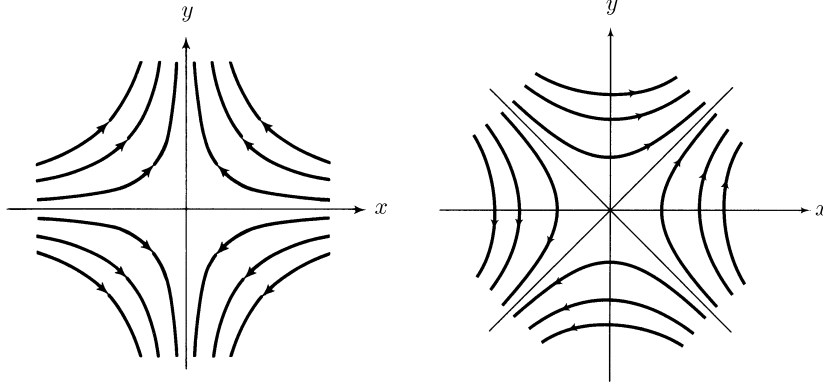


FIGURE 5.11 Field lines of tidal forces of a gravitational wave running along the z -direction with polarization tensor ϵ_+^{ab} and ϵ_x^{ab} , respectively. The field lines change direction with a time dependence $\cos \omega t$.

deformed into an ellipse with a fixed shape which rotates clockwise or counter-clockwise around the direction of the wave. The wave is circularly polarized. This is seen by taking again two particles at positions

$$\pm \left(0, \frac{d}{2} \cos \phi, \frac{d}{2} \sin \phi, 0 \right), \quad (5.219)$$

and measuring their distances with the metric

$$g_{\mu\nu} = \eta_{\mu\nu} + [\epsilon_\mu(+)\epsilon_\nu(+)]e^{i(kz-\omega t)} + \text{c.c.} \quad (5.220)$$

As a function of time t , the square distance of the two particles behaves like

$$\begin{aligned} d^2 &= d_0^2 \left\{ 1 - [(\cos^2 \phi - \sin^2 \phi) + i2 \cos \phi \sin \phi] a e^{-i\omega t} + \text{c.c.} \right\} \\ &= d_0^2 [1 - |a| \cos(\omega t - 2\phi - \delta)], \end{aligned} \quad (5.221)$$

implying the above-described rotations of the necklace, the azimuthal angle ϕ acting merely as a phase shift.

The time-dependence of the length measured by the metric $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ has a direct experimental equivalence. If we take a piezoelectric crystal, then it shows a pulsating voltage due to the distance changes between the atoms, even though its atoms remain at rest in the Minkowski coordinates. The distance is given by the minima of the interatomic potentials. Since the atomic interactions are due to electromagnetism which spreads through a space with the metric $g_{\mu\nu}$, the distances of these minima change according to changes in $g_{\mu\nu}$, and this gives rise to the piezoelectric voltage.

How large are the distortions caused by a gravitational wave? If we assume a typical astrophysical source (for the emission mechanism see the next section) with an energy flux of $\approx 10^{10}$ erg/(cm²sec) at $\omega \sim 10^4$ /sec, we calculate the distortion of the metric to be of the order

$$h_{\mu\nu} \approx 10^{-7}. \quad (5.222)$$

By analyzing seismometer data of the Earth's vibrations, J. Weber estimated in 1967 [10] an upper limit for the flux of gravitational waves:

$$\frac{\text{energy flux}}{\text{frequency}} < 3 \times 10^7 \frac{\text{erg}}{\text{cm}^2 \text{sec Hertz}}, \quad (5.223)$$

at a frequency 3.1×10^{-4} Hz. This would make the Earth-Moon distance oscillate by $\approx 10^{-7} \text{cm} = 10 \text{\AA}$ around the average distance $3.8 \times 10^{10} \text{cm}$. This amplitude is of the same order as the distance between the atoms in matter.

Other possible observable effects are quadrupole vibrations which can be excited by incoming gravitational waves within the Earth or the Moon themselves. Their natural frequencies are 54 minutes or 15 minutes, respectively. In 1972, J. Weber built a gravitational detector consisting of a cylindrical aluminum block of 1.53 m length and 0.66 m diameter (weight $\approx 1.41 \times 10^6 \text{g}$). The block has an eigenfrequency of 1.66 Hz. By a piezoelectric strain transducer, Weber measured length changes in the material of the block. Setting up one block at the University of Maryland and another one at Argonne National Laboratory and looking at coincidences between the two, he eliminated random vibrations caused by the daily activities in the neighborhood of each detector [11].

In 1972, he observed two sudden simultaneous excitations which he interpreted as a possible response to a gravitational wave passing through. Unfortunately, his observation has not found any recurrence in spite of collective efforts of several laboratories [12]. A new approach was necessary to become sensitive to such small effects. This approach has finally led to the so-far undisputed discovery of the waves [13]. More details will be discussed in the forthcoming Section.

5.6 Inspiralling Plunge of One Black Hole into another

An extremely dramatic event which can release gigantic gravitational energies is the merger of a black hole with another in an inspiralling plunge. Such an event has been studied by many theorists using computer simulations of Einstein's equation [18]. Analytically, it has been possible to develop an effective one-body approach to general-relativistic two-body problems that has made it possible to calculate the plunge of one body into a larger one as a powers series in the inverse distance [19]. If translated into an acoustical signal, the accelerating motion with the final merger should be hearable as a short chirp [20]. Such signals have recently been detected by the experimental collaboration LIGO (see the heading of Fig. 5.3), where more than 1000 researchers were linked via internet. The chirp was heard simultaneously in Hanford, Washington and in Livingston, Louisiana, and looks exactly [13] as expected from the theoretical computer simulations [18]. When the black holes are still far apart from each other, the signal has the general form calculated for two mass point in Fig. 31.15. As the inspiralling of the two bodies proceeds, the frequency increases, until one black hole merges with the other.

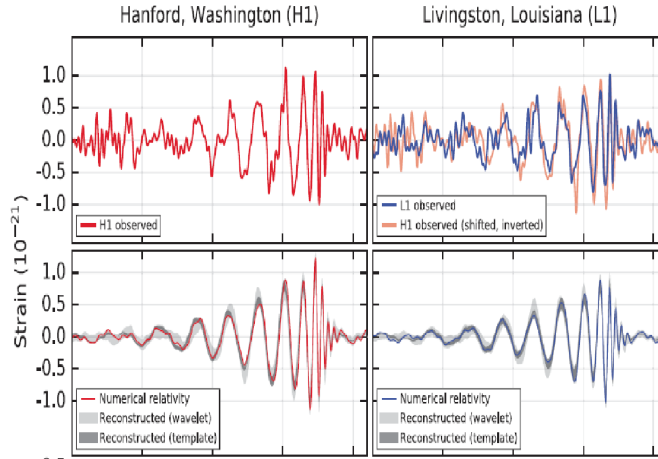


FIGURE 5.12 Two correlated chirps detected by the LIGO collaboration in Hanford, Washington and Livingston, Louisiana.

Appendix 5A Attractive Gravity versus Repulsive Electric Forces between Like Charges

The energy of gravitational waves gives a simple insight into why the fields lead to an attraction between masses (which are always positive) while electromagnetism is repulsive between line charges. The physical components of gravitational waves are the purely spatial ones ϕ^{ij} . Their energy has to be positive, and hence the field energy carries a plus sign when expressed in momentum space:

$$E_{\text{grav}} \propto \mathbf{k}^2 (\phi^{ij})^2. \quad (5A.1)$$

In electromagnetism, the same is true for the spatial part of the electromagnetic field A^i :

$$E_{\text{elm}} \propto \mathbf{k}^2 (A^i)^2. \quad (5A.2)$$

As a simple consequence of Lorentz invariance, the components ϕ^{00} and A^0 have to appear with opposite signs in E :

$$\begin{aligned} E_{\text{grav}} &\propto \mathbf{k}^2 \phi^{00^2}, \\ E_{\text{em}} &\propto -\mathbf{k}^2 A^{0^2}. \end{aligned} \quad (5A.3)$$

But these components are the relevant ones coupling to the mass density T^{00} or to the charge density j^0 , respectively, thereby giving rise to Newton's or to Coulomb's law. The opposite signs cause the forces to point in opposite directions.

Appendix 5B Nonlinear Gravitational Waves

Plane gravitational waves are such simple phenomena that they can easily be found as solutions to the full nonlinear Einstein equations in the vacuum

$$G_{\mu\nu} = 0. \quad (5B.1)$$

If the wave runs in the z -direction we can make a two-dimensional ansatz for the invariant distance

$$(ds)^2 = (dt)^2 - L^2 [e^{2\beta} (dx)^2 + e^{-2\beta} (dy)^2] - (dz)^2, \quad (5B.2)$$

where L and β are functions which depend only on z and t . It is useful to go to so-called *light cone coordinates*:

$$\begin{aligned} u &= t - z, \\ v &= t + z, \end{aligned} \quad (5B.3)$$

which sit on wave crests moving along the positive and negative z -directions. It can easily be verified that the only non-zero component of the Ricci tensor is

$$R_{uu} = -2L^{-1}(L'' + \beta'^2 L), \quad (5B.4)$$

so that the nonlinear wave equation in empty space reads

$$L'' + \beta'^2 L = 0. \quad (5B.5)$$

Our previous linear waves correspond to the equation

$$L'' \approx 0, \quad (5B.6)$$

which can be solved by

$$L \approx 1. \quad (5B.7)$$

In this limit, the square of the line elements are equal to

$$ds^2 \approx -(1 + 2\beta)dx^2 - (1 - 2\beta)dy^2 - dz^2, \quad (5B.8)$$

corresponding to a small metric distortion

$$h_{ab} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2\beta & 0 \\ 2\beta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (5B.9)$$

i.e., a wave with a polarization tensor $\epsilon_+(k_z)_{ab}$.

Going back to the nonlinear case, we assume the space to be flat before the wave arrives, say at

$$t - z = -T, \quad (5B.10)$$

i.e., we take

$$\beta = 0, \quad L = 1 \quad \text{for } u < -T. \quad (5B.11)$$

We shall assume that the wave comes as a pulse of width $2T$ and that, after the pulse has passed, the final spacetime is left again flat. While the pulse passes, i.e., for $T > u > -T$, we allow for an arbitrary $\beta(u)$ but assume, for simplicity, that the pulse is not sharp:

$$|\beta'(u)| \ll \frac{1}{T}. \quad (5B.12)$$

Then we do not have to solve the full differential equation. While the pulse is passing, we have

$$\beta(u) = \text{arbitrary, with } |\beta'| \ll \frac{1}{T}, \quad (5B.13)$$

$$L(u) = 1 - \int_{-T}^u du' \int_{-T}^{u'} du'' [\beta'(u'')]^2 + \mathcal{O}((\beta'T)^4) \quad \text{for } u \in (-T, T).$$

After it has passed, $\beta(u)$ is again zero by assumption, and

$$L(u) = 1 - \frac{u}{a}, \quad \text{with } a \equiv \frac{1}{\int_{-T}^T \beta'^2 du} + \mathcal{O}((\beta'T)^2) \quad \text{for } u > T. \quad (5B.14)$$

The change in L from 1 to $-u/a$ is physically not observable. The space is flat after the pulse has passed. This is seen by going to new coordinates X, Y and U, V defined by

$$x = \frac{X}{1 - U/a}, \quad y = \frac{Y}{1 - U/a} \quad \text{and} \quad u = U, \quad v = V + \frac{1}{a} \frac{X^2 + Y^2}{1 - U/a}, \quad (5B.15)$$

which transforms the invariant distance to the Minkowski form:

$$ds^2 = dU dV - d^2 - (dY)^2. \quad (5B.16)$$

Appendix 5C Nonexistence of Gravitational Waves in $D=3$ and $D=2$ Spacetime Dimensions

The counting procedure of physical degrees of freedom has an immediate consequence for the existence of gravitational waves in a hypothetical lower-dimensional world. In three dimensions, the symmetric tensor $\phi^{\mu\nu}$ has six independent components, three of which are eliminated by the Hilbert condition $\partial_\mu \phi^{\mu\nu} = 0$. This leaves only three components. These, however, are just as many as there are gauge degrees of freedom:

$$\phi^{\mu\nu} \rightarrow \phi^{\mu\nu} + \partial^\mu \xi^\nu + \partial^\nu \xi^\mu - \eta^{\mu\nu} \partial_\lambda \xi^\lambda. \quad (5C.1)$$

In fact, all field degrees of freedom are gauge degrees of freedom. We see this by choosing $\mathbf{k}$ in the z -direction, where polarization vectors can be written as

$$\begin{aligned} \epsilon^\mu(l) &= \frac{1}{\sqrt{2}} \frac{1}{|\mathbf{k}|} k^\mu = \frac{1}{\sqrt{2}} (1, 0, 1), \\ \epsilon^\mu(l') &= \frac{1}{\sqrt{2}} (1, 0, -1), \\ \epsilon^\mu(1) &= (0, 1, 0). \end{aligned} \quad (5C.2)$$

They allow us to form the three symmetric polarization tensors which satisfy the Hilbert condition:

$$\begin{aligned} &\epsilon^\mu(l) \epsilon^\nu(l) \\ &\epsilon^\mu(1) \epsilon^\nu(l) + (a \leftrightarrow b) \\ &\epsilon^\mu(1) \epsilon^\nu(1). \end{aligned} \quad (5C.3)$$

The first is proportional to $k^\mu k^\nu$, i.e., to a pure gauge of the form (5C.1) with $\xi^\mu = k^\mu$. The second is a pure gauge with $\xi^\mu = \epsilon^\mu(1)$. The third, finally, is equal to

$$\eta^{\mu\nu} - [\epsilon^\mu(l) \epsilon^\nu(l') + \epsilon^\mu(l') \epsilon^\nu(l)], \quad (5C.4)$$

which has the pure gauge form (5C.1) with $\xi^\mu = \epsilon^\mu(l')/\sqrt{2}|\mathbf{k}|$.

This implies that the three-dimensional gravitational field has no dynamical degrees of freedom. There exist no freely propagating gravitational waves in three spacetime dimensions.

A three-dimensional Einstein theory would have a further disease. It would not even possess a Newtonian weak-field limit. To see this, we suppose to have found a field $\phi^{\mu\nu}$ from the equation

$$\partial^2 \phi^{\mu\nu} = -2\kappa \overset{\text{m}}{T}{}^{\mu\nu}. \quad (5C.5)$$

From the solution we calculate in D -dimensions

$$h^{\mu\nu} = \phi^{\mu\nu} - \frac{1}{D-2} \eta^{\mu\nu} \phi. \quad (5C.6)$$

In order to guarantee Newton's equation of motion in the weak-field limit, it is necessary that a massive point particle at the origin produces a field h^{00} satisfying the Poisson differential equation

$$\partial^2 h^{00}(x) = GM\delta^{(3)}(\mathbf{x}). \quad (5C.7)$$

Moreover, $T^{\mu\nu}$ has only a T^{00} -component appearing in (5C.7). Hence $\phi^{\mu\nu}$ has only a single non-vanishing component ϕ^{00} . In three dimensions this implies that

$$h^{00} = \phi^{00} - \frac{1}{D-2} \eta^{00} \phi = \frac{D-3}{D-2} \phi^{00}. \quad (5C.8)$$

But ϕ^{00} must satisfy (5C.5)! Hence the Newton potential vanishes identically.

Another equivalent place where this disease manifests itself is in the coupling of the gravitational field $\phi^{\mu\nu}$ to the energy-momentum tensor of a massive particle. Since this coupling is

$$H^{\mu\nu} T_{\mu\nu}, \quad (5C.9)$$

we see that

$$h^{\mu\nu} T_{\mu\nu} = \left(\phi^{\mu\nu} - \frac{\eta_{ab}}{D-2} \phi \right) T_{\mu\nu} = \phi^{\mu\nu} \left(T_{\mu\nu} - \frac{\eta_{\mu\nu}}{D-2} T_{\lambda}^{\lambda} \right). \quad (5C.10)$$

With the particle being at rest and T_{ab} having only a 00-component, the interaction becomes

$$\phi^{00} \left(T_{00} - \frac{\eta_{00}}{D-2} T_{00} \right), \quad (5C.11)$$

which vanishes for $D = 3$.

Only by a technical trick can we obtain a nonzero limit. The theory has to be defined for continuous dimensions D in the neighborhood of 3 with a coupling constant which diverges at $D - 3$:

$$\kappa = \kappa_0 / (D - 3).$$

The above-described diseases are not a consequence of the linear approximation to gravity. We have mentioned before that in three dimensions, the full curvature tensor $R_{\mu\nu\lambda\kappa}$ is completely determined in terms of the Ricci tensor

$$R_{\mu\nu} = G_{\mu\nu} - \frac{1}{D-2} g_{\mu\nu} G, \quad (5C.12)$$

and thus in terms of the Einstein tensor $G_{\mu\nu} = \kappa T_{\mu\nu}$. Due to Einstein's equation $G_{\mu\nu} = \kappa \overset{m}{T}_{\mu\nu}$, the Ricci tensor $R_{\mu\nu}$ vanishes identically everywhere, except right at the mass point. This implies, in particular, that the empty-space field equation

$$G_{\mu\nu} = 0, \quad (5C.13)$$

which we have used in four dimensions to find the Schwarzschild metric, can have only the trivial solution $g_{\mu\nu} = \eta_{\mu\nu}$, up to an irrelevant reparametrization of spacetime.⁴

It is curious to note that this disease makes it possible to develop a quantum theory of gravity, in contrast to four dimensions where such a theory does not yet exist. Thus it is possible to define

⁴For a detailed discussion see S. Giddings, J. Abbott, and K. Kuchar, *Rel. Grav.* **16**, 751 (1986); see also S. Deser, R. Jackson, and S. Templeton, *Am. Phys. (NY)* **140**, 372 (1982).

a wave function for the universe. In the absence of matter, the entire Hilbert space consists only of one state, the vacuum $|0\rangle$.⁵

Let us take a look at gravitational waves in two dimensions. There the only polarization tensor satisfying Hilbert's constraint is

$$\epsilon^{\mu\nu}(k) = \frac{1}{|\mathbf{k}|^2} k^\mu k^\nu, \quad (5C.14)$$

and this is obviously a pure gauge. As far as the equation (5C.6) is concerned, the situation is even worse than in three dimensions. It is impossible to recover from $\phi^{\mu\nu}$ the metric $g_{\mu\nu}$ since the equation

$$h_{\mu\nu} = \phi_{\mu\nu} - \frac{\eta_{\mu\nu}}{D-2} \phi \quad (5C.15)$$

is meaningless for $D = 2$. In order to see the origin of the problem let us choose a gauge different from Hilbert's, and use the gauge freedom

$$\begin{aligned} h_{00} &\rightarrow h_{00} + 2\partial_0 \xi_0, \\ h_{01} &\rightarrow h_{01} + \partial_0 \xi_1 + \partial_1 \xi_0, \end{aligned} \quad (5C.16)$$

to make h_{00} and h_{01} vanish. For the remaining component $h_{11} \equiv h$ we find from (4.371) the Lagrangian density:

$$\stackrel{\text{f}}{\mathcal{L}} = \frac{1}{4} [(\partial h)^2 - 2(\partial_1 h)^2 + 2(\partial_1 h)^2 - (\partial h)^2] = 0, \quad (5C.17)$$

which vanishes identically. In fact, this property could have been anticipated. It is well known in differential geometry that, in two dimensions, the Einstein action

$$\stackrel{\text{f}}{\mathcal{A}} = \frac{1}{2\kappa} \int d^2\xi \sqrt{g} R \quad (5C.18)$$

is a pure surface term. By the Gauss-Bonnet theorem, it is entirely determined by the global topological properties of the space. For closed surfaces, it is equal to $(4\pi/2\kappa)(1-h)$, where h is the number of handles of the surface. This makes it impossible to derive equations of motion from such an action.

For completeness, let us compare the situation with the electromagnetism case. In three dimensions, the vector potential has three components minus one, due to the Lorentz condition. This leaves two degrees of freedom. One of them is a pure gauge mode, the other is physical. Hence there exists a freely propagating photon in three dimensions.

In two dimensions, the Lorenz gauge allows A^μ to be written in the form of a two-dimensional curl:

$$A^\mu = \epsilon^{\mu\nu} \partial_\nu \phi. \quad (5C.19)$$

In empty space, it satisfies the free field equation

$$\partial^2 A^\mu = 0. \quad (5C.20)$$

In terms of the field ϕ , the field strength is

$$F^{01} = \partial^0 A^1 - \partial^1 A^0 = -\partial^2 \phi. \quad (5C.21)$$

Note the relation with the theory of complex functions. For a zero field, ϕ is a harmonic function. It can therefore be considered as the real part of an analytic function

$$\phi(x) = \text{Re } f(z), \quad (5C.22)$$

⁵See H. Leutwyler, Phys. Rev. B *134*, 1755 (1964).

where

$$z = x + iy. \quad (5C.23)$$

The vector A^μ is the real part of the gradient of this function

$$A^\mu = \epsilon^{\mu\nu} \partial_\nu \operatorname{Re} f(z). \quad (5C.24)$$

Now, the real and imaginary part of f satisfy the Cauchy-Riemann differential equations

$$\begin{aligned} \partial_1 \operatorname{Re} f &= \partial_2 \operatorname{Im} f, \\ \partial_1 \operatorname{Im} f &= -\partial_2 \operatorname{Re} f. \end{aligned} \quad (5C.25)$$

Hence we can also write

$$A^\mu = \partial^\mu \operatorname{Im} f. \quad (5C.26)$$

This shows that A^μ is a pure gauge which, therefore, carries no electromagnetic field, in agreement with the assumption we started out from.

It is important to point out that the nonexistence of propagating electromagnetic waves does not rule out Coulomb forces. They do not need the exchange of physical electromagnetic waves. The exchange of virtual electromagnetic fields with zero momentum is sufficient. The inhomogeneous equation

$$\partial^2 A^\mu = -\frac{1}{c} j^\mu \quad (5C.27)$$

has, outside the charge distribution, only the solution $\partial^2 A^\mu = 0$, and we have seen before that the only field satisfying this is a pure gauge field. Still, the Maxwell equation

$$\partial_1 F^{01} = \frac{1}{2} j^0 \quad (5C.28)$$

allows a nonvanishing constant field:

$$F^{01} = \text{const.} \quad (5C.29)$$

It is carried by the $k = 0$ -components of A_μ to which the previous polarization discussions do not apply. It is this component which gives rise to the Coulomb force in two spacetime dimensions. Another way to see this is by considering the Maxwell action

$$\mathcal{A} = \frac{1}{2c} \int d^2 x F_{ab} F^{\mu\nu} + \frac{1}{c^2} \int d^2 x j^\mu A_\mu, \quad (5C.30)$$

and by going to the Lorenz gauge,

$$A^\mu = \epsilon^{\mu\nu} \partial_\nu \phi, \quad (5C.31)$$

in which it becomes (up to surface terms)

$$\mathcal{A} = \frac{1}{2c} \int d^2 x (\partial^2 \phi)^2 + \frac{1}{c^2} \int d^2 x \epsilon^{\mu\nu} (\partial_\mu j_\nu) \phi. \quad (5C.32)$$

Extremizing this in the field ϕ gives the field equation

$$(\partial^2)^2 \phi = \frac{1}{c} \epsilon^{\mu\nu} \partial_\mu j_\nu. \quad (5C.33)$$

Reinserting this into the action, the extremum is found to be

$$\mathcal{A}_{\text{extr}} = \frac{1}{c^2} \int d^2x \epsilon^{\mu\nu} \partial_\mu j_\nu \frac{1}{(\partial^2)^2} \epsilon^{\mu'\nu'} \partial_{\mu'} j_{\nu'}. \quad (5C.34)$$

Using

$$\epsilon^{\mu\nu} \epsilon^{\mu'\nu'} = \eta^{\mu\mu'} \eta^{\nu\nu'} - \eta^{\mu\nu'} \eta^{\nu\mu'}, \quad (5C.35)$$

performing a partial integration, and taking advantage of the current conservation law $\partial_\mu j^\mu = 0$, this becomes

$$\mathcal{A}_{\text{extr}} = \frac{1}{c^2} \int d^2x j_\mu \frac{1}{\partial^2} j^\mu, \quad (5C.36)$$

which is precisely the Biot-Savart interaction law between currents. Using once more current conservation in the form

$$\begin{aligned} \int d^2x (j^{02} - j^{12}) &= \int d^2x \left[j^{02} - \partial_1 j^1 \frac{1}{(-\partial_1)^2} \partial_1 j^1 \right] \\ &= \int d^2x \left[\partial_1 j^0 \frac{1}{(-\partial_1)^2} \partial_1 j^0 - \partial_0 j^0 \frac{1}{(-\partial_1)^2} \partial_0 j^0 \right] \\ &= \int d^2x j^0 \frac{\partial^2}{(-\partial_1)^2} j^0, \end{aligned} \quad (5C.37)$$

we can rewrite (5C.36) as

$$\mathcal{A}_{\text{extr}} = \frac{1}{2c^2} \int d^2x j^0 \frac{1}{(-\partial_1)^2} j^0. \quad (5C.38)$$

This is an *instantaneous* linear potential between the charges carried by j_0 . It is due to the constant electric field F^μ allowed in empty space.

In this respect, the situation is quite different from the gravitational case in three dimensions. There the absence of $R_{\mu\nu}$ outside a mass distribution implies a vanishing of the gauge invariant curvature tensor $R_{\mu\nu\lambda\kappa}$ and hence the vanishing of all tidal forces.

Appendix 5D Precession of Gyroscope in a Satellite Orbit

In a comoving frame, the tidal forces cause a precession of a rotating body proportional to its quadrupole moment Q^{kl} . A rotating body without a quadrupole moment does not precess in free fall. However, if we observe such a gyroscope from another frame of reference, for example from a distance observer where the metric is asymptotically flat, the spin vector n^μ does show precession.

Geodetic Precession

In order to be specific, consider a gyroscope in a circular satellite orbit around the earth and let n^i be the unit vector along which its spin points. Its equation of motion is most simple in a comoving frame of reference x'^μ since there $\tau = t$ and $dx'^\mu/dt = c(1, 0, 0, 0)$. In addition, the spin has only spatial components so that the convenient equation of motion $Dn^\mu/d\tau = 0$ reduces to

$$\frac{dn'^i}{dt'} = -\bar{\Gamma}_{0j}{}^{i'} c n'^j. \quad (5D.1)$$

It is possible to use this equation and calculate from it the precession rate of n'^i with respect to the distant star. For this we go into a comoving frame which maintains a fixed orientation with

respect to the distant stars. This is not a falling frame, so that its Christoffel symbols do not vanish, leading to a non-zero precession rate with respect to the distant stars.

Let us focus attention upon a fixed time t'_0 where the orbit is parallel to the x -axis in a coordinate frame anchored to the fixed star. Assume the earth to lie below the gyroscope on the z -axis, at a distance r . The gyroscope will experience an acceleration

$$a = -\frac{GM}{r^2} \quad (5D.2)$$

along the z -axis. Let the velocity with respect to the fixed star be $\mathbf{v} = v\mathbf{e}_x$. It is easy to calculate, for the instant t'_0 , the coordinate transformation to the comoving frame of reference. The motion is stopped by going to the new Lorentz frame with coordinates

$$\begin{aligned} x^0 &= x'^0 + \frac{v}{c}x'^1, \\ x^1 &= x'^1 + \frac{v}{c}x'^0, \\ x^2 &= x'^2, \\ x^3 &= x'^3. \end{aligned} \quad (5D.3)$$

We have assumed $v \ll c$, for simplicity. The acceleration along the negative z -direction is removed by an additional transformation

$$\begin{aligned} x^1 &= x'^1, \\ x^2 &= x'^2, \\ x^3 &= x'^3 + \frac{a}{2c^2}(x'^0)^2. \end{aligned} \quad (5D.4)$$

It is useful to define the comoving frame x', z' such that the transformed metric $g'_{\mu\nu}$ is Minkowskian. This is achieved by the following transformation of time:

$$x^0 = x'^0 + \frac{v}{c}x'^1 + \frac{a}{c^2}x'^0x'^3. \quad (5D.5)$$

The total transformation has the matrix form

$$\frac{\partial x^a}{\partial x'^b} = \begin{pmatrix} 1 + ax'^3/c^2 & v/c & 0 & ax'^0/c^2 \\ v/c & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ ax'^0/c^2 & 0 & 0 & 1 \end{pmatrix} = \alpha^a_b. \quad (5D.6)$$

When subjecting to this transformation the almost Minkowskian metric $g_{ab} = \eta_{ab} + h_{ab}$ around the earth, we obtain

$$\begin{aligned} g'_{ab} &= \frac{\partial x^c}{\partial x'^a} \frac{\partial x^d}{\partial x'^b} g_{cd} \\ &= \alpha^c_a \alpha^d_b \eta_{cd} + \alpha^c_b \alpha^d_a h_{cd}. \end{aligned} \quad (5D.7)$$

Neglecting quantities of the order a^2 and aGM/r , this becomes

$$g'_{ab} = \eta_{ab} + h_{ab} + \begin{pmatrix} 0 & -\frac{4v}{c} \frac{GM}{c^2 r} & 0 & 0 \\ -\frac{4v}{c} \frac{GM}{c^2 r} & 0 & 0 & \frac{v}{c} \frac{a}{c^2} x'^0 \\ 0 & 0 & 0 & 0 \\ 0 & \frac{v}{c} \frac{a}{c^2} x'^0 & 0 & 0 \end{pmatrix}. \quad (5D.8)$$

Adding the weak gravitational field of the earth, the metric reads

$$g'_{ab} = \begin{pmatrix} 1 - 2\frac{GM}{c^2 r} & -\frac{4v}{c} \frac{GM}{c^2 r} & 0 & 0 \\ -\frac{4v}{c} \frac{GM}{c^2 r} & -1 - \frac{2GM}{c^2 r} & 0 & \frac{v}{c} \frac{a}{c^2} x'^0 \\ 0 & 0 & -1 - \frac{2GM}{c^2 r} & 0 \\ 0 & \frac{v}{c} \frac{a}{c^2} x'^0 & 0 & -1 - \frac{2GM}{c^2 r} \end{pmatrix}. \quad (5D.9)$$

From this we calculate the Christoffel symbols

$$\bar{\Gamma}_{03}{}^{1'} = -\bar{\Gamma}_{01}{}^{3'} = -2\frac{v}{c} \frac{GM}{c^2 r^2} - \frac{1}{2} \frac{v}{c} \frac{a}{c^2}. \quad (5D.10)$$

All other components vanish.

The second term has a purely kinematic origin related to the Thomas precession. Inserting (5D.2) we see that it removes 1/4 of the first term caused by the gravitational field,

$$\bar{\Gamma}_{03}{}^{1'} = -\bar{\Gamma}_{01}{}^{3'} = -\frac{3}{2} \frac{v}{c} \frac{GM}{c^2 r^2}. \quad (5D.11)$$

Going back to (5D.1) we find that the rate of change of the spin direction in the comoving frame is given by

$$\begin{aligned} \frac{dn'^1}{dt'} &= \frac{3}{2} \frac{v}{c} \frac{GM}{c^2 r^2} n'^3, \\ \frac{dn'^2}{dt'} &= 0, \end{aligned} \quad (5D.12)$$

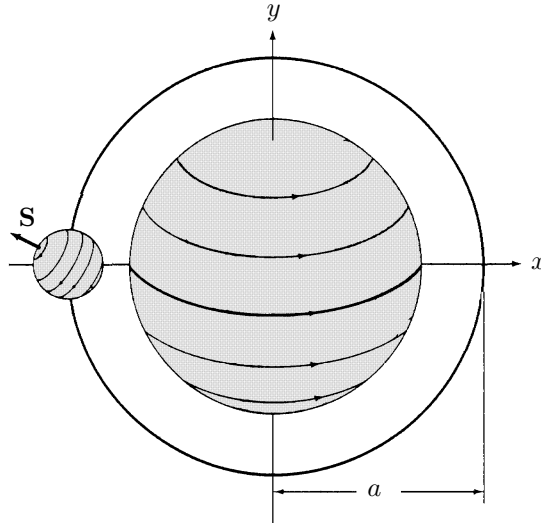


FIGURE 5.13 Gyroscope carrying a frame x', z' around the equator with a fixed orientation with respect to the fixed stars. In an elaborate experiment “Gravity Probe B” launched on April 20, 2004 from Vandenberg air base, gyroscopes were launched into polar orbits whose axes point towards IM Pegasi. If Einstein is correct the axis of rotation of the gyroscope should move by an angle which is as small as the diameter of a hair seen from 1/4 mile away [14].

$$\frac{dn'^3}{dt'} = -\frac{3}{2} \frac{v}{c} \frac{GM}{cr^2} n'^1.$$

In vector notation, this reads

$$\frac{d\mathbf{n}'}{dt'} = \left(\frac{3}{2} \frac{GM}{c^2 r^3} \mathbf{x} \times \mathbf{v} \right) \times \mathbf{n}' \equiv \mathbf{\Omega}_G \times \mathbf{n}', \quad (5D.13)$$

where $\mathbf{\Omega}_G$ is the angular velocity vector of the geodetic precession. The result can also be expressed in terms of the gravitational acceleration vector $\dot{\mathbf{v}}$ as follows

$$\frac{d\mathbf{n}'}{dt'} = \frac{3}{2c^2} (\mathbf{v} \times \dot{\mathbf{v}}) \times \mathbf{n}'. \quad (5D.14)$$

In this form, the result was first obtained by de Sitter in 1916 [15].

Equation (5D.14) may also be interpreted in another way. Since the spin directions can be used to define the orientation of freely falling frames of reference, Eq. (5D.14) tells us how such a frame of reference is rotating with respect to the distant stars.

Just as in atomic physics, we may interpret this result as being the consequence of a gravitational spin-orbit interaction energy

$$U = \frac{2GM}{mc^2 r^3} \mathbf{L} \cdot \mathbf{S} = \frac{2}{mc^2} \frac{1}{r} \frac{\partial U}{\partial r}, \quad (5D.15)$$

which must be corrected by the Thomas precession by replacing the number 2 by $2 - 1/2 = 3/2$.

Note that the existence of such a spin-orbit interaction causes spinning particles to show an apparent violation of the equivalence principle: spinning electrons, protons, etc., *do not* move along geodesics.

For a gyroscope 500 miles above the earth in a polar orbit with a spin orthogonal to the angular momentum (i.e., in the plane of the orbit), the rate of precession is maximal and has the value

$$\frac{3}{2} \frac{GM}{c^2 r^2} \sqrt{\frac{GM}{r}} \approx \frac{6.9''}{\text{year}}. \quad (5D.16)$$

If the spin is parallel to the angular momentum, there is no precession.

Lense-Thirring or Frame-Dragging Precession

These results are only true if we neglect the rotation of the earth around its axis. After the preparatory work in the last section it is easy to take also this effect into account. According to Eq. (5D.9), the gravitational field of the rotating earth has the additional matrix elements:

$$h^{0i} = 2 \frac{G}{r^3} (\mathbf{x} \times \mathbf{S}_E)^i = 2 \frac{G}{r^3} \epsilon^{ijk} x^j S_E^k, \quad (5D.17)$$

where $\mathbf{S}_E$ is the spin angular momentum of the earth. It contributes to the Christoffel symbol a term

$$\bar{\Gamma}_{0j}{}^{i'} = \frac{1}{2} (\partial_j k_{0i} - \partial_i k_{0j}) = -G \epsilon_{ijk} \epsilon_{klm} \partial_l \epsilon^{nms} \frac{x^m}{r^3} S_E^s, \quad (5D.18)$$

which leads to the following contribution to dn'^i/dt' :

$$-\bar{\Gamma}_{0j}{}^{i'} n'^j = \epsilon_{ijl} \frac{G}{r^3} \left[S_E^l - \frac{3x^l}{r^2} (\mathbf{S}_E \cdot \mathbf{x}) \right] n'^j. \quad (5D.19)$$

Writing this as $\Delta \mathbf{\Omega} \times \mathbf{n}'$, we read off the additional precession rate

$$\Delta \mathbf{\Omega} = -\frac{G}{r^3} \left[\mathbf{S}_E - \frac{3\mathbf{x}}{r^2} (\mathbf{x} \cdot \mathbf{S}_E) \right]. \quad (5D.20)$$

This is the *frame-dragging* or *Lense-Thirring effect* [16].

For a gyroscope in polar orbit with the spin axis parallel to the angular momentum, this gives the only contribution to the precession rate of $0.05''$ per year. For nonpolar orbits it is negligible compared with the much larger geodetic precession.

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6

Relativistic Particles and Fields in External Electromagnetic Potential

Given the classical field theory of relativistic particles, we may ask which quantum phenomena arise in a relativistic generalization of the Schrödinger theory of atoms. In a first step we shall therefore study the behavior of the Klein-Gordon and Dirac equations in an external electromagnetic field. Let $A_\mu(x)$ be the four-vector potential that accounts for electric and magnetic field strengths via the equations (4.230) and (4.231). For classical relativistic point particles, an interaction with these external fields is introduced via the so-called *minimal substitution rule*, whose gauge origin and experimental consequences will now be discussed.

An important property of the electromagnetic field is its description in terms of a vector potential $A^\mu(x)$ and the gauge invariance of this description. In Eqs. (4.233) and (4.234) we have expressed electric and magnetic field strength as components of a four-curl $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ of a vector potential $A_\mu(x)$. This four-curl is invariant under gauge transformations

$$A_\mu(x) \rightarrow A_\mu(x) + \partial_\mu \Lambda(x). \quad (6.1)$$

The gauge invariance restricts strongly the possibilities of introducing electromagnetic interactions into particle dynamics and the Lagrange densities (6.92) and (6.94) of charged scalar and Dirac fields. We shall see that the origin of the minimal substitution rule lies precisely in the gauge-invariance of the vector-potential description of electromagnetism.

6.1 Charged Point Particles

A free relativistic particle moving along an arbitrarily parametrized path $x^\mu(\tau)$ in four-space is described by an action

$$\mathcal{A} = -Mc \int d\tau \sqrt{\dot{q}^\mu(\tau) \dot{q}_\mu(\tau)}. \quad (6.2)$$

The physical time along the path is given by $q^0(\tau) = ct$, and the physical velocity by $\mathbf{v}(t) \equiv d\mathbf{q}(t)/dt$. In terms of these, the action reads:

$$\mathcal{A} = \int dt L(t) \equiv -Mc^2 \int dt \left[1 - \frac{\mathbf{v}^2(t)}{c^2} \right]^{1/2}. \quad (6.3)$$

6.1.1 Coupling to Electromagnetism

If the particle has a charge e and lies at rest at some position $\mathbf{x}$, its electric potential energy is

$$V(\mathbf{x}, t) = e\phi(\mathbf{x}, t) \quad (6.4)$$

where

$$\phi(\mathbf{x}, t) = A^0(\mathbf{x}, t). \quad (6.5)$$

In our convention, the charge of the electron e has a negative value to be in agreement with the sign in the historic form of the Maxwell equations:

$$\begin{aligned} \nabla \cdot \mathbf{E}(x) &= -\nabla^2 \phi(x) = \rho(x), \\ \nabla \times \mathbf{B}(x) - \dot{\mathbf{E}}(x) &= \nabla \times \nabla \times \mathbf{A}(x) - \dot{\mathbf{E}}(x) \\ &= -[\nabla^2 \mathbf{A}(x) - \nabla \cdot \nabla \mathbf{A}(x)] - \dot{\mathbf{E}}(x) = \frac{1}{c} \mathbf{j}(x). \end{aligned} \quad (6.6)$$

If the electron moves along a trajectory $\mathbf{q}(t)$, its potential energy is

$$V(t) = e\phi(\mathbf{q}(t), t). \quad (6.7)$$

In the Lagrangian $L = T - V$, this contributes with the opposite sign

$$L^{\text{int}}(t) = -eA^0(\mathbf{q}(t), t), \quad (6.8)$$

giving a potential part of the interaction

$$\mathcal{A}_{\text{pot}}^{\text{int}} = -e \int dt A^0(\mathbf{q}(t), t). \quad (6.9)$$

Since the time t coincides with $q^0(\tau)/c$ of the trajectory, this can be expressed as

$$\mathcal{A}_{\text{pot}}^{\text{int}} = -\frac{e}{c} \int dq^0 A^0. \quad (6.10)$$

In this form it is now quite simple to write down the complete electromagnetic interaction purely on the basis of relativistic invariance. The direct invariant extension of (6.11) is obviously

$$\mathcal{A}^{\text{int}} = -\frac{e}{c} \int dq^\mu A_\mu(q). \quad (6.11)$$

Thus, the full action of a point particle can be written in covariant form as

$$\mathcal{A} = -Mc \int d\tau \sqrt{\dot{q}^\mu(\tau) \dot{q}_\mu(\tau)} - \frac{e}{c} \int dq^\mu A_\mu(q), \quad (6.12)$$

or more explicitly as

$$\mathcal{A} = \int dt L(t) = -Mc^2 \int dt \left[1 - \frac{\mathbf{v}^2}{c^2} \right]^{1/2} - e \int dt \left(A^0 - \frac{1}{c} \mathbf{v} \cdot \mathbf{A} \right). \quad (6.13)$$

The canonical formalism supplies us with the canonically conjugate momenta

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = M \frac{\mathbf{v}}{\sqrt{1 - \mathbf{v}^2/c^2}} + \frac{e}{c} \mathbf{A} \equiv \mathbf{p} + \frac{e}{c} \mathbf{A}. \quad (6.14)$$

The Euler-Lagrange equation obtained by extremizing this equation is

$$\frac{d}{dt} \frac{\partial L}{\partial \mathbf{v}(t)} = \frac{\partial L}{\partial \mathbf{q}(t)}, \quad (6.15)$$

or

$$\frac{d}{dt} \mathbf{p}(t) = -\frac{e}{c} \frac{d}{dt} \mathbf{A}(\mathbf{q}(t), t) - e \nabla A^0(\mathbf{q}(t), t) + \frac{e}{c} v^i \nabla A^i(\mathbf{q}(t), t). \quad (6.16)$$

We now split

$$\frac{d}{dt} \mathbf{A}(\mathbf{q}(t), t) = (\mathbf{v}(t) \cdot \nabla) \mathbf{A}(\mathbf{q}(t), t) + \frac{\partial}{\partial t} \mathbf{A}(\mathbf{q}(t), t), \quad (6.17)$$

and obtain

$$\frac{d}{dt} \mathbf{p}(t) = -\frac{e}{c} (\mathbf{v}(t) \cdot \nabla) \mathbf{A}(\mathbf{q}(t), t) - \frac{e}{c} \frac{\partial}{\partial t} \mathbf{A}(\mathbf{q}(t), t) - e \nabla A^0(\mathbf{q}(t), t) + \frac{e}{c} v^i \nabla A^i(\mathbf{q}(t), t). \quad (6.18)$$

The right-hand side contains the electric and magnetic fields (4.235) and (4.236), in terms of which it takes the well-known form

$$\frac{d}{dt} \mathbf{p} = e \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right). \quad (6.19)$$

This can be rewritten in terms of the proper time $\tau \equiv t/\gamma$ as

$$\frac{d}{d\tau} \mathbf{p} = \frac{e}{Mc} \left(\mathbf{E} p^0 + \mathbf{p} \times \mathbf{B} \right), \quad (6.20)$$

Recalling Eqs. (4.233) and (4.234), this is recognized as the spatial part of the covariant equation

$$\frac{d}{d\tau} p^\mu = \frac{e}{Mc} F^\mu{}_\nu p^\nu. \quad (6.21)$$

The temporal component of this equation

$$\frac{d}{d\tau} p^0 = \frac{e}{Mc} \mathbf{E} \cdot \mathbf{p} \quad (6.22)$$

gives the energy increase of a particle running through an electromagnetic field. In real time this is

$$\frac{d}{dt} p^0 = e \mathbf{E} \cdot \frac{\mathbf{v}}{c}. \quad (6.23)$$

Combining this with (6.19), we find the acceleration

$$\frac{d}{dt} \mathbf{v}(t) = c \frac{d}{dt} \frac{\mathbf{p}}{p^0} = \frac{e}{\gamma M} \left[\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} - \frac{\mathbf{v}}{c} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{E} \right) \right]. \quad (6.24)$$

The velocity is related to the canonical momenta and external field via

$$\frac{\mathbf{v}}{c} = \frac{\mathbf{P} - \frac{e}{c}\mathbf{A}}{\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2}}. \quad (6.25)$$

This can be used to calculate the Hamiltonian via the Legendre transform

$$H = \frac{\partial L}{\partial \mathbf{v}} \mathbf{v} - L = \mathbf{P} \cdot \mathbf{v} - L, \quad (6.26)$$

giving

$$H = c\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2} + eA^0. \quad (6.27)$$

In the non-relativistic limit this has the expansion

$$H = mc^2 + \frac{1}{2m}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + eA^0 + \dots \quad (6.28)$$

Thus, the free theory goes over into the interacting theory by the *minimal substitution rule*

$$\mathbf{p} \rightarrow \mathbf{p} - \frac{e}{c}\mathbf{A}, \quad H \rightarrow H - \frac{e}{c}A^0, \quad (6.29)$$

or, in relativistic notation:

$$p^\mu \rightarrow p^\mu - \frac{e}{c}A^\mu. \quad (6.30)$$

6.1.2 Spin Precession in an Atom

In 1926, Uhlenbeck and Goudsmit noticed that the observed Zeeman splitting of atomic levels could be explained by an electron of spin $\frac{1}{2}$. Its magnetic moment is usually expressed in terms of the combination of fundamental constants which have the dimension of a magnetic moment, the *Bohr magneton* $\mu_B = e\hbar/Mc$. It reads

$$\boldsymbol{\mu} = g\mu_B \frac{\mathbf{S}}{\hbar}, \quad \mu_B \equiv \frac{e\hbar}{2Mc}, \quad (6.31)$$

where $\mathbf{S} = \boldsymbol{\sigma}/2$ is the spin matrix which has the commutation rules

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k, \quad (6.32)$$

and g is a dimensionless number called the *gyromagnetic ratio* or *Landé factor*.

If an electron moves in an orbit under the influence of a torque-free central force, as an electron does in the Coulomb field of an atomic nucleus, the total angular momentum is conserved. The spin, however, shows a precession just like a spinning

top. This precession has two main contributions: one is due to the magnetic coupling of the magnetic moment of the spin to the magnetic field of the electron orbit, called *spin-orbit coupling*. The other part is purely kinematic, it is the Thomas precession discussed in Section (4.15), caused by the slightly relativistic nature of the electron orbit.

The spin-orbit splitting of the atomic energy levels (to be pictured and discussed further in Fig. 6.1) is caused by a magnetic interaction energy

$$H^{LS}(r) = \frac{g}{2M^2c^2} \mathbf{S} \cdot \mathbf{L} \frac{1}{r} \frac{dV(r)}{dr}, \quad (6.33)$$

where $V(r)$ is the atomic potential depending only on $r = |\mathbf{x}|$. To derive this $H^{LS}(r)$, we note that the spin precession of the electron at rest in a given magnetic field $\mathbf{B}$ is given by the *Heisenberg equation*

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\mu} \times \mathbf{B}, \quad (6.34)$$

where $\boldsymbol{\mu}$ is the magnetic moment of the electron. In an atom, the magnetic field in the rest frame of the electron is entirely due to the electric field in the rest frame of the atom. A Lorentz transformation (4.286) that boosts an electron at rest to a velocity $\mathbf{v}$ produces a magnetic field in the electron's rest frame:

$$\mathbf{B} = \mathbf{B}_{\text{el}} = -\gamma \frac{\mathbf{v}}{c} \times \mathbf{E}, \quad \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}. \quad (6.35)$$

Since an atomic electron has a small velocity ratio v/c which is of the order of the fine-structure constant $\alpha \approx 1/137$, the field has the approximate size

$$\mathbf{B}_{\text{el}} \approx -\frac{\mathbf{v}}{c} \times \mathbf{E}. \quad (6.36)$$

The electric field gives the electron an acceleration

$$\dot{\mathbf{v}} = \frac{e}{M} \mathbf{E}, \quad (6.37)$$

so that we may also write

$$\mathbf{B}_{\text{el}} \approx -\frac{Mc}{e} \frac{1}{c^2} \mathbf{v} \times \dot{\mathbf{v}}, \quad (6.38)$$

and Heisenberg's precession equation (6.34) as

$$\frac{d\mathbf{S}}{dt} \approx \frac{g}{2c^2} (\mathbf{v} \times \dot{\mathbf{v}}) \times \mathbf{S}. \quad (6.39)$$

This can be expressed in the form

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\Omega}_{LS} \times \mathbf{S}, \quad (6.40)$$

where $\boldsymbol{\Omega}_{LS}$ is the angular velocity of the spin precession caused by the orbital magnetic field in the rest frame of the electron:

$$\boldsymbol{\Omega}_{LS} \equiv \frac{g}{2c^2} \mathbf{v} \times \dot{\mathbf{v}}. \quad (6.41)$$

In the rest frame of the atom where the electron is accelerated towards the center along its orbit, this result receives a relativistic correction. To lowest order in $1/c$, we must add to $\boldsymbol{\Omega}_{LS}$ the angular velocity $\boldsymbol{\Omega}_T$ of the Thomas precession, such that the total angular velocity of precession becomes

$$\boldsymbol{\Omega} = \boldsymbol{\Omega}_{LS} + \boldsymbol{\Omega}_T \approx \frac{g-1}{2} \mathbf{v} \times \dot{\mathbf{v}}. \quad (6.42)$$

Since g is very close to 2, the Thomas precession explains why the spin-orbit splitting was initially found to be in agreement with a normal gyromagnetic ratio $g = 1$, the characteristic value for a rotating charged sphere.

If there is also an external magnetic field, this is transformed to the electron rest frame by a Lorentz transformation (4.283), where it leads to an approximate equation of motion for the spin

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\mu} \times \mathbf{B}' \approx \boldsymbol{\mu} \times \left(\mathbf{B} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right). \quad (6.43)$$

Expressing $\boldsymbol{\mu}$ via Eq. (6.31), this becomes

$$\frac{d\mathbf{S}}{dt} \equiv -\mathbf{S} \times \boldsymbol{\Omega}_{\text{em}} \approx \frac{eg}{2Mc} \mathbf{S} \times \left(\mathbf{B} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right). \quad (6.44)$$

This equation defines the frequency $\boldsymbol{\Omega}_{\text{em}}$ of precession due to the magnetic and electric fields in the rest frame of the electron. Expressing $\mathbf{E}$ in terms of the acceleration via Eq. (6.37), this becomes

$$\frac{d\mathbf{S}}{dt} \approx \frac{g}{2Mc} \mathbf{S} \times \left[e\mathbf{B} - \frac{M}{c} (\mathbf{v} \times \dot{\mathbf{v}}) \right]. \quad (6.45)$$

The acceleration can be expressed in terms of the central Coulomb potential $V(r)$ as

$$\dot{\mathbf{v}} = -\frac{\mathbf{x}}{r} \frac{1}{M} \frac{dV}{dr}. \quad (6.46)$$

The spin precession rate in the electron's rest frame is

$$\frac{d\mathbf{S}}{dt} = \frac{g}{2Mc} \mathbf{S} \times \left(e\mathbf{B} + \mathbf{v} \times \frac{\mathbf{x}}{r} \frac{1}{c} \frac{dV}{dr} \right) = \frac{g}{2Mc} \mathbf{S} \times \left(e\mathbf{B} - \frac{1}{Mc} \mathbf{L} \frac{dV}{dr} \right). \quad (6.47)$$

There exists a simple Hamiltonian operator for the spin-orbit interaction $H^{\text{LS}}(t)$, from which this equation can be derived via Heisenberg's equation (1.280):

$$\dot{\mathbf{S}}(t) = \frac{i}{\hbar} [\mathbf{S}(t), H^{\text{LS}}(t)]. \quad (6.48)$$

The operator is

$$\begin{aligned} H^{LS}(r) &= -\boldsymbol{\mu} \cdot \left(\mathbf{B} - \frac{1}{Mc} \mathbf{L} \frac{dV}{dr} \right) \\ &= -\frac{ge}{2Mc} \mathbf{S} \cdot \mathbf{B} + \frac{g}{2M^2c^2} \mathbf{S} \cdot \mathbf{L} \frac{1}{r} \frac{dV}{dr}. \end{aligned} \quad (6.49)$$

Indeed, using the commutation rules (6.32), we find immediately (6.46). Historically, the interaction energy (6.49) was used to explain the experimental level splittings assuming a gyromagnetic ratio $g \approx 1$ for the electron.

Without the external magnetic field, the angular velocity of precession caused by spin-orbit coupling is

$$\boldsymbol{\Omega}_{LS} = \frac{g}{2M^2c^2} \mathbf{L} \frac{1}{r} \frac{\partial V}{\partial r}. \quad (6.50)$$

It was realized by Thomas in 1927 that the relativistic motion of the electron changes the factor g to $g - 1$, as in (6.42), so that the true precession frequency is

$$\boldsymbol{\Omega} = \boldsymbol{\Omega}_{LS} + \boldsymbol{\Omega}_T = \frac{g - 1}{2M^2c^2} \mathbf{L} \frac{1}{r} \frac{\partial V}{\partial r}. \quad (6.51)$$

This implied that the experimental data should give $g - 1 \approx 1$, so that g is really twice as large as expected for a rotating charged sphere. Indeed, the value $g \approx 2$ was predicted by the Dirac theory of the electron.

In Section 12.15 we shall find that the magnetic moment of the electron has a g -factor slightly larger than the Dirac value 2, the relative deviations $a \equiv (g - 2)/2$ being defined as the *anomalous magnetic moments*. From measurements of the above precession rate, experimentalists have deduced the values

$$a(e^-) = (115\,965.77 \pm 0.35) \times 10^{-8}, \quad (6.52)$$

$$a(e^+) = (116\,030 \pm 120) \times 10^{-8}, \quad (6.53)$$

$$a(\mu^\pm) = (116\,616 \pm 31) \times 10^{-8}. \quad (6.54)$$

In quantum electrodynamics, the gyromagnetic ratio will receive further small corrections, as will be discussed in detail in Chapter 12.

6.1.3 Relativistic Equation of Motion for Spin Vector and Thomas Precession

If an electron moves in an orbit under the influence of a torque-free central force, such as an electron in the Coulomb field of an atomic nucleus, the total angular momentum is conserved. The spin, however, performs a Thomas precession as discussed in the previous section. There exists a covariant equation of motion for the spin four-vector introduced in Eq. (4.767) which describes this precession. Along a particle orbit parametrized by a parameter τ , for instance the proper time, we form

the derivative with respect to τ , assuming that the motion proceeds at a fixed total angular momentum:

$$\frac{d\hat{S}_\mu}{d\tau} = \epsilon_{\mu\nu\lambda\kappa} \hat{J}^{\nu\lambda} \frac{dp^\kappa}{d\tau}. \quad (6.55)$$

The right-hand side can be simplified by multiplying it with the trivial expression

$$\frac{1}{M^2 c^2} g^{\sigma\tau} p_\sigma p_\tau = 1. \quad (6.56)$$

Now we use the identity for the ϵ -tensor

$$\epsilon_{\mu\nu\lambda\kappa} g_{\sigma\tau} = \epsilon_{\mu\nu\lambda\sigma} g_{\kappa\tau} + \epsilon_{\mu\nu\sigma\kappa} g_{\lambda\tau} + \epsilon_{\mu\sigma\lambda\kappa} g_{\nu\tau} + \epsilon_{\sigma\nu\lambda\kappa} g_{\mu\tau}, \quad (6.57)$$

which can easily be verified using the antisymmetry of the ϵ -tensor and considering $\mu\nu\lambda\kappa = 0123$. Then the right-hand side becomes a sum of the four terms

$$\frac{1}{M^2 c^2} \left(\epsilon_{\mu\nu\lambda\sigma} J^{\nu\lambda} p^\sigma p'^\kappa + \epsilon_{\mu\nu\sigma\kappa} J^{\nu\lambda} p_\lambda p^\sigma p'^\kappa + \epsilon_{\mu\sigma\lambda\kappa} J^{\nu\lambda} p_\nu p^\sigma p'^\kappa + \epsilon_{\sigma\nu\lambda\kappa} J^{\nu\lambda} p^\sigma p_\mu p'^\kappa \right), \quad (6.58)$$

where $p'^\mu \equiv dp^\mu/d\tau$. The first term vanishes, since $p^\kappa p'_\kappa = (1/2)dp^2/d\tau = (1/2)dM^2 c^2/d\tau = 0$. The last term is equal to $-\hat{S}_\kappa p'^\kappa p_\mu/M^2 c^2$. Inserting the identity (6.57) into the second and third terms, we obtain twice the left-hand side of (6.55). Taking this to the left-hand side, we find the equation of motion

$$\frac{dS_\mu}{d\tau} = -\frac{1}{M^2 c^2} S_\lambda \frac{dp^\lambda}{d\tau} p_\mu. \quad (6.59)$$

Note that on account of this equation, the time derivative $dS_\mu/d\tau$ points in the direction of p^μ .

Let us verify that this equation yields indeed the Thomas precession. Denoting the derivatives with respect to the time $t = \gamma\tau$ by a dot, we can rewrite (6.59) as

$$\dot{\mathbf{S}} \equiv \frac{d\mathbf{S}}{dt} = \frac{1}{\gamma} \frac{d\mathbf{S}}{d\tau} = -\frac{1}{M^2 c^2} \left(S^0 \dot{p}^0 + \mathbf{S} \cdot \dot{\mathbf{p}} \right) \mathbf{p} = \frac{\gamma^2}{c^2} (\mathbf{S} \cdot \dot{\mathbf{v}}) \mathbf{v}, \quad (6.60)$$

$$\dot{S}_0 \equiv \frac{dS_0}{dt} = \frac{1}{c} \frac{d}{d\tau} (\mathbf{S} \cdot \mathbf{v}) = \frac{\gamma^2}{c^2} (\mathbf{S} \cdot \dot{\mathbf{v}}). \quad (6.61)$$

We now differentiate Eq. (4.780) with respect to the time using the relation $\dot{\gamma} = \gamma^3 \dot{\mathbf{v}} \cdot \mathbf{v}/c^2$, and find

$$\dot{\mathbf{S}}_R = \dot{\mathbf{S}} - \frac{\gamma}{\gamma+1} \frac{1}{c^2} \dot{S}_0 \mathbf{v} - \frac{\gamma}{\gamma+1} \frac{1}{c^2} S^0 \dot{\mathbf{v}} - \frac{\gamma^3}{(\gamma+1)^2} \frac{1}{c^4} (\mathbf{v} \cdot \dot{\mathbf{v}}) S^0 \mathbf{v}. \quad (6.62)$$

Inserting here Eqs. (6.60) and (6.61), we obtain

$$\dot{\mathbf{S}}_R = \frac{\gamma^2}{\gamma+1} \frac{1}{c^2} (\mathbf{S} \cdot \dot{\mathbf{v}}) \mathbf{v} - \frac{\gamma}{\gamma+1} \frac{1}{c^2} S^0 \dot{\mathbf{v}} - \frac{\gamma^3}{(\gamma+1)^2} (\mathbf{v} \cdot \dot{\mathbf{v}}) S^0 \mathbf{v}. \quad (6.63)$$

On the right-hand side we return to the spin vector $\mathbf{S}_R$ using Eqs. (4.779) and (4.782), and find

$$\dot{\mathbf{S}}_R = \frac{\gamma^2}{\gamma + 1} \frac{1}{c^2} [(\mathbf{S}_R \cdot \dot{\mathbf{v}})\mathbf{v} - (\mathbf{S}_R \cdot \mathbf{v})\dot{\mathbf{v}}] = \boldsymbol{\Omega}_T \times \mathbf{S}_R, \quad (6.64)$$

with the Thomas precession frequency

$$\boldsymbol{\Omega}_T = -\frac{\gamma^2}{(\gamma + 1)} \frac{1}{c^2} \mathbf{v} \times \dot{\mathbf{v}}, \quad (6.65)$$

which agrees with the result (4B.26) derived from purely group-theoretic considerations.

In an external electromagnetic field, there is an additional precession. For slow particles, it is given by Eq. (6.45). If the electron moves fast, we transform the electromagnetic field to the electron rest frame by a Lorentz transformation (4.283), and obtain an equation of motion for the spin:

$$\dot{\mathbf{S}}_R = \boldsymbol{\mu} \times \mathbf{B}' = \boldsymbol{\mu} \times \left[\gamma \left(\mathbf{B} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right) - \frac{\gamma^2}{\gamma + 1} \frac{\mathbf{v}}{c} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{B} \right) \right]. \quad (6.66)$$

Expressing $\boldsymbol{\mu}$ via Eq. (6.31), this becomes

$$\dot{\mathbf{S}}_R \equiv -\mathbf{S}_R \times \boldsymbol{\Omega}_{\text{em}} = \frac{eg}{2Mc} \mathbf{S}_R \times \left[\left(\mathbf{B} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right) - \frac{\gamma}{\gamma + 1} \frac{\mathbf{v}}{c} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{B} \right) \right], \quad (6.67)$$

which is the relativistic generalization of Eq. (6.44). It is easy to see that the associated fully covariant equation is

$$\frac{dS^\mu}{d\tau} = \frac{g}{2Mc} \left[eF^{\mu\nu} S_\nu + \frac{1}{Mc} p^\mu S_\lambda \frac{d}{d\tau} p^\lambda \right] = \frac{eg}{2Mc} \left[F^{\mu\nu} S_\nu + \frac{1}{M^2 c^2} p^\mu S_\lambda F^{\lambda\kappa} p_\kappa \right]. \quad (6.68)$$

On the right-hand side we have inserted the relativistic equation of motion of a point particle (6.21) in an external electromagnetic field.

If we add to this the relativistic Thomas precession rate (6.59), we obtain the covariant Bargmann-Michel-Telegdi equation¹

$$\frac{dS^\mu}{d\tau} = \frac{1}{2Mc} \left[egF^{\mu\nu} S_\nu + \frac{g-2}{Mc} p^\mu S_\lambda \frac{d}{d\tau} p^\lambda \right] = \frac{e}{2Mc} \left[gF^{\mu\nu} S_\nu + \frac{g-2}{M^2 c^2} p^\mu S_\lambda F^{\lambda\kappa} p_\kappa \right]. \quad (6.69)$$

For the spin vector $\mathbf{S}_R$ in the electron rest frame this implies a change in the electromagnetic precession rate in Eq. (6.67) to

$$\dot{\mathbf{S}}_R = -\mathbf{S}_R \times \boldsymbol{\Omega}_{\text{em}}^T \equiv -\mathbf{S}_R \times (\boldsymbol{\Omega}_{\text{em}} + \boldsymbol{\Omega}_T) \quad (6.70)$$

¹V. Bargmann, L. Michel, and V.L. Telegdi, Phys. Rev. Lett. 2, 435 (1959).

with a frequency given by the Thomas equation²

$$\boldsymbol{\Omega}_{\text{em}}^T = -\frac{e}{Mc} \left[\left(\frac{g}{2} - 1 + \frac{1}{\gamma} \right) \mathbf{B} - \left(\frac{g}{2} - 1 \right) \frac{\gamma}{\gamma+1} \left(\frac{\mathbf{v}}{c} \cdot \mathbf{B} \right) \frac{\mathbf{v}}{c} - \left(\frac{g}{2} - \frac{\gamma}{\gamma+1} \right) \frac{\mathbf{v}}{c} \times \mathbf{E} \right]. \quad (6.71)$$

The contribution of the Thomas precession is the part without the gyromagnetic ratio g :

$$\boldsymbol{\Omega}_T = -\frac{e}{Mc} \left[-\left(1 - \frac{1}{\gamma} \right) \mathbf{B} + \frac{\gamma}{\gamma+1} \frac{1}{c^2} (\mathbf{v} \cdot \mathbf{B}) \mathbf{v} + \frac{\gamma}{\gamma+1} \frac{1}{c} \mathbf{v} \times \mathbf{E} \right]. \quad (6.72)$$

This agrees with the Thomas frequency (6.65), after inserting the acceleration (6.24).

The *Thomas equation* (6.71) can be used to calculate the time dependence of the helicity $h \equiv \mathbf{S}_R \cdot \hat{\mathbf{v}}$ of an electron, i.e., its component of the spin in the direction of motion. Using the chain rule of differentiation, we can express the change of the helicity as

$$\frac{dh}{dt} = \frac{d}{dt} (\mathbf{S}_R \cdot \hat{\mathbf{v}}) = \dot{\mathbf{S}}_R \cdot \hat{\mathbf{v}} + \frac{1}{v} [\mathbf{S}_R - (\hat{\mathbf{v}} \cdot \mathbf{S}_R) \hat{\mathbf{v}}] \frac{d}{dt} \mathbf{v}, \quad (6.73)$$

Inserting (6.70) as well as the equation for the acceleration (6.24), we obtain

$$\frac{dh}{dt} = -\frac{e}{Mc} \mathbf{S}_{R\perp} \cdot \left[\left(\frac{g}{2} - 1 \right) \hat{\mathbf{v}} \times \mathbf{B} + \left(\frac{gv}{2c} - \frac{c}{v} \right) \mathbf{E} \right]. \quad (6.74)$$

where $\mathbf{S}_{R\perp}$ is the component of the spin vector orthogonal to $\mathbf{v}$. This equation shows that for a Dirac electron, which has the g -factor $g = 2$, the helicity remains constant in a purely magnetic field. Moreover, if the electron moves ultra-relativistically ($v \approx c$), the value $g = 2$ makes the last term extremely small, $\approx (e/Mc)\gamma^{-2} \mathbf{S}_{R\perp} \cdot \mathbf{E}$, so that the helicity is almost unaffected by an electric field. The anomalous magnetic moment of the electron, however, changes this to a finite value $\approx -(e/Mc)a \mathbf{S}_{R\perp} \cdot \mathbf{E}$. This drastic effect was exploited to measure the experimental values listed in Eqs. (6.52)–(6.54).

6.2 Charged Particle in Schrödinger Theory

When going over from quantum mechanics to second quantized field theories we found the rule that a non-relativistic Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \quad (6.75)$$

becomes an operator

$$H = \int d^3x \psi^\dagger(\mathbf{x}, t) \left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] \psi(\mathbf{x}, t), \quad (6.76)$$

²L.T. Thomas, Phil. Mag. 3, 1 (1927).

where we have omitted the operator hats, for brevity. With the same rules we see that the second quantized form of the interacting nonrelativistic Hamiltonian in a static $A(\mathbf{x})$ field,

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + \frac{e}{c}A^0, \quad (6.77)$$

is given by

$$H = \int d^3x \psi^\dagger(\mathbf{x}, t) \left[-\frac{1}{2m} \left(\nabla - i\frac{e}{c}\mathbf{A} \right)^2 + eA^0(\mathbf{x}) \right] \psi(\mathbf{x}, t). \quad (6.78)$$

When going to the action of this theory we find

$$\begin{aligned} \mathcal{A} = \int dt L = \int dt \int d^3x \left[\psi^\dagger(\mathbf{x}, t) (i\partial_t + eA^0) \psi(\mathbf{x}, t) \right. \\ \left. + \frac{1}{2m} \psi^\dagger(\mathbf{x}, t) \left(\nabla - i\frac{e}{c}\mathbf{A} \right)^2 \psi(\mathbf{x}, t) \right]. \end{aligned} \quad (6.79)$$

It is easy to verify that (6.78) reemerges from the Legendre transform

$$H = \frac{\partial L}{\partial \dot{\psi}(\mathbf{x}, t)} \dot{\psi}(\mathbf{x}, t) - L. \quad (6.80)$$

The action (6.79) holds also for time-dependent $A^\mu(x)$ fields.

We can now deduce the second quantized form of the minimal substitution rule (6.29) which is

$$\begin{aligned} \nabla &\rightarrow \nabla - i\frac{e}{c}\mathbf{A}(\mathbf{x}, t), \\ \partial_t &\rightarrow \partial_t + ieA^0(\mathbf{x}, t), \end{aligned} \quad (6.81)$$

or covariantly:

$$\partial_\mu \rightarrow \partial_\mu + i\frac{e}{c}A_\mu(x). \quad (6.82)$$

This substitution rule has the important property that the gauge invariance of the free photon action is preserved by the interacting theory: If we perform the gauge transformation

$$A^\mu(x) \rightarrow A^\mu(x) + \partial^\mu \Lambda(x), \quad (6.83)$$

i.e.,

$$\begin{aligned} A^0(\mathbf{x}, t) &\rightarrow A^0(\mathbf{x}, t) + \partial_t \Lambda(\mathbf{x}, t) \\ \mathbf{A}(\mathbf{x}, t) &\rightarrow \mathbf{A}(\mathbf{x}, t) - \nabla \Lambda(\mathbf{x}, t), \end{aligned} \quad (6.84)$$

the action remains invariant provided we simultaneously change the fields $\psi(\mathbf{x}, t)$ of the charged particles by a spacetime-dependent phase

$$\psi(\mathbf{x}, t) \rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \psi(\mathbf{x}, t). \quad (6.85)$$

Under this transformation, the derivatives of the field change like

$$\begin{aligned}\partial_t \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} (\partial_t - ie\partial_t \Lambda) \psi(\mathbf{x}, t), \\ \nabla \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left[\nabla - i\frac{e}{c} \nabla \Lambda(\mathbf{x}, t) \right] \psi(\mathbf{x}, t).\end{aligned}\quad (6.86)$$

The modified derivatives appearing in the action have therefore the following simple transformation law:

$$\begin{aligned}\left(\partial_t + i\frac{e}{c} A^0 \right) \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left(\partial_t + ieA^0 \right) \psi(\mathbf{x}, t), \\ \left(\nabla - i\frac{e}{c} \mathbf{A} \right) \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left(\nabla - i\frac{e}{c} \mathbf{A} \right) \psi(\mathbf{x}, t).\end{aligned}\quad (6.87)$$

These combinations of derivatives and gauge fields are called *covariant derivatives*. They occur so frequently in gauge theories that they deserve their own symbols:

$$\begin{aligned}D_t \psi(\mathbf{x}, t) &\equiv \left(\partial_t + ieA^0 \right) \psi(\mathbf{x}, t), \\ \mathbf{D} \psi(\mathbf{x}, t) &\equiv \left(\nabla - i\frac{e}{c} \mathbf{A} \right) \psi(\mathbf{x}, t),\end{aligned}\quad (6.88)$$

or, in four-vector notation,

$$D_\mu \psi(x) = \left(\partial_\mu + i\frac{e}{c} A_\mu \right) \psi(x). \quad (6.89)$$

Here the adjective of the *covariant* derivative does not refer to the Lorentz group but to the gauge group. It records the fact that $D_\mu \psi$ transforms under local gauge changes (6.81) of ψ in the same way as ψ itself in (6.85):

$$D_\mu \psi(x) \rightarrow e^{-i(e/c)\Lambda(x)} D_\mu \psi(x). \quad (6.90)$$

With the help of this covariant derivative, any action that is invariant under a global multiplication change of the field by a constant phase factor $e^{-i\phi}$,

$$\psi(x) \rightarrow e^{-i\phi} \psi(x), \quad (6.91)$$

can also be made invariant under a local version of this transformation, in which ϕ is an arbitrary function $\phi(x)$. For this, we merely have to replace all derivatives by covariant derivatives (6.89), and add to the field action the gauge-invariant photon action (4.237).

6.3 Charged Relativistic Fields

6.3.1 Scalar Field

The Lagrangian density of a free relativistic scalar field was stated in Eq. (4.165):

$$\mathcal{L} = \partial_\mu \phi^*(x) \partial^\mu \phi(x) - M^2 \phi^*(x) \phi(x). \quad (6.92)$$

If the field carries a charge e , the derivatives are simply replaced by the covariant derivatives (6.89), thus leading to a straightforward generalization of the Schrödinger action in (6.79):

$$\begin{aligned}\mathcal{L} &= [D_\mu \phi(x)]^* D^\mu \phi(x) - M^2 \phi^*(x) \phi(x) \\ &= \left[\partial_\mu - i \frac{e}{c} A_\mu(x) \right] \phi(x) \left[\partial^\mu + i \frac{e}{c} A^\mu(x) \right] \phi(x) - M^2 \phi^*(x) \phi(x).\end{aligned}\quad (6.93)$$

The associated scalar field action $\mathcal{A} = \int d^4x \mathcal{L}$ must be extended by the gauge-invariant photon action (4.237).

6.3.2 Dirac Field

The Lagrangian density of a free charged spin-1/2 field was stated in Eq. (4.501):

$$\mathcal{L}(x) = \bar{\psi}(x) (i\partial - M) \psi(x). \quad (6.94)$$

If the particle carries a charge e , we must replace the derivatives in this Lagrangian by their covariant versions (6.89):

$$\partial = \gamma^\mu \partial_\mu \rightarrow \gamma^\mu \left(\partial_\mu + i \frac{e}{c} A_\mu \right) = \left(\partial + i \frac{e}{c} A \right) \equiv \mathcal{D}. \quad (6.95)$$

Adding again the gauge-invariant photon action (4.237), we arrive at the Lagrangian of *quantum electrodynamics* (QED)

$$\mathcal{L}(x) = \bar{\psi}(x) (i\mathcal{D} - M) \psi(x) - \frac{1}{4} F_{\mu\nu}^2. \quad (6.96)$$

The classical field equations can easily be found by extremizing the action under variations of all fields, which gives

$$\frac{\delta \mathcal{A}}{\delta \bar{\psi}(x)} = (i\mathcal{D} - M) \psi(x) = 0, \quad (6.97)$$

$$\frac{\delta \mathcal{A}}{\delta A_\mu(x)} = \partial_\nu F^{\nu\mu}(x) - \frac{1}{c} j^\mu(x) = 0, \quad (6.98)$$

where $j^\mu(x)$ is the *current density*

$$j^\mu(x) \equiv ec \bar{\psi}(x) \gamma^\mu \psi(x). \quad (6.99)$$

Equation (6.98) is the Maxwell equation for the electromagnetic field around a classical four-dimensional vector current $j^\mu(x)$:

$$\partial_\nu F^{\nu\mu}(x) = \frac{1}{c} j^\mu(x). \quad (6.100)$$

In the Lorentz gauge $\partial_\mu A^\mu(x) = 0$, this equation reads simply

$$-\partial^2 A^\mu(x) = \frac{1}{c} j^\mu(x). \quad (6.101)$$

The current j^μ combines the charge density $\rho(x)$ and the current density $\mathbf{j}$ of particles of charge e in a four-vector

$$j^\mu = (c\rho, \mathbf{j}). \quad (6.102)$$

In terms of electric and magnetic fields $E^i = F^{i0}$, $B^i = -F^{jk}$, the field equations (6.100) turn into the Maxwell equations

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \rho = e\bar{\psi}\gamma^0\psi = e\psi^\dagger\psi \\ \nabla \times \mathbf{B} - \dot{\mathbf{E}} &= \frac{1}{c}\mathbf{j} = \frac{e}{c}\bar{\psi}\boldsymbol{\gamma}\psi. \end{aligned} \quad (6.103)$$

The first is Coulomb's law, the second Ampère's law in the presence of charges and currents.

Note that the physical units employed here differ from those used in many books of classical electrodynamics³ by the absence of a factor $1/4\pi$ on the right-hand side. The Lagrangian used in those books is

$$\begin{aligned} \mathcal{L}(x) &= -\frac{1}{8\pi}F_{\mu\nu}^2(x) - \frac{1}{c}j^\mu(x)A_\mu(x) \\ &= \frac{1}{4\pi}[\mathbf{E}^2 - \mathbf{B}^2](x) - \left[\rho\phi - \frac{1}{c}\mathbf{j} \cdot \mathbf{A}\right](x), \end{aligned} \quad (6.104)$$

which leads to Maxwell's field equations

$$\begin{aligned} \nabla \cdot \mathbf{E} &= 4\pi\rho, \\ \nabla \times \mathbf{B} &= \frac{4\pi}{c}\mathbf{j}. \end{aligned} \quad (6.105)$$

The form employed conventionally in quantum field theory arises from this by replacing $A \rightarrow \sqrt{4\pi}A$ and $e \rightarrow \sqrt{4\pi}e$. The charge of the electron in our units has therefore the numerical value

$$e = -\sqrt{4\pi\alpha} \approx -\sqrt{4\pi/137} \quad (6.106)$$

rather than $e = -\sqrt{\alpha}$.

6.4 Pauli Equation from Dirac Theory

It is instructive to take the Dirac equation (6.97) to a two-component form corresponding to (4.567) and (4.569), and further to (4.585). Due to the fundamental nature of the equations to be derived we shall not work with natural units in this section but carry along explicitly all fundamental constants. As in (4.586), we multiply (6.97) by $(i\hbar\mathcal{D} - Mc)$ and work out the product

$$(i\hbar\mathcal{D} - Mc)(i\hbar\mathcal{D} + Mc) = \left[i\gamma^\mu \left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right) + Mc\right] \left[i\gamma^\mu \left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right) - Mc\right]. \quad (6.107)$$

³See for example J.D. Jackson, *Classical Electrodynamics*, Wiley and Sons, New York, 1967.

We now use the relation

$$\gamma^\mu \gamma^\nu = \frac{1}{2}(\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu) + \frac{1}{2}(\gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu) = g^{\mu\nu} - i\sigma^{\mu\nu}, \quad (6.108)$$

with $\sigma^{\mu\nu}$ from (4.517), and find

$$\begin{aligned} \gamma^\mu \gamma^\nu \left(\hbar \partial_\mu + i \frac{e}{c} A_\mu \right) \left(\partial_\nu + i \frac{e}{c} A_\nu \right) \\ = g^{\mu\nu} \left(\hbar \partial_\mu + i \frac{e}{c} A_\mu \right) \left(\partial_\nu + i \frac{e}{c} A_\nu \right) - \frac{i}{2} \sigma^{\mu\nu} [\hbar \partial_\mu + i \frac{e}{c} A_\mu, \hbar \partial_\nu + i \frac{e}{c} A_\nu] \\ = \left(\hbar \partial_\mu + i \frac{e}{c} A_\mu \right)^2 + \frac{1}{2} \frac{e\hbar}{c} \sigma^{\mu\nu} F_{\mu\nu}. \end{aligned} \quad (6.109)$$

Thus we obtain, as a generalization of Eqs. (4.585), the *Pauli equation*:

$$\left[- \left(\hbar \partial_\mu + i \frac{e}{c} A_\mu \right)^2 - \frac{1}{2} \frac{e\hbar}{c} \sigma^{\mu\nu} F_{\mu\nu} - M^2 c^2 \right] \psi(x) = 0, \quad (6.110)$$

and the same equation once more for the other two-component spinor field $\eta(x)$. Note that, in this equation, electromagnetism is not coupled minimally. In fact, there is a non-minimal coupling of the spin via the tensor term

$$\frac{1}{2} \sigma^{\mu\nu} F_{\mu\nu} = -\mathbf{\Sigma} \cdot \mathbf{H} + i\mathbf{\alpha} \cdot \mathbf{E}, \quad (6.111)$$

where in the chiral and Dirac representations, the matrix $\mathbf{\alpha}$ is

$$\mathbf{\alpha} = \begin{pmatrix} -\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \quad \mathbf{\alpha}_D = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad (6.112)$$

respectively. Thus, in the chiral representation, Eq. (6.110) decomposes into two separate two-component equations for the upper and lower spinor components $\xi(x)$ and $\eta(x)$ in $\psi(x)$:

$$\left[- \left(\hbar \partial_\mu + i \frac{e}{c} A_\mu \right)^2 + \boldsymbol{\sigma} \cdot (\mathbf{H} \pm i\mathbf{E}) - M^2 c^2 \right] \begin{Bmatrix} \xi(x) \\ \eta(x) \end{Bmatrix} = 0. \quad (6.113)$$

In the nonrelativistic limit where $c \rightarrow \infty$, we remove the fast oscillations from $\xi(x)$, setting $\xi(x) \equiv e^{-iMc^2t/\hbar} \Psi(\mathbf{x}, t)/\sqrt{2M}$ as in (4.156), and find for $\Psi(\mathbf{x}, t)$ the nonrelativistic Pauli equation

$$\left[i\partial_t + \frac{\hbar^2}{2M} \left(\boldsymbol{\nabla} - i \frac{e}{c\hbar} \mathbf{A} \right)^2 + \frac{e}{2Mc} \boldsymbol{\sigma} \cdot \mathbf{H} - eA^0(x) \right] \Psi(\mathbf{x}, t) = 0. \quad (6.114)$$

This corresponds to a magnetic interaction energy

$$H_{\text{mag}} = -\frac{e\hbar}{2Mc} \boldsymbol{\sigma} \cdot \mathbf{H}. \quad (6.115)$$

For a small magnet with a magnetic moment $\boldsymbol{\mu}$, the magnetic interaction energy is

$$H_{\text{mag}} = -\boldsymbol{\mu} \cdot \mathbf{H}. \quad (6.116)$$

A Dirac particle has therefore a magnetic moment

$$\boldsymbol{\mu} = \frac{e}{Mc} \frac{\hbar \boldsymbol{\sigma}}{2} = 2 \frac{e}{2Mc} \mathbf{S}, \quad (6.117)$$

where $\mathbf{S} = \boldsymbol{\sigma}/2$ is the spin matrix. Experimentally, one parametrizes the magnetic moment of a fundamental particles as

$$\boldsymbol{\mu} = g \frac{e}{2Mc} \mathbf{S}, \quad (6.118)$$

where g is the so-called *gyromagnetic ratio*. It is normalized to unity for a uniformly charged sphere.

Within the Dirac theory, an electron has a gyromagnetic ratio

$$g_e|_{\text{Dirac}} = 2. \quad (6.119)$$

The experimental value is very close to this. A small deviation from it is called *anomalous magnetic moment*. It is a consequence of the quantum nature of the electromagnetic field and will be explained in Chapter 12.

The nonrelativistic Pauli equation (6.114) could also have been obtained by introducing the electromagnetic coupling directly into the nonrelativistic two-component equation (4.582). The minimal substitution rule (6.87) changes $i\partial_t \rightarrow i\partial_t - eA^0$ and $(\boldsymbol{\sigma} \cdot \nabla)^2 \rightarrow [\boldsymbol{\sigma} \cdot (\nabla - ie\mathbf{A})]^2$. The latter is worked out in detail as in Chapter 4, Eq. (4.583), and leads to

$$\begin{aligned} [\boldsymbol{\sigma} \cdot (\nabla - ie\mathbf{A})]^2 &= [\delta^{ij} + i\epsilon_{ijk}\sigma^k] (\nabla_i - ieA_i)(\nabla_j - ieA_j) \\ &= (\nabla - ie\mathbf{A})^2 + i\epsilon_{ijk}\sigma^k (\nabla_i - ieA_i)(\nabla_j - ieA_j) + e\boldsymbol{\sigma} \cdot \mathbf{H}. \end{aligned} \quad (6.120)$$

This brings the free-field equation (4.584) to the nonrelativistic Pauli expression (6.114), after reinserting all fundamental constants.

6.5 Relativistic Wave Equations in the Coulomb Potential

It is now easy to write down field equations for a Klein-Gordon and a Dirac field in the presence of an external Coulomb potential of charge Ze . In natural units we have

$$V_C(\mathbf{x}) = -\frac{Z\alpha}{r}, \quad r = \sqrt{\mathbf{x}^2}, \quad (6.121)$$

corresponding to a four-vector potential

$$eA_\mu(x) = (V_C(\mathbf{x}, 0), \mathbf{0}). \quad (6.122)$$

Since this does not depend on time, we can consider the wave equations for wave functions $\phi(x) = e^{-iEt}\phi_E(\mathbf{x})$ and $\psi(x) = e^{-iEt}\psi_E(\mathbf{x})$, and find the time-independent equations

$$(E^2 + \nabla^2 - M)\phi_E(\mathbf{x}) = 0 \quad (6.123)$$

and

$$(\gamma^0 E + i\boldsymbol{\gamma} \cdot \nabla - M)\psi_E(\mathbf{x}) = 0. \quad (6.124)$$

In these equations we simply perform the minimal substitution

$$E \rightarrow E + \frac{Z\alpha}{r}. \quad (6.125)$$

The energy-eigenvalues obtained from the resulting equations can be compared with those of hydrogen-like atoms. The velocity of an electron in the ground state is of the order αZc . Thus for rather high Z , the electron has a relativistic velocity and there must be significant deviations from the Schrödinger theory. We shall see that the Dirac equation in an external field reproduces quite well a number of features resulting from the relativistic motion.

6.5.1 Reminder of the Schrödinger Equation in a Coulomb Potential

The time-independent Schrödinger equation reads

$$\left(-\frac{1}{2M}\nabla^2 - \frac{Z\alpha}{r} - E\right)\psi_E(\mathbf{x}) = 0. \quad (6.126)$$

The Laplacian may be decomposed into radial and angular parts by writing

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\hat{\mathbf{L}}^2}{r^2}, \quad (6.127)$$

where $\hat{\mathbf{L}} = \mathbf{x} \times \hat{\mathbf{p}}$ are the differential operators for the generators of angular momentum [the spatial part of $L_i = L^{23}$ of (4.97)]. Then (6.126) reads

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{2}{r}\frac{\partial}{\partial r} + \frac{\hat{\mathbf{L}}^2}{r^2} - \frac{2Z\alpha M}{r} - 2ME\right)\psi_E(x) = 0. \quad (6.128)$$

The eigenstates of $\hat{\mathbf{L}}^2$ are the spherical harmonics $Y_{lm}(\theta, \phi)$, which diagonalize also the third component of $\hat{\mathbf{L}}$, with the eigenvalues

$$\begin{aligned} \hat{\mathbf{L}}^2 Y_{lm}(\theta, \phi) &= l(l+1)Y_{lm}(\theta, \phi), \\ \hat{L}_3 Y_{lm}(\theta, \phi) &= mY_{lm}(\theta, \phi). \end{aligned} \quad (6.129)$$

The wave functions may be factorized into a radial wave function $R_{nl}(r)$ and a spherical harmonic:

$$\psi_{nlm}(\mathbf{x}) = R_{nl}(r)Y_{lm}(\theta, \phi). \quad (6.130)$$

Explicitly,

$$\begin{aligned} R_{nl}(r) &= \frac{1}{a_B^{1/2}n} \frac{1}{(2l+1)!} \sqrt{\frac{(n+l)!}{(n-l-1)!}} \\ &\quad \times (2r/na_B)^{l+1} e^{-r/na_B} M(-n+l+1, 2l+2, 2r/na_B) \\ &= \frac{1}{a_B^{1/2}n} \sqrt{\frac{(n-l-1)!}{(n+l)!}} e^{-r/na_B} (2r/na_B)^{l+1} L_{n-l-1}^{2l+1}(2r/na_B), \end{aligned} \quad (6.131)$$

where a_B is the Bohr radius which, in natural units with $\hbar = c = 1$, is equal to

$$a_B = \frac{1}{ZM\alpha}. \quad (6.132)$$

For a hydrogen atom with $Z = 1$, this is about $1/137$ times the Compton wavelength of the electron $\lambda_e \equiv \hbar/M_e c$. The classical velocity of the electron on the lowest Bohr orbit is $v_B = \alpha c$. Thus it is almost nonrelativistic, which is the reason why the Schrödinger equation explains the hydrogen spectrum quite well. The functions $M(a, b, z)$ are confluent hypergeometric functions or Kummer functions, defined by the power series

$$M(a, b, z) \equiv F_{1,1}(a, b, z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)} \frac{z^2}{2!} + \dots \quad (6.133)$$

For $b = -n$, they are polynomials related to the Laguerre polynomials⁴ $L_n^\mu(z)$ by

$$L_n^\mu(z) \equiv \frac{(n+\mu)!}{n!\mu!} M(-n, \mu+1, z). \quad (6.134)$$

The radial wave functions are normalized to

$$\int_0^\infty dr R_{n_r l}(r) R_{n'_r l}(r) = \delta_{n_r n'_r}. \quad (6.135)$$

They have an asymptotic behavior $P_{nl}(r/n)e^{-r/na_B}$, where $P_{nl}(r/n)$ is a polynomial of degree $n_r = n - l - 1$, which defines the *radial quantum number*. The energy eigenvalues depend on n in the well-known way:

$$E_n = -Z^2 \frac{M\alpha^2}{2n^2}. \quad (6.136)$$

⁴I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.970 (our definition differs from that in L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon Press, New York, 1965, Eq. (d.13): Our $L_n^\mu = (-)^\mu / (n+\mu)! L_{n+\mu}^\mu|_{\text{L.L.}}$).

The number $\alpha^2 M/2$ is the Rydberg-constant:

$$\text{Ry} = \frac{\alpha^2 M}{2} \approx \frac{27.21}{2} \text{eV} \approx 3.288 \times 10^{15} \text{Hz}. \quad (6.137)$$

Later in Section 12.21) we shall need the value of the wave function at the origin. It is non-zero only for s -waves where it is equal to

$$|\psi_{n00}(\mathbf{0})| = \frac{1}{\sqrt{\pi}} \sqrt{\frac{ZM\alpha}{n}}^3 = \frac{1}{\sqrt{\pi}} \sqrt{\frac{1}{na_B}}^3. \quad (6.138)$$

6.5.2 Klein-Gordon Field in a Coulomb Potential

After the substitution of (6.125) into (6.123), we find the Klein-Gordon equation in the Coulomb potential (6.121):

$$\left[\left(E + \frac{Z\alpha}{r} \right)^2 + \nabla^2 - M^2 \right] \phi_E(\mathbf{x}) = 0. \quad (6.139)$$

With the angular decomposition (6.127), this becomes

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{\hat{\mathbf{L}}^2 - Z^2 \alpha^2}{r^2} - \frac{2Z\alpha E}{r} - (E^2 - M^2) \right] \phi_E(\mathbf{x}) = 0. \quad (6.140)$$

The solutions of this equation can be obtained from those of the nonrelativistic Schrödinger equation (6.128) by replacing

$$\hat{\mathbf{L}}^2 \rightarrow \hat{\mathbf{L}}^2 - Z^2 \alpha^2, \quad (6.141)$$

$$\alpha \rightarrow \alpha \frac{E}{M}, \quad (6.142)$$

$$E \rightarrow \frac{E^2 - M^2}{2M}. \quad (6.143)$$

The replacement (6.141) is done most efficiently if we define the eigenvalues $l(l+1) - Z^2 \alpha^2$ of the operator $\hat{\mathbf{L}}^2 - Z^2 \alpha^2$ by analogy with those of $\hat{\mathbf{L}}^2$ as

$$\lambda(\lambda+1) \equiv l(l+1) - Z^2 \alpha^2. \quad (6.144)$$

Then the quantum number l of the Schrödinger wave functions is simply replaced by $\lambda_l = l - \delta_l$, where

$$\begin{aligned} \delta_l &= l + \frac{1}{2} - \left[\left(l + \frac{1}{2} \right)^2 - Z^2 \alpha^2 \right]^{1/2} \\ &= \frac{Z^2 \alpha^2}{2l+1} + \mathcal{O}(\alpha^4). \end{aligned} \quad (6.145)$$

The other solution of relation (6.144) with the opposite sign in front of the square root is unphysical since the associated wave functions are too singular at the origin to

be normalizable. As before, the radial quantum number n_r determining the degree of the polynomial $P_{nl}(r/n)$ in the wave functions must be an integer. This is no longer true for the combination of quantum numbers which determines the energy. This is now given by

$$n_r + \lambda + 1 = n_r + l + 1 - \delta_l = n - \delta_l. \quad (6.146)$$

It leads to the equation for the energy eigenvalues

$$\frac{E_{nl}^2 - M^2}{2M} = -\frac{Z^2 M \alpha^2}{2} \frac{E_{nl}^2}{M^2} \frac{1}{(n - \delta_l)^2}, \quad (6.147)$$

with the solution

$$\begin{aligned} E_{nl} &= \pm \frac{M}{\sqrt{1 + Z^2 \alpha^2 / (n - \delta_l)^2}} \\ &= \pm M \left[1 - \frac{(Z\alpha)^2}{2n^2} + \frac{3}{8} \frac{(Z\alpha)^4}{n^4} - \frac{(Z\alpha)^4}{n^3(2l+1)} + \mathcal{O}(Z^6 \alpha^6) \right]. \end{aligned} \quad (6.148)$$

The first two terms correspond to the Schrödinger energies (6.136) including the rest energies of the atom. The next two are relativistic corrections. The first of these breaks the degeneracy between the levels of the same n and different l . This is caused in the Schrödinger theory by the famous Lentz-Runge vector [O(4)-invariance] [1].

The correction terms become large for large central charge Z . In particular, the lowest energy and successively the higher ones become complex for central charges $Z > 137/2$. The physical reason for this is that the large potential gradient near the origin can create pairs of particles from the vacuum. This phenomenon can only be properly understood after quantizing the field theory.

As for the free Klein-Gordon field, the energy appears with both signs.

6.5.3 Dirac Field in a Coulomb Potential

After the substitution (6.125) into (6.124), we find the Dirac equation in the Coulomb potential (6.121):

$$\left[\left(E + \frac{Z\alpha}{r} \right) \gamma^0 + i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} - M \right] \psi_E(\mathbf{x}) = 0. \quad (6.149)$$

In order to find the energy spectrum it is useful to establish contact with the Klein-Gordon case. Multiplying (6.149) by the operator

$$\left(E + \frac{Z\alpha}{r} \right) \gamma^0 + i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M, \quad (6.150)$$

we obtain

$$\left[\left(E + \frac{Z\alpha}{r} \right)^2 + \boldsymbol{\nabla}^2 - i\gamma^0 \boldsymbol{\gamma} \cdot \boldsymbol{\nabla} \frac{Z\alpha}{r} - M^2 \right] \psi_E(\mathbf{x}) = 0. \quad (6.151)$$

In the chiral representation, the 4×4 -matrix $\gamma^0 \boldsymbol{\gamma} = \boldsymbol{\alpha}$ has a block-diagonal form (4.563). We therefore decompose

$$\psi_E(\mathbf{x}) = \begin{pmatrix} \xi_E(\mathbf{x}) \\ \eta_E(\mathbf{x}) \end{pmatrix}, \quad (6.152)$$

and find the equation for the upper two-component spinors

$$\left[\left(E + \frac{Z\alpha}{r} \right)^2 + \nabla^2 + i\boldsymbol{\sigma} \cdot \nabla \frac{Z\alpha}{r} - M^2 \right] \xi_E(\mathbf{x}) = 0. \quad (6.153)$$

The lower bispinor $\eta_E(\mathbf{x})$ satisfies the same equation with i replaced by $-i$. Expressing ∇^2 via (6.127) and writing $\nabla 1/r = -\hat{\mathbf{x}}/r^2$, we obtain the differential equation

$$\left[- \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\hat{\mathbf{L}}^2 - Z^2 \alpha^2 + iZ\alpha \boldsymbol{\sigma} \cdot \hat{\mathbf{x}}}{r^2} - \frac{2Z\alpha E}{r} - (E^2 - M^2) \right] \xi_E(\mathbf{x}) = 0, \quad (6.154)$$

and a corresponding equation for $\eta_E(\mathbf{x})$.

Due to the rotation invariance of $\boldsymbol{\sigma} \cdot \hat{\mathbf{x}}$, the total angular momentum

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \mathbf{S} = \hat{\mathbf{L}} + \frac{\boldsymbol{\sigma}}{2} \quad (6.155)$$

commutes with the differential operator in (6.154). Thus we can diagonalize $\hat{\mathbf{J}}^2$ and $\hat{J}_3$ with eigenvalues $j(j+1)$ and m . For a fixed value of $j = \frac{1}{2}, 1, \frac{3}{2}, \dots$, the orbital angular momentum can have the value $l_+ = j + \frac{1}{2}$ and $l_- = j - \frac{1}{2}$. The two states have opposite parities. The operator $\boldsymbol{\sigma} \cdot \hat{\mathbf{x}}$ is a pseudoscalar, so that multiplication by it will necessarily change the parity of the wave function. Since the square of $\boldsymbol{\sigma} \cdot \hat{\mathbf{x}}$ is the unit matrix, its eigenvalues must be ± 1 . Moreover, the unit vector $\hat{\mathbf{x}}$ changes l by one unit. Thus, in the two-component Hilbert space of fixed quantum numbers j and m , with orbital angular momenta $l = l_{\pm} = j \pm 1/2$, the diagonal matrix elements vanish

$$\langle jm, + | \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} | jm, + \rangle = 0, \quad \langle jm, - | \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} | jm, - \rangle = 0. \quad (6.156)$$

For the off-diagonal elements we easily calculate

$$\langle jm, + | \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} | jm, - \rangle = 1, \quad \langle jm, - | \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} | jm, + \rangle = -1. \quad (6.157)$$

The central parentheses in (6.154) have therefore the matrix elements

$$(\mathbf{L}^2 - Z^2 \alpha^2 \pm iZ\alpha \hat{\mathbf{x}}) = \begin{pmatrix} (j + \frac{1}{2})(j + \frac{3}{2}) - Z^2 \alpha^2 & \pm iZ\alpha \\ \pm iZ\alpha & (j - \frac{1}{2})(j + \frac{1}{2}) - Z^2 \alpha^2 \end{pmatrix}. \quad (6.158)$$

By analogy with the Klein-Gordon case, we denote the eigenvalues of this matrix by $\lambda(\lambda+1)$. The corresponding values of λ are found to be

$$\lambda_{j+} = \left[\left(j + \frac{1}{2} \right)^2 - Z^2 \alpha^2 \right]^{1/2}, \quad \lambda_{j-} = \lambda_{j+} - 1. \quad (6.159)$$

These may be written as

$$\lambda_{j\pm} = j \pm \frac{1}{2} - \delta_j \equiv l_{\pm} - \delta_j, \quad (6.160)$$

where $l_{\pm} \equiv \pm \frac{1}{2}$ is the orbital angular momentum, and

$$\delta_j \equiv j + \frac{1}{2} - \left[\left(j + \frac{1}{2} \right)^2 - Z^2 \alpha^2 \right]^{1/2} = \frac{Z^2 \alpha^2}{2j+1} + \mathcal{O}(Z^4 \alpha^4). \quad (6.161)$$

When solving Eq. (6.154), the solutions consist, as in the nonrelativistic hydrogen atom, of an exponential factor multiplied by a polynomial of degree n_r which is the radial quantum number. It is related to the quantum numbers of spin and orbital angular momentum, and to the principal quantum number n , by

$$n_r + \lambda_{j\pm} + 1 = n_r + l_{\pm} + 1 - \delta_l = n - \delta_j. \quad (6.162)$$

In terms of δ_j , the energies obey the same equation as in (6.148), so that we obtain

$$\begin{aligned} E_{nj} &= \pm \frac{M}{\sqrt{1 + Z^2 \alpha^2 / (n - \delta_j)^2}} \\ &= \pm M \left[1 - \frac{(Z\alpha)^2}{2n^2} + \frac{3}{8} \frac{(Z\alpha)^4}{n^4} - \frac{(Z\alpha)^4}{n^3(2j+1)} + \mathcal{O}(Z^6 \alpha^6) \right]. \end{aligned} \quad (6.163)$$

The condition $n_r \geq 0$ implies that

$$\begin{aligned} j &\leq n - \frac{3}{2} \\ j &\leq n - \frac{1}{2} \end{aligned} \quad \text{for} \quad \begin{aligned} \lambda_{j+} &= j + \frac{1}{2} - \delta_j, \\ \lambda_{j-} &= j - \frac{1}{2} - \delta_j. \end{aligned} \quad (6.164)$$

For $n = 1, 2, 3, \dots$, the total angular momentum runs through $j = \frac{1}{2}, \frac{3}{2}, \dots, n - \frac{1}{2}$.

The spectrum of the hydrogen atom, according to the Dirac theory, is shown in Fig. 6.1. As a remnant of the $O(4)$ -degeneracy of the levels with $l = 0, 1, 2, \dots, n-1$ and fixed n in the Schrödinger spectrum, there is now a twofold degeneracy of levels of equal n and j , with adjacent l -values, which are levels of opposite parity. An exception is the highest total angular momentum $j = n - 1/2$ at each n , which occurs only once. The lowest degenerate pair consists of the levels $2S_{1/2}$ and $2P_{1/2}$.⁵ It was an important experimental discovery to find that this prediction is wrong. There is a splitting of about 10% of the fine-structure splitting. This is called the *Lamb shift*. Its explanation is one of the early triumphs of quantum electrodynamics, which will be discussed in detail in Section 12.21.

As in the Klein-Gordon case, there are complex energies, here for $Z > 137$, with $S_{1/2}$ being the first level to become complex.

⁵Recall the notation in atomic physics for an electronic state: $n^{2S+1}L_J$, where n is the principal quantum number, L the orbital angular momentum, J the total angular momentum, and S the total spin. In a one-electron system such as the hydrogen atom, the trivial superscript $2S+1=2$ may be omitted.

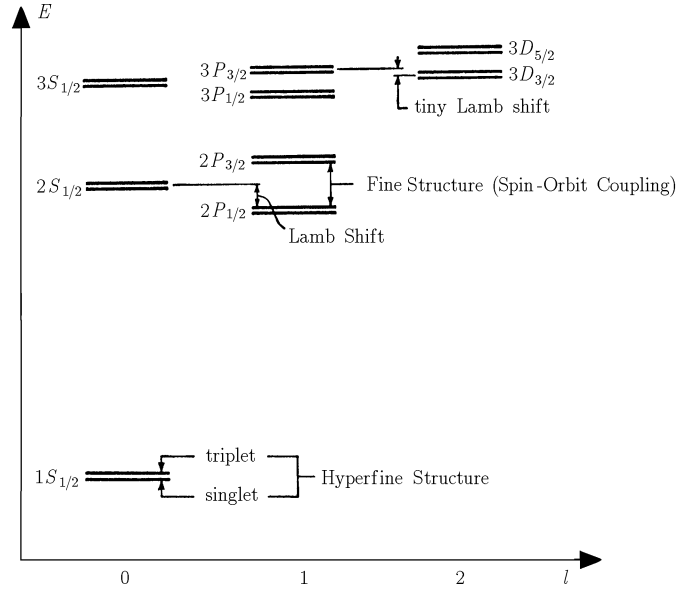


FIGURE 6.1 Hydrogen spectrum according to Dirac's theory. The splittings are shown only schematically. The fine-structure splitting of the $2P$ -levels is about 10 times as big as the hyperfine splitting and Lamb shift.

An important correct prediction of the Dirac theory is the presence of fine structure. States with the same n and l but with different j are split apart by the fourth term in Eq. (6.163) $-MZ^4\alpha^4n^3/(2j+1)$. For the states $2P_{1/2}$ and $2P_{3/2}$, the splitting is

$$\Delta_{\text{fine}}E_{2P} = \frac{Z^4\alpha^2}{32}\alpha^2M. \quad (6.165)$$

In a hydrogen atom, this is equal to

$$\Delta_{\text{fine}}E_{2P} = 3.10.95 \text{ GHz}. \quad (6.166)$$

Thus it is roughly of the order of the splitting caused by the interaction of the magnetic moment of the electron with that of the proton, the so-called *hyperfine-splitting*. For $2S^{1/2}$, $2P^{1/2}$, and $2P^{3/2}$ levels, this is approximately equal to 1, $1/8$, $1/24$, $1/60$ times 1 420 MHz.⁶

In a hydrogen atom, the electronic motion is only slightly relativistic, the velocities being of the order αc , i.e., only about 1% of the light velocity. If one is not only interested in the spectrum but also in the wave functions it is advantageous to solve directly the Dirac equation (6.149) with the gamma matrices in the Dirac

⁶See H.A. Bethe and E.E. Salpeter in *Encyclopedia of Physics (Handbuch der Physik)* 335, Springer, Berlin, 1957, p. 196.

representation (4.550). Multiplying (6.149) by γ^0 and inserting the Dirac matrices (4.562) for $\gamma^0\boldsymbol{\gamma} = \boldsymbol{\alpha}$, we obtain

$$\begin{pmatrix} E - M + \frac{Z\alpha}{r} & i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \\ i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} & E + M + \frac{Z\alpha}{r} \end{pmatrix} \begin{pmatrix} \xi_E(\mathbf{x}) \\ \eta_E(\mathbf{x}) \end{pmatrix} = 0. \quad (6.167)$$

This is of course just the time-independent version of (4.569) extended by the Coulomb potential according to the minimal substitution rule (6.125). To lowest order in α , the lower spinor is related to the upper by

$$\eta_E(\mathbf{x}) \approx -i \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}}{2M} \xi_E(\mathbf{x}). \quad (6.168)$$

We may take care of rotational symmetry of the system by splitting the spinor wave functions into radial and angular parts

$$\psi_E(\mathbf{x}) = \begin{pmatrix} i \frac{G_{jl}(r)}{r} y_{j,m}^l(\theta, \phi) \\ \frac{F_{jl}(r)}{r} \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} y_{j,m}^l(\theta, \phi) \end{pmatrix}, \quad (6.169)$$

where $y_{j,m}^l(\theta, \phi)$ denotes the *spinor spherical harmonics*. They are composed from the ordinary spherical harmonics $Y_{lm}(\theta, \phi)$ and the basis spinors $\chi(s_3)$ of (4.446) via *Clebsch-Gordan coefficients* (see Appendix 4E):

$$y_{j,m}^l(\theta, \phi) = \langle j, m | l, m'; \frac{1}{2}, s_3 \rangle Y_{lm'}(\theta, \phi) \chi(s_3). \quad (6.170)$$

The derivation is given in Appendix 6A.

The explicit form of the spinor spherical harmonics (6.170) is for $l = l_{\pm}$:

$$y_{j,m}^{l_+}(\theta, \phi) = \frac{1}{\sqrt{2l_+ + 1}} \begin{pmatrix} \sqrt{l_+ - m + \frac{1}{2}} Y_{l_+, m - \frac{1}{2}}(\theta, \phi) \\ -\sqrt{l_+ + m + \frac{1}{2}} Y_{l_+, m + \frac{1}{2}}(\theta, \phi) \end{pmatrix}, \quad (6.171)$$

$$y_{j,m}^{l_-}(\theta, \phi) = \frac{1}{\sqrt{2l_- + 1}} \begin{pmatrix} \sqrt{l_- + m + \frac{1}{2}} Y_{l_-, m - \frac{1}{2}}(\theta, \phi) \\ \sqrt{l_- - m + \frac{1}{2}} Y_{l_-, m + \frac{1}{2}}(\theta, \phi) \end{pmatrix}. \quad (6.172)$$

On these eigenfunctions, the operator $\mathbf{L} \cdot \boldsymbol{\sigma}$ has the eigenvalues

$$\mathbf{L} \cdot \boldsymbol{\sigma} y_{j,m}^{l_{\pm}}(\theta, \phi) = -(1 + \kappa_{\pm}) y_{j,m}^{l_{\pm}}(\theta, \phi), \quad (6.173)$$

with

$$\kappa_{\pm} = \mp(j + \frac{1}{2}), \quad j = l \pm \frac{1}{2}. \quad (6.174)$$

We can now go from Eqs. (6.167) to radial differential equations by using the trivial identity,

$$i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \frac{f(r)}{r} y_{l,m}^{l_+} \equiv \frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{r^2} (\boldsymbol{\sigma} \cdot \mathbf{x}) i(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) \frac{f(r)}{r} y_{l,m}^{l_+}, \quad (6.175)$$

and the algebraic relation Eq. (4.464) in the form

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}) + i(\mathbf{a} \cdot \mathbf{b}), \quad (6.176)$$

to bring the right-hand side to

$$\frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{r^2} (ir\partial_r - i\boldsymbol{\sigma} \cdot \mathbf{L}) \frac{f(r)}{r} y_{l,m}^{l+} = \left[i\partial_r \frac{f(r)}{r} - i(1+\kappa) \frac{f(r)}{r^2} \right] \boldsymbol{\sigma} \cdot \hat{\mathbf{x}} y_{l,m}^{l+}. \quad (6.177)$$

In this way we find the radial differential equations for the functions $F_{jl}(r)$ and $G_{jl}(r)$:

$$\left(E - M + \frac{Z\alpha}{r} \right) G_{jl}(r) = -\frac{d}{dr} F_{jl}(r) \mp (j+1/2) \frac{1}{r} F_{jl}(r), \quad (6.178)$$

$$\left(E + M + \frac{Z\alpha}{r} \right) F_{jl}(r) = \frac{d}{dr} G_{jl}(r) \mp (j+1/2) \frac{1}{r} G_{jl}(r). \quad (6.179)$$

To solve these, dimensionless variables $\rho \equiv 2r/\lambda$ are introduced, with $\lambda = 1/\sqrt{M^2 - E^2}$, writing

$$F(r) = \sqrt{1 - E/M} e^{-\rho/2} (F_1 - F_2)(\rho), \quad G(r) = \sqrt{1 + E/M} e^{-\rho/2} (F_1 + F_2)(\rho). \quad (6.180)$$

The functions $F_{1,2}(\rho)$ satisfy a degenerate hypergeometric differential equation of the form

$$\left[\rho \frac{d^2}{d\rho^2} + (b - \rho) \frac{d}{d\rho} - a \right] F(a, b; \rho) = 0, \quad (6.181)$$

and the solutions are

$$\begin{aligned} F_2(\rho) &= \rho^l F(\gamma - Z\alpha E\lambda, 2\gamma + 1; \rho), \\ F_1(\rho) &= \rho^l \frac{\gamma - Z\alpha E\lambda}{-1/\lambda + Z\alpha E\lambda} F(\gamma + 1 - Z\alpha E\lambda, 2\gamma + 1; \rho). \end{aligned} \quad (6.182)$$

The constant γ is Einstein's gamma parameter $\gamma = \sqrt{1 - v^2/c^2}$ for the atomic unit velocity $v = Z\alpha c$. It has the expansion $\gamma = 1 - Z^2\alpha^2/2$.

As an example, we write down explicitly the ground state wave functions of the $1S^{1/2}$ state:

$$\psi_{1S^{1/2}, \pm \frac{1}{2}} = \sqrt{\frac{(2MZ\alpha)^3}{4\pi} \frac{1+\gamma}{2\Gamma(1+2\gamma)}} \frac{e^{-mZ\alpha r}}{(2MZ\alpha)^{1-\gamma}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ i\frac{1-\gamma}{Z\alpha} \cos \theta & i\frac{1-\gamma}{Z\alpha} \sin \theta e^{-i\phi} \\ i\frac{1-\gamma}{Z\alpha} \sin \theta e^{i\phi} & -i\frac{1-\gamma}{Z\alpha} \cos \theta \end{pmatrix}. \quad (6.183)$$

The first column is for $m = 1/2$, the second for $m = -1/2$. For small α , Einstein's gamma parameter has the expansion $\gamma = 1 - Z^2\alpha^2/2$, and we see that for $\alpha \rightarrow 0$, the upper components of the spinor wave functions tend to the nonrelativistic Schrödinger wave function $2\sqrt{(Z\alpha M)^3/4\pi} e^{-\rho}$, multiplied by Pauli spinors (4.446). In general,

$$\xi_{j,m}^l(\mathbf{x}) = \langle j, m | l, m; \frac{1}{2}, s_3 \rangle \psi_{nlm}(\mathbf{x}) \chi(s_3). \quad (6.184)$$

The lower (small) components vanish.

6.6 Green Function in an External Electromagnetic Field

An important physical object of a field theory is the Green function, defined as the solution of the equation of motion having a δ -function source term [recall (1.315) and (2.402)]. For external electromagnetic fields which are constant or plane waves, this Green function can be calculated exactly.

6.6.1 Scalar Field in a Constant Electromagnetic Field

For a scalar field, the Green function $G(x, x')$ is defined by the inhomogeneous differential equation

$$(-\partial^2 - M^2)G(x, x') = i\delta^{(4)}(x - x'), \quad (6.185)$$

whose solution can immediately be expressed as a Fourier integral:

$$G(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')} = \int_0^\infty d\tau \int \frac{d^4p}{(2\pi)^4} e^{-ip(x-x') + i\tau(p^2 - M^2 + i\eta)}. \quad (6.186)$$

A detailed discussion of this function will be given in Subsection 7.2.2.

Here we shall address the problem of calculating the corresponding Green function in the presence of a static electromagnetic field, which obeys the more complicated differential equation

$$\{[i\partial - eA(x)]^2 - M^2\} G(x, x') = i\delta^{(4)}(x - x'), \quad (6.187)$$

for which a Fourier decomposition is no longer helpful. For either a constant or an oscillating electromagnetic field, however, this equation can be solved by an elegant method due to Fock and Schwinger [2].

Generalizing the right-hand side of (6.186), we find the representation

$$G(x - x') = \int_0^\infty d\tau \langle x | e^{i\tau[(i\partial - eA)^2 - M^2 + i\eta]} | x' \rangle. \quad (6.188)$$

The integrand contains the time-evolution operator associated with the Hamiltonian operator

$$\hat{H}(x, i\partial) \equiv -(i\partial - eA)^2 + M^2. \quad (6.189)$$

This is the Schrödinger representation of the operator

$$\hat{H} = H(\hat{x}, \hat{p}) = -\hat{P}^2 + M^2, \quad (6.190)$$

where $\hat{P}_\mu \equiv \hat{p}_\mu - eA_\mu(\hat{x})$ is the canonical momentum in the presence of electromagnetism.

We shall calculate the evolution operator in (6.188) by introducing time-dependent Heisenberg operators for position and momentum. These obey the Heisenberg-Ehrenfest equations of motion [recall (1.277)]:

$$\frac{d\hat{x}^\mu(\tau)}{d\tau} = i [\hat{H}, \hat{x}^\mu(\tau)] = 2\hat{P}^\mu(\tau) \quad (6.191)$$

$$\frac{d\hat{P}^\mu(\tau)}{d\tau} = i [\hat{H}, \hat{P}^\mu(\tau)] = 2eF^\mu{}_\nu(\hat{x}(\tau))\hat{P}^\nu(\tau) + ie\partial^\nu F_{\mu\nu}(\hat{x}(\tau)). \quad (6.192)$$

In a constant field where $F^\mu{}_\nu(\hat{x}(\tau))$ is a constant matrix $F^\mu{}_\nu$, the last term in the second equation is absent, and we find directly the solution

$$\hat{P}^\mu(\tau) = \left(e^{2eF\tau}\right)^\mu{}_\nu \hat{P}^\nu(0). \quad (6.193)$$

Here the matrix $\left(e^{2eF\tau}\right)^\mu{}_\nu$ is defined by its formal power series expansion

$$\left(e^{2eF\tau}\right)^\mu{}_\nu = \delta^\mu{}_\nu + 2eF^\mu{}_\nu\tau + 4e^2F^\mu{}_\lambda F^\lambda{}_\nu \frac{\tau^2}{2} + \dots \quad (6.194)$$

Inserting (6.193) into Eq. (6.191), we find the time-dependent operator $\hat{x}^\mu(\tau)$:

$$\hat{x}^\mu(\tau) - \hat{x}^\mu(0) = \left(\frac{e^{2eF\tau} - 1}{eF}\right)^\mu{}_\nu \hat{P}^\nu(0), \quad (6.195)$$

where the matrix on the right-hand side is again defined by its formal power series

$$\left(\frac{e^{2eF\tau} - 1}{eF}\right)^\mu{}_\nu = 2\tau + e^2F^\mu{}_\lambda F^\lambda{}_\nu \frac{(2\tau)^3}{3!} + \dots \quad (6.196)$$

Note that division by eF is *not* a matrix multiplication by the inverse of the matrix eF but indicates the reduction of the expansion powers of eF by one unit. This is defined also if eF does not have an inverse.

We can invert Eq. (6.195) to find

$$\hat{P}^\nu(0) = \frac{1}{2} \left[eF \frac{e^{-eF\tau}}{\sinh eF\tau} \right]^\mu{}_\nu [\hat{x}(\tau) - \hat{x}(0)]^\nu, \quad (6.197)$$

and, using (6.193),

$$\hat{P}^\nu(\tau) = L^\mu{}_\nu(eF\tau) [\hat{x}(\tau) - \hat{x}(0)]^\nu, \quad (6.198)$$

with the matrix

$$L^\mu{}_\nu(eF\tau) \equiv \frac{1}{2} \left[eF^\mu{}_\nu \frac{e^{eF\tau}}{\sinh eF\tau} \right]^\mu{}_\nu. \quad (6.199)$$

By squaring (6.198) we obtain

$$\hat{P}^2(\tau) = [\hat{x}(\tau) - \hat{x}(0)]^\mu K_\mu{}^\nu(eF\tau) [\hat{x}(\tau) - \hat{x}(0)]_\nu, \quad (6.200)$$

where

$$K_\mu{}^\nu(eF\tau) = L^\lambda{}_\mu(eF\tau) L_\lambda{}^\nu(eF\tau). \quad (6.201)$$

Using the antisymmetry of the matrix $F_{\mu\nu}$, we can rewrite this as

$$K_\mu{}^\nu(eF\tau) = L_\mu{}^\lambda(-eF\tau) L_\lambda{}^\nu(eF\tau) = \frac{1}{4} \left[\frac{e^2 F^2}{\sinh^2 eF\tau} \right]^\nu{}_\mu. \quad (6.202)$$

The commutator between two operators $\hat{x}(\tau)$ at different times is

$$[\hat{x}^\mu(\tau), \hat{x}_\nu(0)] = i \left(\frac{e^{2eF\tau} - 1}{eF} \right)^\mu{}_\nu, \quad (6.203)$$

and

$$\begin{aligned} [\hat{x}^\mu(\tau), \hat{x}_\nu(0)] + [\hat{x}_\nu(\tau), \hat{x}^\mu(0)] &= i \left(\frac{e^{2eF\tau} - 1}{eF} \right)^\mu{}_\nu + i \left(\frac{e^{2eF^T\tau} - 1}{eF^T} \right)^\mu{}_\nu \\ &= i \left(\frac{e^{2eF\tau} - e^{-2eF\tau}}{eF} \right)^\mu{}_\nu = 2i \left[\frac{\sinh 2eF\tau}{eF} \right]^\mu{}_\nu. \end{aligned} \quad (6.204)$$

With the help of this commutator, we can expand (6.200) in powers of operators $\hat{x}(\tau)$ and $\hat{x}(0)$. We must be sure to let the later operators $\hat{x}(\tau)$ lie to the left of the earlier operators $\hat{x}(0)$ as follows:

$$\begin{aligned} H(\hat{x}(\tau), \hat{x}(0); \tau) &= -\hat{x}^\mu(\tau) K_\mu{}^\nu(eF\tau) \hat{x}_\nu(\tau) - \hat{x}^\mu(0) K_\mu{}^\nu(eF\tau) \hat{x}_\nu(0) \\ &+ 2\hat{x}^\mu(\tau) K_\mu{}^\nu(eF\tau) \hat{x}_\nu(0) - \frac{i}{2} \text{tr} [eF \coth eF\tau] + M^2. \end{aligned} \quad (6.205)$$

Given this form of the Hamiltonian operator, it is easy to calculate the time evolution amplitude in Eq. (6.188):

$$\langle x, \tau | x' 0 \rangle \equiv \langle x | e^{-i\hat{H}\tau} | x' \rangle. \quad (6.206)$$

It satisfies the differential equation

$$\begin{aligned} i\partial_\tau \langle x, \tau | x' 0 \rangle &\equiv \langle x | \hat{H} e^{-i\hat{H}\tau} | x' \rangle = \langle x | e^{-i\hat{H}\tau} [e^{i\hat{H}\tau} \hat{H} e^{-i\hat{H}\tau}] | x' \rangle \\ &= \langle x, \tau | \hat{H}(\hat{x}(\tau), \hat{P}(\tau)) | x', 0 \rangle. \end{aligned} \quad (6.207)$$

Replacing the operator $H(\hat{x}(\tau), \hat{P}(\tau))$ by $H(\hat{x}(\tau), \hat{x}(0); \tau)$ of Eq. (6.205), the matrix elements on the right-hand side can immediately be evaluated, using the property

$$\langle x, \tau | \hat{x}(\tau) = x \langle x, \tau |, \quad \hat{x}(0) | x', 0 \rangle = x' | x', 0 \rangle, \quad (6.208)$$

and the differential equation (6.209) becomes

$$i\partial_\tau \langle x, \tau | x' 0 \rangle \equiv H(x, x'; \tau) \langle x, \tau | x' 0 \rangle, \quad (6.209)$$

or

$$\langle x, \tau | x' 0 \rangle = C(x, x') E(x, x'; \tau) \equiv C(x, x') e^{-i \int d\tau H(x, x'; \tau)}. \quad (6.210)$$

The prefactor $C(x, x')$ contains a possible constant of integration in the exponent which may have an arbitrary dependence on x and x' . The following integrals are needed:

$$\int d\tau K(eF\tau) = \frac{1}{4} \int d\tau \frac{e^2 F^2}{\sinh^2 eF\tau} = -\frac{1}{4} eF \coth eF\tau, \quad (6.211)$$

and

$$\int d\tau \operatorname{tr} [eF \coth eF\tau] = \operatorname{tr} \log \frac{\sinh eF\tau}{eF} = \operatorname{tr} \log \frac{\sinh eF\tau}{eF\tau} + 4 \log \tau. \quad (6.212)$$

These results follow again from a Taylor expansion of both sides. As a consequence, the exponential factor $E(x, x'; \tau)$ in (6.210) becomes

$$E(x, x'; \tau) = \frac{1}{\tau^2} \exp \left\{ -\frac{i}{4} (x-x')^\mu [eF \coth eF\tau]_\mu{}^\nu (x-x')_\nu - iM^2\tau - \frac{1}{2} \operatorname{tr} \log \frac{\sinh eF\tau}{eF\tau} \right\}. \quad (6.213)$$

The last term produces a prefactor

$$\det^{-1/2} \left(\frac{\sinh eF\tau}{eF\tau} \right). \quad (6.214)$$

The time-independent integration constant is fixed by the differential equation with respect to x :

$$\begin{aligned} [i\partial_\mu - eA_\mu(x)] \langle x, \tau | x' 0 \rangle &= \langle x | \hat{P}_\mu e^{-i\hat{H}\tau} | x' \rangle = \langle x | e^{-i\hat{H}\tau} [e^{i\hat{H}\tau} \hat{P}_\mu e^{-i\hat{H}\tau}] | x' \rangle \\ &= \langle x, \tau | \hat{P}_\mu(\tau) | x' 0 \rangle, \end{aligned} \quad (6.215)$$

which becomes, after inserting (6.198):

$$[i\partial_\mu - eA_\mu(x)] \langle x, \tau | x' 0 \rangle = L_\mu{}^\nu(eF\tau)(x-x')_\nu \langle x, \tau | x' 0 \rangle. \quad (6.216)$$

Calculating the partial derivative we find

$$\begin{aligned} i\partial_\mu \langle x, \tau | x' 0 \rangle &= [i\partial_\mu C(x, x')] E(x, x'; \tau) + C(x, x') [i\partial_\mu E(x, x'; \tau)] \\ &= [i\partial_\mu C(x, x')] E(x, x'; \tau) + C(x, x') \frac{1}{2} [eF \coth eF\tau]_\mu{}^\nu (x-x')_\nu E(x, x'; \tau). \end{aligned}$$

Subtracting from this $eA_\mu(x) \langle x, \tau | x' 0 \rangle$, and inserting (6.210), the right-hand side of (6.216) is equal to $[i\partial_\mu C(x, x')] E(x, x'; \tau)$ plus

$$\left\{ L_\mu{}^\nu(eF\tau)(x-x')_\nu - \frac{1}{2} [eF \coth eF\tau]_\mu{}^\nu (x-x')_\nu \right\} C(x, x') E(x, x'; \tau). \quad (6.217)$$

Inserting Eq. (6.199), this simplifies to

$$\frac{e}{2} F_\mu{}^\nu (x-x')_\nu C(x, x') E(x, x'; \tau), \quad (6.218)$$

so that $C(x, x')$ satisfies the time-independent differential equation

$$\left[i\partial^\mu - eA^\mu(x) - \frac{e}{2} F^\mu{}_\nu (x-x')^\nu \right] C(x, x') = 0. \quad (6.219)$$

This is solved by

$$C(x, x') = C \exp \left\{ -ie \int_{x'}^x d\xi^\mu \left[A_\mu(\xi) + \frac{1}{2} F_\mu{}^\nu (\xi - x')_\nu \right] \right\}. \quad (6.220)$$

The contour of integration is arbitrary since $A'(\xi) \equiv A_\mu(\xi) + \frac{1}{2}F_\mu{}^\nu(\xi - x')_\nu$ has a vanishing curl:

$$\partial_\mu A'_\nu(x) - \partial_\nu A'_\mu(x) = 0. \quad (6.221)$$

We can therefore choose the contour to be a straight line connecting x' and x , in which case the F -term does not contribute in (6.220), since $d\xi^\mu$ points in the same direction of $x^\mu - x'^\mu$ as $\xi^\mu - x'^\mu$ and $F_{\mu\nu}$ is antisymmetric. Hence we may write for a straight-line connection

$$C(x, x') = C \exp \left[-ie \int_{x'}^x d\xi^\mu A_\mu(\xi) \right]. \quad (6.222)$$

The normalization constant C is finally fixed by the initial condition

$$\lim_{\tau \rightarrow 0} \langle x, \tau | x' 0 \rangle = \delta^{(4)}(x - x'), \quad (6.223)$$

which requires

$$C = -\frac{i}{(4\pi)^2}. \quad (6.224)$$

Collecting all terms we obtain

$$\begin{aligned} \langle x, \tau | x' 0 \rangle &= -\frac{i}{(4\pi\tau)^2} \exp \left[-ie \int_{x'}^x d\xi^\mu A_\mu(\xi) \right] \det^{-1/2} \left(\frac{\sinh eF\tau}{eF\tau} \right) \\ &\times \exp \left\{ -\frac{i}{4} (x - x')^\mu [eF \coth eF\tau]_\mu{}^\nu (x - x')_\nu - iM^2\tau \right\}. \end{aligned} \quad (6.225)$$

For a vanishing field $F_\mu{}^\nu$, this reduces to the relativistic free-particle amplitude

$$\langle x, \tau | x' 0 \rangle = -\frac{i}{(4\pi\tau)^2} \exp \left[-\frac{i}{2} \frac{(x - x')^2}{2\tau} - iM^2\tau \right]. \quad (6.226)$$

According to relation (6.188), the Green function of the scalar field is given by the integral

$$G(x, x') = \int_0^\infty d\tau \langle x, \tau | x' 0 \rangle. \quad (6.227)$$

The functional trace of (6.225),

$$\text{Tr} \langle x, \tau | x 0 \rangle = V \Delta t \frac{i}{(4\pi\tau)^2} \frac{eE\tau}{\sinh eE\tau}, \quad (6.228)$$

will be needed below. Due to translation invariance in spacetime, it carries a factor equal to the total spacetime volume $V \times \Delta t$ of the universe.

The result (6.228) can be checked by a more elementary derivation [3]. We let the constant electric field point in the z -direction, and represent it by a vector potential to have only a zeroth component

$$A^3(x) = -Ex^0. \quad (6.229)$$

Then the Hamiltonian (6.190) becomes

$$\hat{H} = -\hat{p}_0^2 + \hat{\mathbf{p}}_\perp^2 + (\hat{p}^3 + eEx_0)^2 + M^2, \quad (6.230)$$

where $\mathbf{p}_\perp$ are the two-dimensional momenta in the xy -plane. Using the commutation rule $[p_0, x_0] = i$, this can be rewritten as

$$\hat{H} = e^{-i\hat{p}_0 p^3/eE} \hat{H}' e^{i\hat{p}_0 p^3/eE}, \quad (6.231)$$

where $\hat{H}'$ is the sum of two commuting Hamiltonians:

$$\hat{H}' = -(\hat{p}_0^2 - e^2 E^2 x_0^2) + \mathbf{p}_\perp^2 + M^2 \equiv \hat{H}_{\omega_E} + \hat{H}_\perp. \quad (6.232)$$

The first is a harmonic Hamiltonian with imaginary frequency $\omega_E = ieE$ and an energy spectrum $-2(n + 1/2)ieE$. The second describes a free particle in the xy -plane. This makes it easy to calculate the functional trace. We insert a complete set of momentum states on either side of (6.206), so that the functional trace becomes

$$\text{Tr} \langle x, \tau | x 0 \rangle = \int d^4x \int \frac{d^4p}{(2\pi)^4} \int \frac{d^4p'}{(2\pi)^4} e^{-i(p-p')x} \langle p | e^{-i\tau(\hat{H}_{\omega_E} + \hat{H}_\perp)} | p' \rangle. \quad (6.233)$$

The matrix elements are

$$\begin{aligned} \langle p | e^{-i\tau\hat{H}} | p' \rangle &= e^{-ip_0(x_0 + p^3/eE)} \langle p_0 | e^{-is\hat{H}_{\omega_E}} | p'_0 \rangle e^{-i\tau(p_\perp^2 + M^2 - i\eta)} e^{ip'_0(x_0 + p'^3/eE)} \\ &\times (2\pi)^2 \delta^{(2)}(\mathbf{p}_\perp - \mathbf{p}'_\perp) (2\pi) \delta(p^3 - p'^3). \end{aligned} \quad (6.234)$$

Inserting this into (6.233) and performing the integrals over the spatial parts of p' appearing in the δ -functions of (6.234) yields

$$\begin{aligned} \text{Tr} \langle x, \tau | x 0 \rangle &= V \int dx_0 \int \frac{d^2p_\perp}{(2\pi)^2} e^{-i\tau(p_\perp^2 + M^2 - i\eta)} \\ &\times \int \frac{dp_0 dp^3 dp'_0}{(2\pi)^3} e^{-i(p_0 - p'_0)(x_0 + p^3/eE)} \langle p_0 | e^{-is\hat{H}_{\omega_E}} | p'_0 \rangle, \end{aligned} \quad (6.235)$$

which can be reduced to

$$\text{Tr} \langle x, \tau | x 0 \rangle = V \Delta t \frac{-i}{4\pi\tau} e^{-i\tau(M^2 - i\eta)} \frac{eE}{2\pi} \left[\int \frac{dp_0}{2\pi} \langle p_0 | e^{-i\tau\hat{H}_{\omega_E}} | p_0 \rangle \right]. \quad (6.236)$$

The expression in brackets is the trace of $e^{-i\tau\hat{H}_{\omega_E}}$, which is conveniently calculated in the eigenstates $|n\rangle$ of the harmonic oscillator with eigenvalues $-2(n + 1/2)\omega_E$:

$$\text{Tr} e^{-i\tau\hat{H}_{\omega_E}} = \sum_{n=0}^{\infty} e^{i\tau 2(n+1/2)eE} = \frac{i}{2 \sin \omega_E} = \frac{1}{2 \sinh \tau eE}. \quad (6.237)$$

Thus we obtain

$$\text{Tr} \langle x, \tau | x 0 \rangle = V \Delta t \frac{-i}{4(2\pi)^2 \tau^2} \frac{eE\tau}{\sinh \tau eE}. \quad (6.238)$$

6.6.2 Dirac Field in a Constant Electromagnetic Field

For a Dirac field we have to solve the inhomogeneous differential equation

$$\{i\gamma^\mu[\partial_\mu - eA_\mu(x)] - M\}S(x, x') = i\delta^{(4)}(x - x'), \quad (6.239)$$

rather than (6.187). The solution can formally be written as

$$S(x, x') = \{i\gamma^\mu[\partial_\mu - eA_\mu(x)] + M\}\bar{G}(x, x') = i\delta^{(4)}(x - x'), \quad (6.240)$$

where $\bar{G}(x, x')$ solves a slight generalization of Eq. (6.187):

$$\left\{[i\partial - eA(x)]^2 - \frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu - M^2\right\}\bar{G}(x, x') = i\delta^{(4)}(x - x'). \quad (6.241)$$

This is the Green function of the Pauli equation (6.110), in natural units. For a constant field, the extra term enters the final result (6.240) in a trivial way. We recall the relations (6.188) and (6.227) to the Green function, and see that $\bar{G}(x, x')$ contains the fields as follows:

$$\bar{G}(x, x') = \int_0^\infty d\tau \exp\left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau\right) \langle x, \tau | x' 0 \rangle. \quad (6.242)$$

Constant Electric Background Field

For a constant electric field in the z -direction, we choose the vector potential to have only a zeroth component

$$A^3(x) = -Ex^0. \quad (6.243)$$

Then, since $F^{30} = E$, we have $F_3^0 = -E$ and $F_0^3 = -E$. The field tensor $F_\mu{}^\nu$ is given by the matrix

$$F = -E \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = iE M_3, \quad (6.244)$$

where M_3 is the generator (4.60) of pure Lorentz transformations in the z -direction. The exponential $e^{eF\tau}$ is therefore equal to the boost transformation (4.59) $B_3(\zeta) = e^{-iM_3\zeta}$ with a rapidity $\zeta = -E\tau$. From (14.285) we find the explicit matrices

$$e^{eF\tau} = \begin{pmatrix} \cosh eE\tau & 0 & 0 & -\sinh eE\tau \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh eE\tau & 0 & 0 & \cosh eE\tau \end{pmatrix}, \quad (6.245)$$

and hence

$$\sinh eF\tau = \begin{pmatrix} 0 & 0 & 0 & -\sinh eE\tau \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\sinh eE\tau & 0 & 0 & 0 \end{pmatrix}, \quad (6.246)$$

$$\frac{\sinh eF\tau}{eF\tau} = \begin{pmatrix} \frac{\sinh eE\tau}{eE} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \frac{\sinh eE\tau}{eE} \end{pmatrix}, \quad (6.247)$$

and

$$eF \coth eF\tau = eE \begin{pmatrix} \coth eE\tau & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \coth eE\tau \end{pmatrix}. \quad (6.248)$$

Thus we obtain

$$\begin{aligned} \langle x, \tau | x' 0 \rangle &= \frac{i}{(4\pi\tau)^2} \frac{eE\tau}{\sinh eE\tau} \exp \left[-ie \int_{x'}^x d\xi^\mu A_\mu(\xi) \right] \\ &\times e^{\frac{i}{4} [-(x-x')^0 eE \coth eE\tau (x-x')^0 + (x-x')^T \frac{1}{\tau} (x-x')^T + (x-x')^3 eE \coth eE\tau (x-x')^3] - iM^2\tau}, \end{aligned} \quad (6.249)$$

where the superscript T indicates transverse directions to $\mathbf{E}$. The prefactor $\exp[-ie \int_{x'}^x d\xi^\mu A_\mu(\xi)]$ is found by inserting (6.243) and integrating along the straight line

$$\xi = x' + s(x - x'), \quad s \in [0, 1], \quad (6.250)$$

to be

$$\exp \left[-ie \int_{x'}^x d\xi^\mu A_\mu(\xi) \right] = e^{-ieE(x_0-x'_0) \int_0^1 ds [z' + s(z-z')]} = e^{-ieE(x_0-x'_0)(z+z')}. \quad (6.251)$$

The exponential prefactor in the fermionic Green function (6.242) is calculated in the chiral representation of the Dirac algebra where, due to (6.111) and (6.112),

$$\exp \left(-i\frac{e}{2} \sigma^\mu{}_\nu F_\mu{}^\nu \tau \right) = \exp(e\boldsymbol{\alpha}\mathbf{E}\tau) = \begin{pmatrix} e^{-\sigma\mathbf{e}\mathbf{E}\tau} & 0 \\ 0 & e^{\sigma\mathbf{e}\mathbf{E}\tau} \end{pmatrix}, \quad (6.252)$$

which is equal to

$$\exp \left(-i\frac{e}{2} \sigma^\mu{}_\nu F_\mu{}^\nu \tau \right) = \begin{pmatrix} \cosh eE\tau - \sinh eE\tau \boldsymbol{\sigma}\hat{\mathbf{E}} & 0 \\ 0 & \cosh eE\tau + \sinh eE\tau \boldsymbol{\sigma}\hat{\mathbf{E}} \end{pmatrix}. \quad (6.253)$$

Comparison with (4.506) shows that this is the Dirac representation of a Lorentz boost into the direction of $\mathbf{E}$ with rapidity $\zeta = 2e|\mathbf{E}|\tau$. The Dirac trace of the evolution amplitude for Dirac fields is then simply

$$\text{tr} \langle x, \tau | x 0 \rangle = -\frac{i}{(4\pi\tau)^2} \frac{eE\tau}{\sinh eE\tau} \times 4 \cosh eE\tau, \quad (6.254)$$

and the functional trace of this carries simply a total spacetime volume factor $V\Delta t$ that appeared before in Eq. (6.228).

Note that the Lorentz-transformation (6.253) has twice the rapidity of the transformation (6.245) in the defining representation, this being a manifestation of the gyromagnetic ratio of the electron in Dirac's theory which is equal to two [recall (6.119)].

The process of pair creation in a space- and time-dependent electromagnetic field is discussed in Ref. [4].

The above discussion becomes especially simple in 1+1 spacetime dimensions, the so-called *massive Schwinger model* [5].

6.6.3 Dirac Field in an Electromagnetic Plane-Wave Field

The results for constant-background fields in the last subsection simplify drastically if electric and magnetic fields have the same size and are orthogonal to each other. This is the case for a travelling plane wave of arbitrary shape [10] running along some direction n^μ with $n^2 = 0$. If ξ denotes the spatial coordinate along n , we may write the vector potential as

$$A_\mu(x) = \epsilon_\mu f(\xi), \quad \xi \equiv nx, \quad (6.255)$$

where ϵ^μ is some polarization vector with the normalization $\epsilon^2 = -1$ in the gauge $\epsilon n = 0$. The field tensor is

$$F_{\mu\nu} = \epsilon_{\mu\nu} f'(\xi), \quad \epsilon_{\mu\nu} \equiv n_\mu \epsilon_\nu - n_\nu \epsilon_\mu, \quad (6.256)$$

where the constant tensor $\epsilon_{\mu\nu}$ satisfies

$$\epsilon_{\mu\nu} n^\mu = 0, \quad \epsilon_{\mu\nu} \epsilon^\mu = 0, \quad \epsilon_{\mu\nu} \epsilon^{\nu\lambda} = n_\mu n_\lambda. \quad (6.257)$$

The Heisenberg equations of motion (6.191) and (6.192) take the form

$$\frac{d\hat{x}^\mu(\tau)}{d\tau} = i [\hat{H}, \hat{x}^\mu(\tau)] = 2\hat{P}^\mu(\tau) \quad (6.258)$$

$$\frac{d\hat{P}^\mu(\tau)}{d\tau} = i [\hat{H}, \hat{P}^\mu(\tau)] = 2e\epsilon^\mu_\nu \hat{P}^\nu(\tau) f'(\hat{\xi}(\tau)) + \frac{e}{2} n^\mu \epsilon_{\lambda\kappa} \sigma^{\lambda\kappa} f''(\hat{\xi}(\tau)). \quad (6.259)$$

Note that the last term in (6.259) vanishes for a sourceless plane wave: $\partial^\nu F_{\mu\nu} = 0$. Multiplying these equations by n_μ we see that

$$n_\mu \frac{d\hat{\xi}^\mu(\tau)}{d\tau} = 2n_\mu \hat{P}^\mu(\tau), \quad n_\mu \frac{d\hat{P}^\mu(\tau)}{d\tau} = 0. \quad (6.260)$$

Hence

$$n\hat{P}(\tau) = n\hat{P}(0) = \text{const}, \quad \hat{\xi}(\tau) - \hat{\xi}(0) = n\hat{x}(\tau) - n\hat{x}(0) = 2\tau n\hat{P}(\tau). \quad (6.261)$$

Whereas the components of $\hat{P}(\tau)$ parallel to n are time independent, those orthogonal to n have a nontrivial time dependence. To find it we multiply (6.259) by $\epsilon_{\mu\nu}$ and find

$$\frac{d}{d\tau} \epsilon_{\nu\mu} \hat{P}^\mu(\tau) = 2e\epsilon_{\nu\mu} \epsilon^{\mu\rho} \hat{P}_\rho f'(\hat{\xi}) = en_\nu f'(\hat{\xi}) (2n\hat{P}) = en_\nu f'(\hat{\xi}) \frac{d\hat{\xi}}{d\tau} = en_\nu \frac{df(\hat{\xi})}{d\tau}, \quad (6.262)$$

which is integrated to

$$\epsilon_{\nu\mu}\hat{P}^\mu(\tau) = en_\nu f(\hat{\xi}) + \hat{C}_\nu, \quad (6.263)$$

with an operator integration constant $\hat{C}_\nu$, that commutes with the constant $n\hat{P}$, and satisfies the relations $n^\nu\hat{C}^\nu = 0$ and

$$\epsilon^{\mu\nu}\hat{C}_\nu = n^\mu(n\hat{P}) = n^\mu \frac{\hat{\xi}(\tau) - \hat{\xi}(0)}{2\tau}. \quad (6.264)$$

Inserting this into (6.259), and integrating the resulting equation yields

$$\hat{P}_\mu(\tau) = \frac{1}{2\pi n} \left[2eC_\mu f(\hat{\xi}) + e^2 n_\mu f^2(\xi) + \frac{e}{2} n_\mu \epsilon_{\mu\nu} \sigma^{\mu\nu} f'(\hat{\xi}) \right] + \hat{D}_\mu, \quad (6.265)$$

where $\hat{D}_\mu$ is again an interaction constant commuting with $n\hat{P}$. Now we can integrate the equation of motion (6.258) over $d\tau = d\hat{\xi}/2n\hat{P}$, and find

$$\frac{1}{2} [\hat{x}(\tau) - \hat{x}(0)] = \frac{1}{(2n\hat{P})^2} \int_{\hat{\xi}(0)}^{\hat{\xi}(\tau)} d\hat{\xi} \left[2eC_\mu f(\hat{\xi}) + e^2 n_\mu f^2(\xi) + \frac{e}{2} n_\mu \epsilon_{\mu\nu} \sigma^{\mu\nu} f'(\hat{\xi}) \right] + \hat{D}_\mu \tau. \quad (6.266)$$

We determine $\hat{D}_\mu$, and insert it into (6.265) to find

$$\begin{aligned} \hat{P}_\mu(\tau) &= \frac{1}{2\tau} [\hat{x}_\mu(\tau) - \hat{x}_\mu(0)] \\ &\quad - \frac{\tau}{[\hat{\xi}(\tau) - \hat{\xi}(0)]^2} \int_{\hat{\xi}(0)}^{\hat{\xi}(\tau)} d\hat{\xi} \left[2e\hat{C}_\mu f(\hat{\xi}) + e^2 n_\mu f^2(\hat{\xi}) + \frac{e}{2} n_\mu \epsilon_{\rho\nu} \sigma^{\rho\nu} f'(\hat{\xi}) \right] \\ &\quad + \frac{\tau}{\hat{\xi}(\tau) - \hat{\xi}(0)} \left[2e\hat{C}_\nu f(\hat{\xi}(\tau)) + e^2 n_\mu f^2(\hat{\xi}(\tau)) + \frac{e}{2} n_\mu \epsilon_{\rho\nu} \sigma^{\rho\nu} f'(\hat{\xi}(\tau)) \right]. \end{aligned} \quad (6.267)$$

After multiplication by $\epsilon^{\nu\mu}$, and recalling (6.257) and (6.264), we obtain

$$\begin{aligned} \epsilon^{\nu\mu}\hat{P}_\mu(\tau) &= \frac{1}{2\tau} \epsilon^{\nu\mu} [\hat{x}_\mu(\tau) - \hat{x}_\mu(0)] + \\ &\quad - \frac{en^\nu}{\xi(\tau) - \hat{\xi}(0)} \int_{\hat{\xi}(0)}^{\hat{\xi}(\tau)} d\hat{\xi} f(\hat{\xi}) + en^\nu f(\hat{\xi}(\tau)). \end{aligned} \quad (6.268)$$

Inserting this into (6.263) determines the integration constant $\hat{C}^\nu$:

$$\hat{C}^\nu = \frac{1}{2\tau} \epsilon^{\nu\mu} [\hat{x}_\mu(\tau) - \hat{x}_\mu(0)] - \frac{en^\nu}{\xi(\tau) - \hat{\xi}(0)} \int_{\hat{\xi}(0)}^{\hat{\xi}(\tau)} d\hat{\xi} f(\hat{\xi}). \quad (6.269)$$

It is useful to introduce the notations

$$\langle f \rangle \equiv \frac{1}{\xi(\tau) - \hat{\xi}(0)} \int_{\hat{\xi}(0)}^{\hat{\xi}(\tau)} d\hat{\xi} f(\hat{\xi}) \quad (6.270)$$

and

$$\langle (\delta f)^2 \rangle \equiv \langle (f - \langle f \rangle)^2 \rangle = \langle f^2 \rangle - \langle f \rangle^2. \quad (6.271)$$

In order to calculate the matrix elements

$$\langle x \tau | \hat{H} | x 0 \rangle = \left\langle x \tau \left| -\hat{P}^2 + \frac{e}{2} \sigma^\mu{}_\nu F_\mu{}^\nu + M^2 \right| x 0 \right\rangle, \quad (6.272)$$

we must time-order the operators $\hat{x}(\tau), \hat{x}(0)$. For this we need the commutator

$$[\hat{x}_\mu(\tau), \hat{x}_\nu(0)] = 2i\tau g_{\mu\nu}. \quad (6.273)$$

This is deduced from Eq. (6.267) by commuting it with $\hat{x}(\tau)$ and using the trivially vanishing equal-time commutator $[\hat{\xi}(\tau), \hat{x}^\nu(\tau)] = 0$, as well as the nonequal-time commutator $[\hat{\xi}(0), \hat{x}^\nu(\tau)] = 2in^\nu\tau$. The latter implies that $[\hat{\xi}(\tau), \hat{x}^\nu(0)] = 0$, which is also needed for time-ordering. The result is

$$\langle x \tau | \hat{H} | x 0 \rangle = -\frac{1}{4\tau^2}(x-x')^2 - 2\frac{i}{\tau} + \left(M^2 + e^2\langle(\delta\phi)^2\rangle\right)^2 + e\epsilon_{\mu\nu}\sigma^{\mu\nu}\frac{f(\xi) - f(\xi')}{\xi - \xi'}. \quad (6.274)$$

Integrating this over τ we obtain the exponential factor of the time-evolution amplitude (6.210):

$$E(x, x'; \tau) = \frac{1}{\tau^2} \exp \left\{ -\frac{i}{4\tau}(x-x')^2 + \left(M^2 + e^2\langle(\delta f)^2\rangle\right)^2 - i\tau e\epsilon_{\mu\nu}\sigma^{\mu\nu}\frac{f(\xi) - f(\xi')}{\xi - \xi'} \right\}. \quad (6.275)$$

The time-independent prefactor $C(x, x')$ is again determined by the differential equation Eq. (6.215), which reduces here to

$$[i\partial_\mu - eA_\mu(x)] \langle x, \tau | x' 0 \rangle = \left[\frac{\epsilon^{\mu\nu}(x-x')_\nu}{\xi - \xi'} \langle f \rangle - f(\xi) \right] \langle x, \tau | x' 0 \rangle, \quad (6.276)$$

and is solved by

$$C(x, x') = \frac{-i}{(4\pi)^2} \exp \left(ie \int_{x'}^x dy_\mu \left\{ A^\mu(y) - \frac{\epsilon^{\mu\nu}(x-x')_\nu}{\xi - \xi'} \left[\int_\xi^{ny} dy' \frac{f(y')}{ny - \xi'} - f(ny) \right] \right\} \right). \quad (6.277)$$

For a straight-line integration contour, the second term does not contribute, as before.

Observe that in Eq. (6.275), the mass term M^2 is replaced by

$$M_{\text{eff}}^2 = M^2 + e^2\langle(\delta f)^2\rangle, \quad (6.278)$$

implying that, in an electromagnetic wave, a particle acquires a larger effective mass. If the wave is periodic with frequency ω and wavelength $\lambda = 2\pi c/\omega$, the right-hand side becomes $M^2 + e^2\langle f^2 \rangle$. If the photon number density is ρ , their energy density is $\rho\omega$ (in units with $\hbar = 1$), and we can calculate

$$e^2\langle f^2 \rangle = 4\pi\alpha \frac{\langle E^2 \rangle}{\omega^2} = 4\pi\alpha \frac{\rho}{\omega}. \quad (6.279)$$

Hence we find a relative mass shift:

$$\frac{\Delta M^2}{M^2} = 4\pi\alpha\lambda_e^2\lambda\rho, \quad (6.280)$$

where $\lambda_e \equiv \hbar/M_e c = 3.861592642(28) \times 10^{-3} \text{\AA}$ is the Compton wavelength of the electron. For visible light, the right-hand side is of the order of $\text{\AA}^3 \rho / 100$. Present lasers achieve energy densities of 10^9 W/sec corresponding to a photon density

$$\rho = \frac{1}{\hbar\omega} \times 10^9 \frac{\text{W}}{\text{sec}} \equiv 2.082 \times 10^{-7} \frac{1}{\text{\AA}^3} \frac{\text{eV}}{\hbar\omega}, \quad (6.281)$$

which is too small to make $\Delta M^2/M^2$ observable.

Appendix 6A Spinor Spherical Harmonics

Equation (6.170) defines spinor spherical harmonics. In these, an orbital wave function of angular momentum $l_{\pm}$ is coupled with spin $1/2$ to a total angular momentum $j = l_{\mp} \pm 1/2$. For the configurations $j = l_- + 1/2$ with $m_2 = -1/2$ the recursion relation (4E.20) for the Clebsch-Gordan coefficients $\langle s_1 m_1; s_2 m_2 | s m \rangle$ becomes simple by having no second term. Inserting $s_1 = l_-$, $s_2 = 1/2$, and $s = j = l_- + 1/2$, we find

$$\langle l_-, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_- - m + 1/2}{l_- - m + 3/2}} \langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l_- + \tfrac{1}{2}, m - 1 \rangle. \quad (6A.1)$$

This has to be iterated with the initial condition

$$\langle l_-, -l_-; \tfrac{1}{2}, -\tfrac{1}{2} | l_- + \tfrac{1}{2}, -l_- - \tfrac{1}{2} \rangle = 1, \quad (6A.2)$$

which follows from the fact that the state $\langle l_-, -l_-; \tfrac{1}{2}, -\tfrac{1}{2} \rangle$ carries a unique magnetic quantum number $m = -l_- - 1/2$ of the irreducible representation of total angular momentum $s = j = l_- + 1/2$. The result of the iteration is

$$\langle l_+, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_+ - m + 1/2}{2l_+ + 1}}. \quad (6A.3)$$

Similarly we may simplify the recursion relation (4E.21) for the configurations $j = l_+ - 1/2$ with $m_2 = 1/2$ to

$$\langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_- + m + 1/2}{l_- + m + 3/2}} \langle l_-, m + \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m + 1 \rangle, \quad (6A.4)$$

and iterate this with the initial condition

$$\langle l_-, l_-; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, l_- + \tfrac{1}{2} \rangle = 1, \quad (6A.5)$$

which expresses the fact that the state $\langle l_- l_-; \tfrac{1}{2}, \tfrac{1}{2} \rangle$ is the state of the maximal magnetic quantum number $m = l_- + 1/2$ in the irreducible representation of total angular momentum $s = j = l_- + 1/2$. The result of the iteration is

$$\langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_- + m + 1/2}{2l_- + 1}}. \quad (6A.6)$$

Using (6A.3) and (6A.6), the expression (6.170) for the spinor spherical harmonic of total angular momentum $j = l_- + 1/2$ reads

$$\begin{aligned} y_{j,m}^{l-}(\theta, \phi) &= \langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle Y_{l_{m-1/2}}(\theta, \phi) \chi(\tfrac{1}{2}) \\ &+ \langle l_- m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle Y_{l_{m+1/2}}(\theta, \phi) \chi(-\tfrac{1}{2}). \end{aligned} \quad (6A.7)$$

Separating the spin-up and spin-down components, we obtain precisely (6.172).

In order to find the corresponding result for $j = l_+ - 1/2$, we use the orthogonality relation for states with the same l but different $j = l \pm 1/2$:

$$\langle l + \tfrac{1}{2}, m | l - \tfrac{1}{2}, m \rangle = 0. \quad (6A.8)$$

Inserting a complete set of states in the direct product space yields

$$\begin{aligned} &\langle l + \tfrac{1}{2}, m | l, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} \rangle \langle l m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l - \tfrac{1}{2}, m \rangle \\ &+ \langle l + \tfrac{1}{2}, m | l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} \rangle \langle l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l - \tfrac{1}{2}, m \rangle = 0. \end{aligned} \quad (6A.9)$$

Together with (6A.3) and (6A.6) we find

$$\begin{aligned} \langle l_+, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle &= \sqrt{\frac{l_+ + m + 1/2}{2l_+ + 1}}, \\ \langle l_+, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle &= -\sqrt{\frac{l_+ - m + 1/2}{2l_+ + 1}}. \end{aligned} \quad (6A.10)$$

With this, the expression (6.170) for the spinor spherical harmonics written as

$$\begin{aligned} y_{j,m}^{l+}(\theta, \phi) &= \langle l_+, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle Y_{l_{m-1/2}}(\theta, \phi) \chi(\tfrac{1}{2}) \\ &+ \langle l_+, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle Y_{l_{m+1/2}}(\theta, \phi) \chi(-\tfrac{1}{2}) \end{aligned} \quad (6A.11)$$

has the components given in (6.171).

Notes and References

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*Life can only be understood backwards,
but it must be lived forwards.*
S. KIERKEGAARD (1813-1855)

7

Quantization of Relativistic Free Fields

In Chapter 2 we have shown that quantum mechanics of the N -body Schrödinger equation can be replaced by a Schrödinger *field theory*, where the fields are operators satisfying canonical equal-time commutation rules. They were given in Sections 2.8 and 2.10 for bosons and fermions, respectively. A great advantage of this reformulation of Schrödinger theory was that the field quantization leads automatically to symmetric or antisymmetric N -body wave functions, which in Schrödinger theory must be imposed from the outside in order to explain atomic spectra and Bose-Einstein condensation. Here we shall generalize the procedure to relativistic particles by quantizing the free relativistic fields of the previous section following the above general rules. For each field $\phi(\mathbf{x}, t)$ in a classical Lagrangian $L(t)$, we define a canonical field momentum as the functional derivative (2.156)

$$\pi(\mathbf{x}, t) = p_{\mathbf{x}}(t) = \frac{\delta L(t)}{\delta \dot{\phi}(\mathbf{x}, t)}. \quad (7.1)$$

The fields are now turned into field operators by imposing the canonical equal-time commutation rules (2.143):

$$[\phi(\mathbf{x}, t), \phi(\mathbf{x}', t)] = 0, \quad (7.2)$$

$$[\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = 0, \quad (7.3)$$

$$[\pi(\mathbf{x}, t), \phi(\mathbf{x}', t)] = -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.4)$$

For fermions, one postulates corresponding anticommutation rules.

In these equations we have omitted the hat on top of the field operators, and we shall do so from now on, for brevity, since most field expressions will contain quantized fields. In the few cases which do not deal with field operators, or where it is not obvious that the fields are classical objects, we shall explicitly state this. We shall also use natural units in which $c = 1$ and $\hbar = 1$, except in some cases where CGS-units are helpful.

Before implementing the commutation rules explicitly, it is useful to note that all free Lagrangians constructed in the last chapter are local, in the sense that they are given by volume integrals over a Lagrangian density

$$L(t) = \int d^3x \mathcal{L}(\mathbf{x}, t), \quad (7.5)$$

where $\mathcal{L}(\mathbf{x}, t)$ is an ordinary function of the fields and their first spacetime derivatives. The functional derivative (7.1) may therefore be calculated as a partial derivative of the density $\mathcal{L}(x) = \mathcal{L}(\mathbf{x}, t)$:

$$\pi(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{\phi}(x)}. \quad (7.6)$$

Similarly, the Euler-Lagrange equations may be written down using only partial derivatives

$$\partial^\mu \frac{\partial \mathcal{L}(x)}{\partial [\partial^\mu \phi(x)]} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)}. \quad (7.7)$$

Here and in the sequel we employ a four-vector notation for all spacetime objects such as $x = (x^0, \mathbf{x})$, where $x^0 = ct$ coincides with the time t in natural units.

The locality is an important property of all present-day quantum field theories of elementary particles. The spacetime derivatives appear usually only in quadratic terms. Since a derivative measures the difference of the field between neighboring spacetime points, the field described by a local Lagrangian propagates through spacetime via a “nearest-neighbor hopping”. In field-theoretic models of solid-state systems, such couplings are useful lowest approximations to more complicated short-range interactions. In field theories of elementary particles, the locality is an essential ingredient which seems to be present in all fundamental theories. All nonlocal effects arise from higher-order perturbation expansions of local theories.

7.1 Scalar Fields

We begin by quantizing the field of a spinless particle. This is a scalar field $\phi(x)$ that can be real or complex.

7.1.1 Real Case

The action of the real field was given in Eq. (4.167). As we shall see in Subsec. 7.1.6, and even better in Subsec. 8.11.1, the quanta of the real field are *neutral spinless particles*. For the canonical quantization we must use the real-field Lagrangian density (4.169) in which only first derivatives of the field occur:

$$\mathcal{L}(x) = \frac{1}{2} \{ [\partial \phi(x)]^2 - M^2 \phi^2(x) \}. \quad (7.8)$$

The associated Euler-Lagrange equation is the *Klein-Gordon equation* (4.170):

$$(-\partial^2 - M^2)\phi(x) = 0. \quad (7.9)$$

7.1.2 Field Quantization

According to the rule (7.6), the canonical momentum of the field is

$$\pi(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{\phi}(x)} = \partial^0 \phi(x) = \dot{\phi}(x). \quad (7.10)$$

As in the case of non-relativistic fields, the quantization rules (7.2)–(7.4) will eventually render a multiparticle Hilbert space. To find it we expand the field operator $\phi(x, t)$ in normalized plane-wave solutions (4.180) of the field equation (7.9):

$$\phi(x) = \sum_{\mathbf{p}} \left[f_{\mathbf{p}}(x) a_{\mathbf{p}} + f_{\mathbf{p}}^*(x) a_{\mathbf{p}}^\dagger \right]. \quad (7.11)$$

Observe that in contrast to a corresponding expansion (2.209) of the nonrelativistic Schrödinger field, the right-hand side contains operators for the creation and annihilation of particles. This is an automatic consequence of the fact that the quantizations of $\phi(x)$ and $\pi(x)$ lead to Hermitian field operators, and this is natural for quantum fields in the relativistic setting, which necessarily allow for the creation and annihilation of particles. Inserting for $f_{\mathbf{p}}(x)$ and $f_{\mathbf{p}}^*(x)$ the explicit wave functions (4.180), the expansion (7.11) reads

$$\phi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} (e^{-ipx} a_{\mathbf{p}} + e^{ipx} a_{\mathbf{p}}^\dagger). \quad (7.12)$$

Since the zeroth component of the four-momentum p^μ in the exponent is on the mass shell, we should write px more explicitly as $px = \omega_{\mathbf{p}} t - \mathbf{p}\mathbf{x}$. However, the notation px is shorter, and there is little danger of confusion. If there is such a danger, we shall explicitly state the off- or on-shell property $p^0 = \omega_{\mathbf{p}}$.

The expansions (7.11) and (7.12) are complete in the Hilbert space of free particles. They may be inverted for $a_{\mathbf{p}}$ and $a_{\mathbf{p}}^\dagger$ with the help of the orthonormality relations (4.177), which lead to the scalar products

$$a_{\mathbf{p}}^\dagger = (f_{\mathbf{p}}, \phi)_t, \quad a_{\mathbf{p}} = -(f_{\mathbf{p}}^*, \phi). \quad (7.13)$$

More explicitly, these can be written as

$$\begin{Bmatrix} a_{\mathbf{p}} \\ a_{\mathbf{p}}^\dagger \end{Bmatrix} = e^{\pm ip^0 x_0} \frac{1}{\sqrt{2V p^0}} \int d^3x e^{\mp i\mathbf{p}\mathbf{x}} \left[\pm i\pi(x) + p^0 \phi(x) \right], \quad (7.14)$$

where we have inserted $\pi(x) = \dot{\phi}(x)$.

Using the canonical field commutation rules (7.2)–(7.4) between $\phi(x)$ and $\pi(x)$, we find for the coefficients of the plane-wave expansion (7.12) the commutation relations

$$\begin{aligned} [a_{\mathbf{p}}, a_{\mathbf{p}'}] &= [a_{\mathbf{p}}^\dagger, a_{\mathbf{p}'}^\dagger] = 0, \\ [a_{\mathbf{p}}, a_{\mathbf{p}'}^\dagger] &= \delta_{\mathbf{p}, \mathbf{p}'}, \end{aligned} \quad (7.15)$$

making them creation and annihilation operators of particles of momentum $\mathbf{p}$ on a vacuum state $|0\rangle$ defined by $a_{\mathbf{p}}|0\rangle = 0$. Conversely, reinserting (7.15) into (7.12), we verify the original local field commutation rules (7.2)–(7.4).

In an infinite volume one often uses, in (7.11), the wave functions (4.181) with continuous momenta, and works with a plane-wave decomposition in the form of a Fourier integral

$$\phi(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} \left(e^{-ipx} a_{\mathbf{p}} + e^{ipx} a_{\mathbf{p}}^\dagger \right), \quad (7.16)$$

with the identification [recall (2.217)]

$$a_{\mathbf{p}} = \sqrt{2p^0 V} a_{\mathbf{p}}, \quad a_{\mathbf{p}}^\dagger = \sqrt{2p^0 V} a_{\mathbf{p}}^\dagger. \quad (7.17)$$

The inverse of the expansion is now

$$\left\{ \begin{array}{c} a_{\mathbf{p}} \\ a_{\mathbf{p}}^\dagger \end{array} \right\} = e^{\pm ip^0 x_0} \int d^3x e^{\mp i\mathbf{p}\mathbf{x}} \left[\pm i\pi(x) + p^0 \phi(x) \right]. \quad (7.18)$$

This can of course be written in the same form as in (7.13), using the orthogonality relations (4.182) for continuous-momentum wave functions (4.181):

$$a_{\mathbf{p}}^\dagger = (f_{\mathbf{p}}, \phi)_t, \quad a_{\mathbf{p}} = -(f_{\mathbf{p}}^*, \phi)_t. \quad (7.19)$$

In the expansion (7.11), the commutators (7.15) are valid after the replacement

$$\delta_{\mathbf{p},\mathbf{p}'} \rightarrow 2p^0 \delta^{(3)}(\mathbf{p} - \mathbf{p}') = 2p^0 (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}'), \quad (7.20)$$

which is a consequence of (1.190) and (1.196).

In the following we shall always prefer to work with a finite volume and sums over $\mathbf{p}$. If we want to find the large-volume limit of any formula, we can always go over to the continuum limit by replacing the sums, as in (2.257), by phase space integrals:

$$\sum_{\mathbf{p}} \rightarrow \int d^3p \frac{V}{(2\pi\hbar)^3}, \quad (7.21)$$

$$\delta_{\mathbf{p},\mathbf{p}'} \rightarrow \frac{(2\pi\hbar)^3}{V} \delta^{(3)}(\mathbf{p} - \mathbf{p}'). \quad (7.22)$$

After the replacement (7.17), the volume V disappears in all physical quantities.

A single-particle state of a fixed momentum $\mathbf{p}$ is created by

$$|\mathbf{p}\rangle = a_{\mathbf{p}}^\dagger |0\rangle. \quad (7.23)$$

Its wave function is obtained from the matrix elements of the field

$$\begin{aligned} \langle 0 | \phi(x) | \mathbf{p} \rangle &= \frac{1}{\sqrt{2Vp^0}} e^{-ipx} = f_{\mathbf{p}}(x), \\ \langle \mathbf{p} | \phi(x) | 0 \rangle &= \frac{1}{\sqrt{2Vp^0}} e^{ipx} = f_{\mathbf{p}}^*(x). \end{aligned} \quad (7.24)$$

As in the nonrelativistic case, the second-quantized Hilbert space is obtained by applying the particle creation operators $a_{\mathbf{p}}^\dagger$ to the vacuum state $|0\rangle$, defined by $a_{\mathbf{p}}^\dagger|0\rangle = 0$. This produces basis states (2.219):

$$|n_{\mathbf{p}_1} n_{\mathbf{p}_2} \dots n_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A} (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \dots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} |0\rangle. \quad (7.25)$$

Multiparticle wave functions are obtained by matrix elements of the type (2.221).

The single-particle states are

$$|\mathbf{p}\rangle = a_{\mathbf{p}}^\dagger |0\rangle. \quad (7.26)$$

They satisfy the orthogonality relation

$$(\mathbf{p}'|\mathbf{p}) = 2p^0 \delta^{(3)}(\mathbf{p}' - \mathbf{p}). \quad (7.27)$$

Their wave functions are

$$\begin{aligned} (0|\phi(x)|\mathbf{p}) &= e^{-ipx} = f_{\mathbf{p}}(x), \\ (\mathbf{p}|\phi(x)|0) &= e^{ipx} = f_{\mathbf{p}}^*(x). \end{aligned} \quad (7.28)$$

Energy of Free Neutral Scalar Particles

On account of the local structure (7.5) of the Lagrangian, also the Hamiltonian can be written as a volume integral

$$H = \int d^3x \mathcal{H}(x). \quad (7.29)$$

The Hamiltonian density is the Legendre transform of the Lagrangian density

$$\begin{aligned} \mathcal{H}(x) &= \pi(x) \partial^0 \phi(x) - \mathcal{L}(x) \\ &= \frac{1}{2} [\partial^0 \phi(x)]^2 + \frac{1}{2} [\partial_{\mathbf{x}} \phi(x)]^2 + \frac{M^2}{2} \phi^2(x). \end{aligned} \quad (7.30)$$

Inserting the expansion (7.12), we obtain the Hamilton operator

$$\begin{aligned} H &= \sum_{\mathbf{p}, \mathbf{p}'} \left\{ \frac{1}{2\sqrt{p^0 p'^0}} \delta_{\mathbf{p}, \mathbf{p}'} (p^0 p'^0 + \mathbf{p} \cdot \mathbf{p}' + M^2) (a_{\mathbf{p}}^\dagger a_{\mathbf{p}'} + a_{\mathbf{p}} a_{\mathbf{p}'}^\dagger) \right. \\ &\quad \left. + \frac{1}{2\sqrt{p^0 p'^0}} \delta_{\mathbf{p}, -\mathbf{p}'} (-p^0 p'^0 - \mathbf{p} \cdot \mathbf{p}' + M^2) [a_{\mathbf{p}}^\dagger a_{\mathbf{p}'}^\dagger e^{i(p^0 + p'^0)t} + a_{\mathbf{p}} a_{\mathbf{p}'} e^{-i(p^0 + p'^0)t}] \right\} \\ &= \sum_{\mathbf{p}} p^0 \left(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{1}{2} \right). \end{aligned} \quad (7.31)$$

The vacuum state $|0\rangle$ has an energy

$$E_0 \equiv \langle 0|H|0\rangle = \frac{1}{2} \sum_{\mathbf{p}} p^0 = \frac{1}{2} \sum_{\mathbf{p}} \omega_{\mathbf{p}}. \quad (7.32)$$

It contains the sum of the energies $\frac{1}{2}\hbar\omega_{\mathbf{p}}$ of the zero-point oscillations of all “oscillator quanta” in the second quantization formalism. It is the result of all the so-called *vacuum fluctuations* of the field. In the limit of large volume, the momentum sum turns into an integral over the phase space according to the usual rule (7.21).

This energy is infinite. Fortunately, in most circumstances this infinity is unobservable. It is therefore often subtracted out of the Hamiltonian, replacing H by

$$:H:\equiv H - \langle 0|H|0\rangle. \quad (7.33)$$

The double dots to the left-hand side define what is called the *normal product* form of H . It is obtained by the following prescription for products of operators $a, a^\dagger$. Given an arbitrary product of creation and annihilation operators enclosed by double dots

$$:a^\dagger \cdots a \cdots a^\dagger \cdots a:, \quad (7.34)$$

the product is understood to be re-ordered in a way that all creation operators stand to the left of all annihilation operators. For example,

$$:a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{\mathbf{p}} a_{\mathbf{p}}^\dagger: = 2a_{\mathbf{p}}^\dagger a_{\mathbf{p}}, \quad (7.35)$$

so that the normally-ordered free-particle Hamiltonian is

$$:H:= \sum_{\mathbf{p}} \omega_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}. \quad (7.36)$$

A prescription like this is necessary to make sure that the vacuum is invariant under time translations.

When following this ad hoc procedure, care has to be taken that one is not dealing with phenomena that are sensitive to the omitted zero-point oscillations. Gravitational interactions, for example, couple to zero-point energy. The infinity creates a problem when trying to construct quantum field theories in the presence of a classical gravitational field, since the vacuum energy gives rise to an infinite cosmological constant, which can be determined experimentally from solutions of the cosmological equations of motion, to have a finite value. A possible solution of this problem will appear later in Section 7.4 when quantizing the Dirac field. We shall see in Eq. (7.248) that for a Dirac field, the vacuum energy has the same form as for the scalar field, but with an *opposite sign*. In fact, this opposite sign is a consequence of the Fermi-Dirac statistics of the electrons. As will be shown in Section 7.10, all particles with half-integer spins obey Fermi-Dirac statistics and require a different quantization than that of the Klein-Gordon field. They all give a *negative* contribution $-\hbar\omega_{\mathbf{p}}/2$ to the vacuum energy for each momentum and spin degree of freedom. On the other hand, all particle with integer spins are bosons as the scalar particles of the Klein-Gordon field and will be quantized in a similar way, thus contributing a *positive* vacuum energy $\hbar\omega_{\mathbf{p}}/2$ for each momentum and spin degree of freedom.

The sum of bosonic and fermionic vacuum energies is therefore

$$E_{\text{vac}}^{\text{tot}} = \frac{1}{2} \sum_{\mathbf{p}, \text{bosons}} \omega_{\mathbf{p}} - \frac{1}{2} \sum_{\mathbf{p}, \text{fermions}} \omega_{\mathbf{p}}. \quad (7.37)$$

Expanding $\omega_{\mathbf{p}}$ as

$$\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2} = |\mathbf{p}| \left(1 + \frac{1}{2} \frac{M^2}{\mathbf{p}^2} - \frac{1}{8} \frac{M^4}{\mathbf{p}^4} + \dots \right), \quad (7.38)$$

we see that the vacuum energy can be finite if the universe contains as many Bose fields as Fermi fields, and if the masses of the associated particles satisfy the sum rules

$$\begin{aligned} \sum_{\text{bosons}} M^2 &= \sum_{\text{fermions}} M^2, \\ \sum_{\text{bosons}} M^4 &= \sum_{\text{fermions}} M^4. \end{aligned} \quad (7.39)$$

The higher powers in M contribute with finite momentum sums in (7.37).

If these cancellations do not occur, the sums are divergent and a cutoff in momentum space is needed to make the sum over all vacuum energies finite. Summing over all momenta inside a momentum sphere $|\mathbf{p}|$ of radius Λ will lead to a divergent energy proportional to Λ^4 .

Many authors have argued that all quantum field theories may be valid only if the momenta are smaller than the Planck momentum $P_{\text{P}} \equiv m_{\text{P}}c = \hbar/\lambda_{\text{P}}$, where m_{P} is the Planck mass (4.356) and λ_{P} the associated Compton wavelength

$$\lambda_{\text{P}} = \sqrt{\hbar G/c^3} = 1.616252(81) \times 10^{-33} \text{cm}, \quad (7.40)$$

which is also called *Planck length*. Then the vacuum energy would be of the order $m_{\text{P}}^4 \approx 10^{76} \text{GeV}^4$. From the present cosmological reexpansion rate one estimates a cosmological constant of the order of 10^{-47}GeV^4 . This is smaller than the vacuum energy by a factor of roughly 10^{123} . The authors conclude that, in the absence of cancellations of Bose and Fermi vacuum energies, field theory gives a too large cosmological constant by a factor 10^{123} . This conclusion is, however, definitely false. As we shall see later when treating other infinities of quantum field theories, divergent quantities may be made finite by including an infinity in the initial bare parameters of the theory. Their values may be *chosen* such that the final result is equal to the experimentally observed quantity [1]. The cutoff indicates that the quantity depends on ultra-short-distance physics which we shall never know. For this reason one must always restrict one's attention to theories which do not depend on ultra-short-distance physics. These theories are called *renormalizable theories*. The quantum electrodynamics to be discussed in detail in Chapter 12 was historically the first theory of this kind. In this theory, which is experimentally the most accurate theory ever, the situation of the vacuum is precisely the same as for the mass of the

electron. Also here the mass emerging from the interactions needs a cutoff to be finite. But all cutoff dependence is absorbed into the initial bare mass parameter so that the final result is the experimentally observed quantity (see also the later discussion on p. 1512).

If boundary conditions cause a modification of the sums over momenta, the vacuum energy leads to finite observable effects which are independent of the cutoff. These are the famous *Casimir forces* on conducting walls, or the *van der Waals forces* between different dielectric media. Both will be discussed in Section 7.12.

7.1.3 Propagator of Free Scalar Particles

The free-particle propagator of the scalar field is obtained from the vacuum expectation

$$G(x, x') = \langle 0 | T \phi(x) \phi(x') | 0 \rangle. \quad (7.41)$$

As for nonrelativistic fields, the propagator coincides with the Green function of the free-field equation. This follows from the explicit form of the time-ordered product

$$T \phi(x) \phi(x') = \Theta(x_0 - x'_0) \phi(x) \phi(x') + \Theta(x'_0 - x_0) \phi(x') \phi(x). \quad (7.42)$$

Multiplying $G(x, x')$ by the operator ∂^2 , we obtain

$$\begin{aligned} \partial^2 T \phi(x) \phi(x') &= T [\partial^2 \phi(x)] \phi(x') \\ &\quad + 2\delta(x_0 - x'_0) [\partial_0 \phi(x), \phi(x')] + \delta'(x_0 - x'_0) [\phi(x), \phi(x')]. \end{aligned} \quad (7.43)$$

The last term can be manipulated according to the usual rules for distributions: It is multiplied by an arbitrary smooth test function of x_0 , say $f(x_0)$, and becomes after a partial integration:

$$\begin{aligned} \int dx_0 f(x_0) \delta'(x_0 - x'_0) [\phi(x), \phi(x')] &= \\ - \int dx_0 f'(x_0) \delta(x_0 - x'_0) [\phi(x), \phi(x')] &- \int dx_0 f(x_0) \delta(x_0 - x'_0) [\dot{\phi}(x), \phi(x')]. \end{aligned} \quad (7.44)$$

The first term on the right-hand side does not contribute, since it contains the commutator of the fields only at equal-times, $[\phi(x), \phi(x')]_{x^0=x'^0}$, where it vanishes. Thus, dropping the test function $f(x_0)$, we have the equality between distributions

$$\delta'(x_0 - x'_0) [\phi(x), \phi(x')] = -\delta(x_0 - x'_0) [\dot{\phi}(x), \phi(x')], \quad (7.45)$$

and therefore with (7.4), (7.10), (7.41)–(7.43):

$$(-\partial^2 - M^2)G(x, x') = i\delta(x_0 - x'_0)\delta^{(3)}(\mathbf{x} - \mathbf{x}') = i\delta^{(4)}(x - x'). \quad (7.46)$$

To calculate $G(x, x')$ explicitly, we insert (7.12) and (7.42) into (7.41), and find

$$\begin{aligned} G(x, x') &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{\sqrt{p^0 p'^0}} e^{-i(px - p'x')} \langle 0 | a_{\mathbf{p}} a_{\mathbf{p}'}^\dagger | 0 \rangle \\ &+ \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{\sqrt{p^0 p'^0}} e^{i(px - p'x')} \langle 0 | a_{\mathbf{p}'} a_{\mathbf{p}}^\dagger | 0 \rangle \\ &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{-ip(x - x')} + \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{ip(x - x')}. \end{aligned} \quad (7.47)$$

It is useful to introduce the functions

$$G^{(\pm)}(x, x') = \sum_{\mathbf{p}} \frac{1}{2p^0 V} e^{\mp ip(x - x')}. \quad (7.48)$$

They are equal to the commutators of the positive- and negative-frequency parts of the field $\phi(x)$ defined by

$$\phi^{(+)}(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} e^{-ipx} a_{\mathbf{p}}, \quad \phi^{(-)}(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} e^{ipx} a_{\mathbf{p}}^\dagger. \quad (7.49)$$

They annihilate and create free single-particle states, respectively. In terms of these,

$$G^{(+)}(x, x') = [\phi^{(+)}(x), \phi^{(-)}(x')], \quad G^{(-)}(x, x') = -[\phi^{(-)}(x), \phi^{(+)}(x')] = G^{(-)}(x', x). \quad (7.50)$$

The commutators on the right-hand sides can also be replaced by the corresponding expectation values. They can also be rewritten as Fourier integrals

$$G^{(\pm)}(x, x') = \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2p^0} e^{\pm i\mathbf{p}(\mathbf{x} - \mathbf{x}')} G^{(\pm)}(\mathbf{p}, t - t'), \quad (7.51)$$

with the Fourier components

$$G^{(\pm)}(\mathbf{p}, t - t') \equiv e^{\mp ip^0(t - t')}. \quad (7.52)$$

These are equal to the expectation values

$$\begin{aligned} G^{(+)}(\mathbf{p}, t - t') &= \langle 0 | a_{\mathbf{pH}}(t) a_{\mathbf{pH}}^\dagger(t') | 0 \rangle, \\ G^{(-)}(\mathbf{p}, t - t') &= \langle 0 | a_{\mathbf{pH}}(t') a_{\mathbf{pH}}^\dagger(t) | 0 \rangle \end{aligned} \quad (7.53)$$

of Heisenberg creation and annihilation operators [recall the definition (1.286), and (2.132)], whose energy is $p^0 = \omega_{\mathbf{p}}$:

$$a_{\mathbf{pH}}(t) \equiv e^{iHt} a_{\mathbf{p}} e^{-iHt} = e^{-ip^0 t} a_{\mathbf{p}}, \quad a_{\mathbf{pH}}^\dagger(t) \equiv e^{iHt} a_{\mathbf{p}}^\dagger e^{-iHt} = e^{ip^0 t} a_{\mathbf{p}}^\dagger. \quad (7.54)$$

In the infinite-volume limit, the functions (7.48) have the Fourier representation

$$G^{(\pm)}(x, x') = \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2p^0} e^{\mp ip(x - x')}. \quad (7.55)$$

The full commutator $[\phi(x), \phi(x')]$ receives contributions from both functions. It is given by the difference:

$$[\phi(x), \phi(x')] = G^{(+)}(x - x') - G^{(-)}(x - x') \equiv C(x - x'). \quad (7.56)$$

The right-hand side defines the *commutator function*, which has the Fourier representation

$$C(x - x') = -i \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} e^{ip(\mathbf{x} - \mathbf{x}')} \sin[p^0(x^0 - x'^0)]. \quad (7.57)$$

This representation is convenient for verifying the canonical equal-time commutation rules (7.2) and (7.4), which imply that

$$C(x - x') = 0, \quad \dot{C}(x - x') = -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad \text{for } x^0 = x'^0. \quad (7.58)$$

Indeed, for $x^0 = x'^0$, the integrand in (7.57) is zero, so that the integral vanishes. The time derivative of $C(x - x')$ removes p^0 in the denominator, leading at $x^0 = x'^0$ directly to the Fourier representation of the spatial δ -function.

Another way of writing (7.57) uses a four-dimensional momentum integral

$$C(x - x') = \int \frac{d^4p}{(2\pi)^4} 2\pi \Theta(p^0) \delta(p^2 - M^2) e^{-ip(x - x')}. \quad (7.59)$$

In contrast to the Feynman propagator which satisfies the inhomogenous Klein-Gordon equation, the commutator function (7.56) satisfies the homogenous equation:

$$(-\partial^2 - M^2)C(x - x') = 0. \quad (7.60)$$

The Fourier representation (7.59) satisfies this equation since multiplication from the left by the Klein-Gordon operator produces an integrand proportional to $(p^2 - M^2)\delta(p^2 - M^2) = 0$.

The equality of the two expressions (7.56) and (7.59) follows directly from the property of the δ -function

$$\delta(p^2 - M^2) = \delta(p^0{}^2 - \omega_{\mathbf{p}}^2) = \frac{1}{2\omega_{\mathbf{p}}} [\delta(p^0 - \omega_{\mathbf{p}}) + \delta(p^0 + \omega_{\mathbf{p}})]. \quad (7.61)$$

Due to $\Theta(p^0)$ in (7.59), the integral over p^0 runs only over positive $p^0 = \omega_{\mathbf{p}}$, thus leading to (7.57).

In terms of the functions $G^{(\pm)}(x, x')$, the propagator can be written as

$$G(x, x') = G(x, x') = \Theta(x_0 - x'_0)G^{(+)}(x, x') + \Theta(x'_0 - x_0)G^{(-)}(x, x'). \quad (7.62)$$

As follows from (7.55) and (7.62), all three functions $G(x, x')$, $G^{(+)}(x, x')$, and $G^{(-)}(x, x')$ depend only on $x - x'$, thus exhibiting the translational invariance of the vacuum state. In the following, we shall therefore always write one argument $x - x'$ instead of x, x' .

As in the nonrelativistic case, it is convenient to use the integral representation (1.319) for the Heaviside functions:

$$\begin{aligned}\Theta(x_0 - x'_0) &= \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{i}{E - p^0 + i\eta} e^{-i(E-p^0)(x_0-x'_0)}, \\ \Theta(x'_0 - x_0) &= - \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{i}{E + p^0 - i\eta} e^{-i(E+p^0)(x_0-x'_0)},\end{aligned}\quad (7.63)$$

with an infinitesimal parameter $\eta > 0$. This allows us to reexpress $G(x, x')$ more compactly using (7.55), (7.52), and (7.62) as

$$G(x - x') = \int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} \left(\frac{i}{E - p^0 + i\eta} - \frac{i}{E + p^0 - i\eta} \right) e^{-iE(x_0-x'_0) + i\mathbf{p}(\mathbf{x}-\mathbf{x}')}.\quad (7.64)$$

Here we have used the fact that p^0 is an even function of $\mathbf{p}$, thus permitting us to change the integration variables $\mathbf{p}$ to $-\mathbf{p}$ in the second integral. By combining the denominators, we find

$$G(x - x') = \int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{i}{E^2 - \mathbf{p}^2 - M^2 + i\eta} e^{-iE(x_0-x'_0) + i\mathbf{p}(\mathbf{x}-\mathbf{x}')}.\quad (7.65)$$

This has a relativistically invariant form in which it is useful to rename E as p^0 , and write

$$G(x - x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')}.\quad (7.66)$$

Note that in this expression, p^0 is integrated over the entire p^0 -axis. In contrast to all earlier formulas in this section, the energy variable p^0 is no longer constrained to satisfy the mass shell conditions $(p^0)^2 = p^{02} = \mathbf{p}^2 + M^2$.

The integral representation (7.66) shows very directly that $G(x, x')$ is the Green function of the free-field equation (7.9). An application of the differential operator $(-\partial^2 - M^2)$ cancels the denominator in the integrand and yields

$$\begin{aligned}(-\partial^2 - M^2)G(x - x') &= \int \frac{d^4p}{(2\pi)^4} (p^2 - M^2) \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')} \\ &= i\delta^{(4)}(x - x').\end{aligned}\quad (7.67)$$

This calculation gives rise to a simple *mnemonic rule* for calculating the Green function of an arbitrary free-field theory. We write the Lagrangian density (7.8) as

$$\mathcal{L}(x) = \frac{1}{2} \phi(x) L(i\partial) \phi(x),\quad (7.68)$$

with the differential operator

$$L(i\partial) \equiv (-\partial^2 - M^2).\quad (7.69)$$

The Euler-Lagrange equation (7.9) can then be expressed as

$$L(i\partial)\phi(x) = 0. \quad (7.70)$$

And the Green function is the Fourier transform of the inverse of $L(i\partial)$:

$$G(x - x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{L(p)} e^{-ip(x-x')}, \quad (7.71)$$

with an infinitesimal $-i\eta$ added to the mass of the particle. This rule can directly be generalized to all other free-field theories to be discussed in the sequel.

7.1.4 Complex Case

Here we use the Lagrangian (4.165):

$$\mathcal{L}(x) = \partial^\mu \varphi^*(x) \partial_\mu \varphi(x) - M^2 \varphi^*(x) \varphi(x), \quad (7.72)$$

whose Euler-Lagrange equation is the same as in the real case, i.e., it has the form (7.9). We shall see later in Subsec. 8.11.1, that the complex scalar field describes *charged spinless particles*.

Field Quantization

According to the canonical rules, the complex fields possess complex canonical momenta

$$\begin{aligned} \pi_\varphi(x) &\equiv \pi(x) \equiv \frac{\partial \mathcal{L}(x)}{\partial [\partial^0 \varphi(x)]} = \partial^0 \varphi^*(x), \\ \pi_{\varphi^*}(x) &\equiv \pi^*(x) \equiv \frac{\partial \mathcal{L}(x)}{\partial [\partial^0 \varphi^*(x)]} = \partial^0 \varphi(x). \end{aligned} \quad (7.73)$$

The associated operators are required to satisfy the equal-time commutation rules

$$\begin{aligned} [\pi(\mathbf{x}, t), \varphi(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\pi^\dagger(\mathbf{x}, t), \varphi^\dagger(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (7.74)$$

All other equal-time commutators vanish. We now expand the field operator into its Fourier components

$$\varphi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}} \left(e^{-ipx} a_{\mathbf{p}} + e^{ipx} b_{\mathbf{p}}^\dagger \right), \quad (7.75)$$

where, in contrast to the real case (7.12), $b_{\mathbf{p}}^\dagger$ is no longer equal to $a_{\mathbf{p}}^\dagger$. The reader may wonder why we do not just use another set of annihilation operators $d_{-\mathbf{p}}$ rather than creation operators $b_{\mathbf{p}}^\dagger$. A negative sign in the momentum label would be appropriate since the associated wave function $f_{\mathbf{p}}^*(x) = e^{ipx}/\sqrt{2Vp^0}$ has a negative momentum.

One formal reason for using $b_{\mathbf{p}}^\dagger$ instead of $d_{-\mathbf{p}}$ is that this turns the expansion (7.75) into a straightforward generalization of the expansion (7.12) of the real field. A more physical reason will be seen below when discussing Eq. (7.88).

By analogy with (7.14), we invert (7.75) to find

$$\begin{Bmatrix} a_{\mathbf{p}} \\ b_{\mathbf{p}}^\dagger \end{Bmatrix} = e^{\pm i p^0 x_0} \sqrt{\frac{1}{2V p^0}} \int d^3x e^{\mp i \mathbf{p} \cdot \mathbf{x}} [\pm i \pi^\dagger(x) + p^0 \varphi(x)]. \quad (7.76)$$

Corresponding equations hold for Hermitian-adjoint operators $a_{\mathbf{p}}^\dagger$ and $b_{\mathbf{p}}$. From these equations we find that the operators $a_{\mathbf{p}}$, $a_{\mathbf{p}}^\dagger$, $b_{\mathbf{p}}$, and $b_{\mathbf{p}}^\dagger$ all commute with each other, except for

$$[a_{\mathbf{p}}, a_{\mathbf{p}'}^\dagger] = \delta_{\mathbf{p}, \mathbf{p}'}, \quad [b_{\mathbf{p}}, b_{\mathbf{p}'}^\dagger] = \delta_{\mathbf{p}, \mathbf{p}'}. \quad (7.77)$$

Thus there are two types of particle states, created as follows:

$$|\mathbf{p}\rangle \equiv a_{\mathbf{p}}^\dagger |0\rangle, \quad |\bar{\mathbf{p}}\rangle \equiv b_{\mathbf{p}}^\dagger |0\rangle, \quad (7.78)$$

$$\langle \mathbf{p}| \equiv \langle 0| a_{\mathbf{p}}, \quad \langle \bar{\mathbf{p}}| \equiv \langle 0| b_{\mathbf{p}}. \quad (7.79)$$

They are referred to as particle and antiparticle states, respectively, and have the wave functions

$$\langle 0| \varphi(x) | \mathbf{p}\rangle = \frac{1}{\sqrt{2V p^0}} e^{-i p x} = f_{\mathbf{p}}(x), \quad \langle 0| \varphi^\dagger(x) | \bar{\mathbf{p}}\rangle = \frac{1}{\sqrt{2V p^0}} e^{-i p x} = f_{\mathbf{p}}(x), \quad (7.80)$$

$$\langle \bar{\mathbf{p}}| \varphi(x) | 0\rangle = \frac{1}{\sqrt{2V p^0}} e^{i p x} = f_{\mathbf{p}}^*(x), \quad \langle \mathbf{p}| \varphi^\dagger(x) | 0\rangle = \frac{1}{\sqrt{2V p^0}} e^{i p x} = f_{\mathbf{p}}^*(x), \quad (7.81)$$

which by analogy with (2.212) may be abbreviated as

$$\langle 0| \varphi(x) | \mathbf{p}\rangle = \langle 0| \mathbf{p}\rangle, \quad \langle 0| \varphi^\dagger(x) | \bar{\mathbf{p}}\rangle = \langle x| \bar{\mathbf{p}}\rangle, \quad (7.82)$$

$$\langle \bar{\mathbf{p}}| \varphi(x) | 0\rangle = \langle \bar{\mathbf{p}}| x\rangle, \quad \langle \mathbf{p}| \varphi^\dagger(x) | 0\rangle = \langle \mathbf{p}| x\rangle. \quad (7.83)$$

We are now prepared to justify why we associated a creation operator for antiparticles $b_{\mathbf{p}}^\dagger$ with the second term in the expansion (7.75), instead of an annihilation operator for particles $d_{-\mathbf{p}}$. First, this is in closer analogy with the real field in (7.12), which contains a creation operator $a_{\mathbf{p}}^\dagger$ accompanied by the negative-frequency wave function $e^{i p x}$. Second, only the above choice leads to commutation rules (7.77) with the correct sign between $b_{\mathbf{p}}$ and $b_{\mathbf{p}}^\dagger$. The choice $d_{\mathbf{p}}$ would have led to the commutator $[d_{\mathbf{p}}, d_{\mathbf{p}'}^\dagger] = -\delta_{\mathbf{p}, \mathbf{p}'}$. For the second-quantized Hilbert space, this would imply a negative norm for the states created by $d_{\mathbf{p}}^\dagger$. Third, the above choice ensures that the wave functions of incoming states $|\mathbf{p}\rangle$ and $|\bar{\mathbf{p}}\rangle$ are both $e^{-i p x}$, i.e., they both oscillate in time with a *positive* frequency like $e^{-i p^0 t}$, thus having a positive energy. With annihilation operators $d_{\mathbf{p}}$ instead of $b_{\mathbf{p}}^\dagger$, the energy of a state created by $d_{\mathbf{p}}^\dagger$ would have been negative. This will also be seen in the calculation of the second-quantized energy to be performed now.

Multiparticle states are formed in the same way as in the real-field case in Eq. (7.25), except that creation operators $a_{\mathbf{p}}^\dagger$ and $b_{\mathbf{p}}^\dagger$ have to be applied to the vacuum state $|0\rangle$:

$$|n_{\mathbf{p}_1} n_{\mathbf{p}_2} \dots n_{\mathbf{p}_k}; \bar{n}_{\mathbf{p}_1} \bar{n}_{\mathbf{p}_2} \dots \bar{n}_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A} (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \dots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} (b_{\mathbf{p}_1}^\dagger)^{\bar{n}_{\mathbf{p}_1}} \dots (b_{\mathbf{p}_k}^\dagger)^{\bar{n}_{\mathbf{p}_k}} |0\rangle. \quad (7.84)$$

As in the real-field case, we shall sometimes work in an infinite volume and use the single-particle states

$$|\mathbf{p}\rangle = a_{\mathbf{p}}^\dagger |0\rangle, \quad |\bar{\mathbf{p}}\rangle = b_{\mathbf{p}}^\dagger |0\rangle, \quad (7.85)$$

with the vacuum $|0\rangle$ defined by $a_{\mathbf{p}}|0\rangle = 0$ and $b_{\mathbf{p}}|0\rangle = 0$. These states satisfy the same orthogonality relation as those in (7.27), and possess wave functions normalized as in Eq. (7.28).

7.1.5 Energy of Free Charged Scalar Particles

The second-quantized energy density reads

$$\begin{aligned} \mathcal{H}(x) &= \pi(x) \partial^0 \varphi(x) + \pi^\dagger(x) \partial^0 \varphi^\dagger(x) - \mathcal{L}(x) \\ &= 2 \partial^0 \varphi^\dagger(x) \partial^0 \varphi(x) - \mathcal{L}(x) \\ &= \partial^0 \varphi^\dagger(x) \partial^0 \varphi(x) + \partial_{\mathbf{x}} \varphi^\dagger(x) \partial_{\mathbf{x}} \varphi(x) + M^2 \varphi^\dagger(x) \varphi(x). \end{aligned} \quad (7.86)$$

Inserting the expansion (7.75), we find the Hamilton operator [analogous to (7.31)]

$$\begin{aligned} H = \int d^3x \mathcal{H}(x) &= \sum_{\mathbf{p}} \left[\frac{p^{02} + \mathbf{p}^2 + M^2}{2p^0} (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + b_{\mathbf{p}} b_{\mathbf{p}}^\dagger) \right. \\ &\quad \left. + \frac{-p^{02} + \mathbf{p}^2 + M^2}{2p^0} (a_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger e^{2ip^0 t} + b_{-\mathbf{p}} a_{\mathbf{p}} e^{-2ip^0 t}) \right] \\ &= \sum_{\mathbf{p}} p^0 (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{\mathbf{p}} + 1). \end{aligned} \quad (7.87)$$

Note that the mixed terms in the second line appear with opposite momentum labels, since H does not change the total momentum. Had we used $d_{-\mathbf{p}}$ rather than $b_{\mathbf{p}}^\dagger$ in the field expansion, the energy would have been

$$\begin{aligned} H = \int d^3x \mathcal{H}(x) &= \sum_{\mathbf{p}} \left[\frac{p^{02} + \mathbf{p}^2 + M^2}{2p^0} (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + d_{\mathbf{p}}^\dagger d_{\mathbf{p}}) \right. \\ &\quad \left. + \frac{-p^{02} + \mathbf{p}^2 + M^2}{2p^0} (a_{\mathbf{p}}^\dagger d_{\mathbf{p}} e^{2ip^0 t} + d_{\mathbf{p}}^\dagger a_{\mathbf{p}} e^{-2ip^0 t}) \right] \\ &= \sum_{\mathbf{p}} p^0 (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + d_{\mathbf{p}}^\dagger d_{\mathbf{p}}). \end{aligned} \quad (7.88)$$

Here the mixed terms have subscripts with equal momenta. Since the commutation rule of $d_{\mathbf{p}}, d_{\mathbf{p}}^\dagger$ have the wrong sign, the eigenvalues of $d_{\mathbf{p}}^\dagger d_{\mathbf{p}}$ take *negative* integer values implying the energy of the particles created by $d_{\mathbf{p}}^\dagger$ to be negative. For an arbitrary number of such particles, this would have implied an energy spectrum without lower bound, which is unphysical (since it would allow one to build a perpetuum mobile).

Taking the vacuum expectation value of the positive-definite energy (7.87), we obtain, as in Eq. (7.32),

$$E_0 \equiv \langle 0|H|0\rangle = \sum_{\mathbf{p}} p^0 = \sum_{\mathbf{p}} \omega_{\mathbf{p}}. \quad (7.89)$$

In comparison with Eq. (7.32), there is a factor 2 since the complex field has twice as many degrees of freedom as a real field. As in the real case, we may subtract this infinite vacuum energy to obtain finite expressions via the earlier explained normal-ordering prescription. Only the gravitational interaction is sensitive to the vacuum energy.

What is the difference between the particle states $|\mathbf{p}\rangle$ and $|\bar{\mathbf{p}}\rangle$ created by $a_{\mathbf{p}}^\dagger$ and $b_{\mathbf{p}}^\dagger$? We shall later see that they couple with opposite sign to the electromagnetic field. Here we only observe that they have the same intrinsic properties under the Poincaré group, i.e., the same mass and spin. They are said to be *antiparticles* of each other.

Propagator of Free Charged Scalar Particles

The propagator of the complex scalar field can be calculated in the same fashion as for real-fields with the result

$$\begin{aligned} G(x, x') &\equiv G(x - x') = \langle 0|T\varphi(x)\varphi^\dagger(x')|0\rangle \\ &= \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')}. \end{aligned} \quad (7.90)$$

As before, the propagator is equal to the Green function of the free-field equation (7.9). It may again be obtained following the mnemonic rule on p. 484, by Fourier transforming the inverse of the differential operator $L(i\partial)$ in the field equation [recall (7.365) and (7.71)].

7.1.6 Behavior under Discrete Symmetries

Let us now see how the discrete operations of space inversion, time reversal, and complex conjugation of Subsecs. 4.5.2–4.5.4 act in the Hilbert space of quantized scalar fields.

Space Inversion

Under space inversion, defined by the transformation

$$x \xrightarrow{P} x' = \tilde{x} = (x_0, -\mathbf{x}), \quad (7.91)$$

a real or complex scalar field is transformed according to

$$\varphi(x) \xrightarrow{P} \varphi'_P(x) = \eta_P \varphi(\tilde{x}), \quad (7.92)$$

with

$$\eta_P = \pm 1. \quad (7.93)$$

For a real-field operator $\phi(x)$, this transformation can be achieved by assigning a transformation law

$$\begin{aligned} a_{\mathbf{p}} &\xrightarrow{P} a'_{\mathbf{p}} = \eta_P a_{-\mathbf{p}}, \\ a_{\mathbf{p}}^\dagger &\xrightarrow{P} a'^\dagger_{\mathbf{p}} = \eta_P a_{-\mathbf{p}}^\dagger, \end{aligned} \quad (7.94)$$

to the creation and annihilation operators $a_{\mathbf{p}}^\dagger$ and $a_{\mathbf{p}}$ in the expansion (7.12). Indeed, by inserting (7.94) into (7.12), we find

$$\begin{aligned} \phi'_P(x) &= \eta_P \frac{1}{\sqrt{2p^0 V}} \sum_{\mathbf{p}} \left(e^{-ipx} a_{-\mathbf{p}} + e^{ipx} a_{-\mathbf{p}}^\dagger \right) \\ &= \eta_P \frac{1}{\sqrt{2p^0 V}} \sum_{\mathbf{p}} \left(e^{-ip\tilde{x}} a_{\mathbf{p}} + e^{ip\tilde{x}} a_{\mathbf{p}}^\dagger \right) = \eta_P \phi(\tilde{x}). \end{aligned} \quad (7.95)$$

It is possible to find a *parity operator* $\mathcal{P}$ in the second-quantized Hilbert space which generates the parity in the transformations (7.94), (7.95), i.e., it is defined by

$$\begin{aligned} \mathcal{P} a_{\mathbf{p}} \mathcal{P}^{-1} &\equiv a'_{\mathbf{p}} = \eta_P a_{-\mathbf{p}}, \\ \mathcal{P} a_{\mathbf{p}}^\dagger \mathcal{P}^{-1} &\equiv a'^\dagger_{\mathbf{p}} = \eta_P a_{-\mathbf{p}}^\dagger. \end{aligned} \quad (7.96)$$

An explicit representation of $\mathcal{P}$ is

$$\mathcal{P} = e^{i\pi G_P/2}, \quad G_P = \sum_{\mathbf{p}} \left[a_{-\mathbf{p}}^\dagger a_{\mathbf{p}} - \eta_P a_{\mathbf{p}}^\dagger a_{-\mathbf{p}} \right]. \quad (7.97)$$

In order to prove that this operator has the desired effect, we form the operators

$$a_{\mathbf{p}}^{+\dagger} \equiv a_{\mathbf{p}}^\dagger + \eta_P a_{-\mathbf{p}}^\dagger, \quad a_{\mathbf{p}}^{-\dagger} \equiv a_{\mathbf{p}}^\dagger - \eta_P a_{-\mathbf{p}}^\dagger, \quad (7.98)$$

which are invariant under the parity operation (7.96), with eigenvalues ± 1 :

$$\mathcal{P} a_{\mathbf{p}}^{\pm\dagger} \mathcal{P}^{-1} = \pm a_{\mathbf{p}}^{\pm\dagger}. \quad (7.99)$$

Then we calculate the same property with the help of the unitary operator (7.97), expanding $e^{iG_P\pi/2} a_{\mathbf{p}}^{\pm\dagger} e^{-iG_P\pi/2}$ with the help of Lie's expansion formula (4.105). This turns out to be extremely simple since the first commutators on the right-hand side of (4.105) are

$$[G_P, a_{\mathbf{p}}^{+\dagger}] = 0; \quad [G_P, a_{\mathbf{p}}^{-\dagger}] = -2a_{\mathbf{p}}^{-\dagger}, \quad (7.100)$$

so that the higher ones are obvious. The Lie series yields therefore

$$\begin{aligned} e^{iG_P\pi/2} a_{\mathbf{p}}^{+\dagger} e^{-iG_P\pi/2} &= a_{\mathbf{p}}^{+\dagger}, \\ e^{iG_P\pi/2} a_{\mathbf{p}}^{-\dagger} e^{-iG_P\pi/2} &= a_{\mathbf{p}}^{-\dagger} \left(1 - i\pi + \frac{1}{2!}\pi^2 + \dots \right) = a_{\mathbf{p}}^{-\dagger} e^{-i\pi} = -a_{\mathbf{p}}^{-\dagger}, \end{aligned} \quad (7.101)$$

showing that the operators $a_{\mathbf{p}}^{\pm\dagger}$ do indeed satisfy (7.99).

For a complex field operator $\varphi(x)$, the operator G_P in (7.97) has to be extended by the same expression involving the operators $b_{\mathbf{p}}^\dagger$ and $b_{\mathbf{p}}$.

Let us denote the multiparticle states of the types (7.25) or (7.84) in the second-quantized Hilbert space by $|\Psi\rangle$. In the space of all such states, the operator $\mathcal{P}$ is unitary:

$$\mathcal{P}^\dagger = \mathcal{P}^{-1}, \quad (7.102)$$

i.e., for any two states $|\Psi_1\rangle$ and $|\Psi_2\rangle$, the scalar product remains unchanged by $\mathcal{P}$

$${}_P\langle\Psi'_1|\Psi'_2\rangle_P = \langle\Psi_1|\mathcal{P}^\dagger\mathcal{P}|\Psi_2\rangle = \langle\Psi_1|\Psi_2\rangle. \quad (7.103)$$

With this operator, the transformation (7.92) is generated by

$$\varphi(x) \xrightarrow{P} \mathcal{P}\varphi(x)\mathcal{P}^{-1} = \varphi'_P(x) = \eta_P\varphi(\tilde{x}). \quad (7.104)$$

As an application, consider a state of two identical spinless particles which move in the common center of mass frame with a relative angular momentum l . Such a state is an eigenstate of the parity operation with the eigenvalue

$$\eta_P = (-1)^l. \quad (7.105)$$

This follows directly by applying the parity operator $\mathcal{P}$ to the wave function

$$|\Psi_{lm}\rangle = \int_0^\infty dp R_l(p) \int d^2\hat{\mathbf{p}} Y_{lm}(\hat{\mathbf{p}}) a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger |0\rangle, \quad (7.106)$$

where $R_l(p)$ is some radial wave function of $p = |\mathbf{p}|$. Using (7.96), the commutativity of the creation operators $a_{\mathbf{p}}^\dagger$ and $a_{-\mathbf{p}}^\dagger$ with each other, and the well-known fact¹ that the spherical harmonic for $-\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}$ differ by a phase factor $(-1)^l$, lead to

$$\mathcal{P}|\Psi_{lm}\rangle = (-1)^l |\Psi_{lm}\rangle. \quad (7.107)$$

For two different bosons of parities η_{P_1} and η_{P_2} , the right-hand side is multiplied by $\eta_{P_1}\eta_{P_2}$.

¹This follows from the property of the spherical harmonics $Y_{lm}(\pi - \theta, \phi) = (-1)^{l-m} Y_{lm}(\theta, \phi)$ together with $e^{im(\phi+\pi)} = (-1)^m e^{im\phi}$.

Time Reversal

By time reversal we understand the coordinate transformation

$$x \xrightarrow{T} x' = -\tilde{x} = (-x_0, \mathbf{x}). \quad (7.108)$$

The operator implementation of time reversal is not straightforward. In a time-reversed state, all movements are reversed, i.e., for spin-zero particles all momenta are reversed (see Subsec. 4.5.3). In this respect, there is no difference to the parity operation, and the transformation properties of the creation and annihilation operators are just the same as in (7.96). The associated phase factor is denoted by η_T :

$$\begin{aligned} a_{\mathbf{p}} &\xrightarrow{T} a'_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}, \\ a_{\mathbf{p}}^\dagger &\xrightarrow{T} a'^\dagger_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}^\dagger. \end{aligned} \quad (7.109)$$

We have indicated before [see Eq. (4.226)] and shall see below, that in contrast to the phase factor $\eta_P = \pm 1$ of parity, the phase factor η_T will not be restricted to ± 1 by the group structure. It is unmeasurable and can be chosen to be equal to unity.

If we apply the operation (7.109) to the Fourier components in the expansion (7.12) of the field, we find

$$\begin{aligned} \phi'_T(x) &= \eta_T \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} \left(e^{-ipx} a_{-\mathbf{p}} + e^{ipx} a_{-\mathbf{p}}^\dagger \right) \\ &= \eta_T \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} \left(e^{-ip\tilde{x}} a_{\mathbf{p}} + e^{-ip\tilde{x}} a_{\mathbf{p}}^\dagger \right) \\ &= \eta_T \phi(\tilde{x}). \end{aligned} \quad (7.110)$$

This, however, is not yet the physically intended transformation law that was specified in Eq. (4.206):

$$\phi(x) \xrightarrow{T} \phi'_T(x) = \eta_T \phi(x_T), \quad (7.111)$$

which amounts to

$$\phi(x) \xrightarrow{T} \phi'_T(x) = \eta_T \phi(-\tilde{x}). \quad (7.112)$$

The sign change of the argument is achieved by requiring the time reversal transformation to be an *antilinear operator* $\mathcal{T}$ in the multiparticle Hilbert space. It is defined by

$$\begin{aligned} \mathcal{T} a_{\mathbf{p}} \mathcal{T}^{-1} &\equiv a'_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}, \\ \mathcal{T} a_{\mathbf{p}}^\dagger \mathcal{T}^{-1} &\equiv a'^\dagger_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}^\dagger, \end{aligned} \quad (7.113)$$

in combination with the antilinear property

$$\mathcal{T}(\alpha a + \beta a_{\mathbf{p}}^\dagger) \mathcal{T}^{-1} = \alpha^* \mathcal{T} a_{\mathbf{p}} \mathcal{T}^{-1} + \beta^* \mathcal{T} a_{\mathbf{p}}^\dagger \mathcal{T}^{-1}. \quad (7.114)$$

Whenever the time reversal operation is applied to a combination of creation and annihilation operators, the coefficients have to be switched to their complex conjugates. Under this antilinear operation, we indeed obtain (7.111) rather than (7.110):

$$\phi(x) \xrightarrow{T} \mathcal{T} \phi(x) \mathcal{T}^{-1} = \phi'_T(x) = \eta_T \phi(x_T). \quad (7.115)$$

The same transformation law is found for complex scalar fields by defining for particles and antiparticles

$$\begin{aligned} \mathcal{T} a_{\mathbf{p}} \mathcal{T}^{-1} &\equiv a'_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}, \\ \mathcal{T} b_{\mathbf{p}}^\dagger \mathcal{T}^{-1} &\equiv b'^\dagger_{\mathbf{p}} = \eta_T b_{-\mathbf{p}}^\dagger. \end{aligned} \quad (7.116)$$

In the second-quantized Hilbert space consisting of states (7.25) and (7.84), the antiunitarity has the consequence that all scalar products are changed into their complex conjugates:

$$\langle \Psi_2 | \Psi_1 \rangle \xrightarrow{T} {}_T \langle \Psi'_2 | \Psi'_1 \rangle_T = \langle \Psi_1 | \Psi_2 \rangle^*, \quad (7.117)$$

thus complying with the property (4.209) of scalar products of ordinary quantum mechanics (to which the second-quantized formalism reduces in the one-particle subspace). This makes the operator $\mathcal{T}$ antiunitary.

To formalize operations with the antiunitary operator $\mathcal{T}$ in the Dirac bra-ket language, it is useful to introduce an antilinear unit operator $\mathbf{1}_A$ which has the effect

$$\langle \Psi_2 | \mathbf{1}_A | \Psi_1 \rangle \equiv \mathbf{1}_A \langle \Psi_2 | \Psi_1 \rangle \equiv \langle \Psi_2 | \Psi_1 \rangle^*. \quad (7.118)$$

The antiunitarity of the time reversal transformation is then expressed by the equation

$$\mathcal{T}^\dagger = \mathcal{T}^{-1} \mathbf{1}_A, \quad (7.119)$$

the operator $\mathbf{1}_A$ causing all differences with respect to the unitary operator (7.102).

Due to the antilinearity, the factor η_T in the transformation law of the complex field is an arbitrary phase factor. We have mentioned this before in Subsec. 4.5.3. By applying the operator $\mathcal{T}$ twice to the complex field $\phi(x)$, we obtain from (7.114) and (7.115):

$$\mathcal{T}^2 \phi(x) \mathcal{T}^{-2} = \eta_T \eta_T^* \phi(x), \quad (7.120)$$

so that the cyclic property of time reversal $\mathcal{T}^2 = 1$ fixes

$$\eta_T \eta_T^* = 1. \quad (7.121)$$

This is in contrast to the unitary operators $\mathcal{P}$ and $\mathcal{C}$ where the phase factors must be ± 1 .

For real scalar fields, this still holds, since the second transformation law (7.113) must be the complex-conjugate of the first, which requires η_T to be real, leaving only the choices ± 1 .

The antilinearity has the consequence that a Hamilton operator which is invariant under time reversal

$$\mathcal{T} H \mathcal{T}^{-1} = H, \quad (7.122)$$

possesses a time evolution operator $U(t, t_0) = e^{-iH(t-t_0)/\hbar}$ that satisfies

$$\mathcal{T} U(t, t_0) \mathcal{T}^{-1} = U(t_0, t) = U^\dagger(t, t_0), \quad (7.123)$$

in which the time order is inverted.

The antiunitary nature of $\mathcal{T}$ makes the phase factor η_T of a charged field an unmeasurable quantity. This is why we were able to choose $\eta_T = 1$ after Eq. (7.121) [see also (4.226)]. Time reversal invariance does not produce selection rules in the same way as discrete unitary symmetries do, such as parity. This will be discussed in detail in Section 9.7, after having developed the theory of the scattering matrix.

Charge Conjugation

The operator implementation of the transformation (4.227) on a complex scalar field operator

$$\varphi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}} \left(e^{-ipx} a_{\mathbf{p}} + e^{ipx} b_{\mathbf{p}}^\dagger \right) \quad (7.124)$$

is quite simple. We merely have to define a *charge conjugation operator* $\mathcal{C}$ by

$$\begin{aligned} \mathcal{C} a_{\mathbf{p}}^\dagger \mathcal{C}^{-1} &= \eta_C b_{\mathbf{p}}^\dagger, & \mathcal{C} b_{\mathbf{p}}^\dagger \mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}^\dagger, \\ \mathcal{C} a_{\mathbf{p}} \mathcal{C}^{-1} &= \eta_C b_{\mathbf{p}}, & \mathcal{C} b_{\mathbf{p}} \mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}, \end{aligned} \quad (7.125)$$

where $\eta_C = \pm 1$ is the charge parity of the field. Applied to the complex scalar field operator (7.124) the operator $\mathcal{C}$ produces the desired transformation corresponding to (4.227):

$$\varphi(x) \xrightarrow{\mathcal{C}} \mathcal{C} \varphi(x) \mathcal{C}^{-1} = \varphi'_C(x) = \eta_C \varphi^\dagger(x). \quad (7.126)$$

For a real field, we may simply identify $b_{\mathbf{p}}$ with $a_{\mathbf{p}}$, thus making the transformation laws (7.125) trivial:

$$\begin{aligned} \mathcal{C} a_{\mathbf{p}}^\dagger \mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}^\dagger, \\ \mathcal{C} a_{\mathbf{p}} \mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}. \end{aligned} \quad (7.127)$$

The antiparticles created by $b_{\mathbf{p}}^\dagger$ have the same mass as the particles created by $a_{\mathbf{p}}^\dagger$. But they have an opposite charge. The latter follows directly from the transformation law (4.229) of the classical local current. In the present second-quantized formulation it is instructive to calculate the matrix elements of the operator current density (4.171):

$$j_\mu(x) = -i\varphi^\dagger \overset{\leftrightarrow}{\partial}_\mu \varphi. \quad (7.128)$$

Evaluating this between single-particle states created by $a_{\mathbf{p}}^\dagger$ and $b_{\mathbf{p}}^\dagger$, we find

$$\begin{aligned}\langle \mathbf{p}' | j^\mu(x) | \mathbf{p} \rangle &= \langle 0 | a_{\mathbf{p}'} j^\mu(x) a_{\mathbf{p}}^\dagger | 0 \rangle = (p'^\mu + p^\mu) \frac{1}{\sqrt{2p^0 2p'^0}} e^{-i(p-p')x}, \\ \langle \bar{\mathbf{p}}' | j^\mu(x) | \bar{\mathbf{p}} \rangle &= \langle 0 | b_{\mathbf{p}'} j^\mu(x) b_{\mathbf{p}}^\dagger | 0 \rangle = -(p'^\mu + p^\mu) \frac{1}{\sqrt{2p^0 2p'^0}} e^{-i(p-p')x}.\end{aligned}\quad (7.129)$$

The charge of the particle states $|\mathbf{p}\rangle = a_{\mathbf{p}}^\dagger | 0 \rangle$ and $|\bar{\mathbf{p}}\rangle = b_{\mathbf{p}}^\dagger | 0 \rangle$ is given by the diagonal matrix element of the charge operator $Q = \int d^3x j^0(x)$ between these states:

$$\langle \mathbf{p}' | Q | \mathbf{p} \rangle = \int d^3x \langle \mathbf{p}' | j^0(x) | \mathbf{p} \rangle = \delta_{\mathbf{p}', \mathbf{p}}, \quad \langle \bar{\mathbf{p}}' | Q | \bar{\mathbf{p}} \rangle = \int d^3x \langle \bar{\mathbf{p}}' | j^0(x) | \bar{\mathbf{p}} \rangle = -\delta_{\mathbf{p}', \mathbf{p}}. \quad (7.130)$$

The opposite sign of the charges of particles and antiparticles is caused by opposite exponentials accompanying the annihilation and creation operators $a_{\mathbf{p}}$ and $b_{\mathbf{p}}^\dagger$ in the field $\phi(x)$. As far as physical particles are concerned, the states $|\mathbf{p}\rangle = a_{\mathbf{p}}^\dagger | 0 \rangle$ may be identified with π^+ -mesons of momentum $\mathbf{p}$, the states $|\bar{\mathbf{p}}\rangle = b_{\mathbf{p}}^\dagger | 0 \rangle$ with π^- -mesons. The scalar particles associated with the negative frequency solutions of the wave equation are called *antiparticles*. In this nomenclature, the particles of a real field are antiparticles of themselves.

Note that the two matrix elements in (7.129) have the same exponential factors, which is necessary to make sure that particles and antiparticles have the same energies and momenta.

An explicit representation of the unitary operator $\mathcal{C}$ is

$$\mathcal{C} = e^{i\pi G_C/2}, \quad G_C = \sum_{\mathbf{p}} \left[b_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{\mathbf{p}}^\dagger b_{\mathbf{p}} - \eta_P (a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{\mathbf{p}}) \right]. \quad (7.131)$$

The proof is completely analogous to the parity case in Eqs. (7.97)–(7.101).

A bound state of a boson and its antiparticle in a relative angular momentum l has a charge parity $(-1)^l$. This follows directly from the wave function

$$|\Psi\rangle = \int_0^\infty dp R_l(p) \int d^2\hat{\mathbf{p}} Y_{lm}(\hat{\mathbf{p}}) a_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger | 0 \rangle, \quad (7.132)$$

where $R_l(p)$ is some radial wave function of $p = |\mathbf{p}|$. Applying $\mathcal{C}$ to this we have

$$\mathcal{C} a_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger | 0 \rangle = b_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger | 0 \rangle. \quad (7.133)$$

Note that we must interchange the order of $b_{\mathbf{p}}^\dagger$ and $a_{-\mathbf{p}}^\dagger$, as well as the momenta $\mathbf{p}$ and $-\mathbf{p}$, to get back to the original state. This results in a sign factor $(-1)^l$ from the spherical harmonic. An example is the ρ -meson which is a p -wave resonance of a π^+ - and a π^- -meson, and has therefore a charge parity $\eta_C = -1$.

7.2 Spacetime Behavior of Propagators

Let us evaluate the integral representations (7.66) and (7.90) for the propagators of real and complex scalar fields. To do this we use two methods which will be

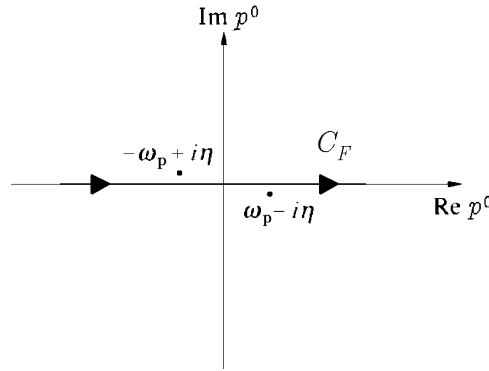


FIGURE 7.1 Pole positions in the complex p^0 -plane in the integral representations (7.66) and (7.90) of Feynman propagators.

applied many times in this text. The integrands in (7.66) and (7.90) have two poles in the complex p^0 -plane as shown in Fig. 7.1, one at $p^0 = \sqrt{\mathbf{p}^2 + M^2} - i\eta$, the other at $p^0 = -\sqrt{\mathbf{p}^2 + M^2} + i\eta$, both with infinitesimal $\eta > 0$. The first is due to the intermediate single-particle state propagating in the positive time direction, the other comes from an antiparticle propagating in the negative time direction. A propagator with such pole positions is called a *Feynman propagator*.

7.2.1 Wick Rotation

The special pole positions make it possible to rotate the contour of integration in the p^0 -plane without crossing a singularity so that it runs along the imaginary axis $dp^0 = idp^4$. This procedure is called a *Wick rotation*, and is illustrated in Fig. 7.2. Volume elements $d^4p = dp^0 dp^1 dp^2 dp^3$ in Minkowski space go over into volume elements $i dp^1 dp^2 dp^3 dp^4 \equiv i d^4p_E$ in euclidean space.

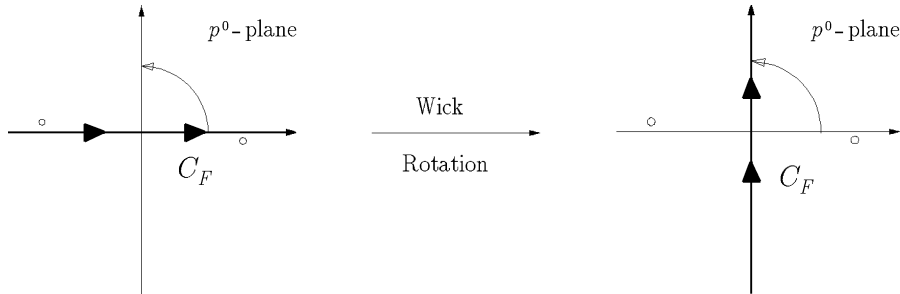


FIGURE 7.2 Wick rotation of the contour of integration in the complex p^0 -plane.

By this procedure, the integral representations (7.66) and (7.90) for the propagator become

$$G(x - x') = \int \frac{d^4 p_E}{(2\pi)^4} \frac{1}{p_E^2 + M^2} e^{-ip_E(x-x')_E}, \quad (7.134)$$

where p_E^μ is the four-momentum

$$p_E^\mu = (p^1, p^2, p^3, p^4 = -ip^0), \quad (7.135)$$

and p_E^2 the square of the momentum p_E^μ calculated in the euclidean metric, i.e., $p_E^2 \equiv p^{1^2} + p^{2^2} + p^{3^2} + p^{4^2}$. The vector x_E^μ is the corresponding euclidean spacetime vector

$$x_E^\mu = (x^1, x^2, x^3, x^4 = -ix^0), \quad (7.136)$$

so that $px = -p_E x_E$. With $p_E^2 + M^2$ being strictly positive, the integral (7.134) is now well-defined. Moreover, the denominator possesses a simple integral representation in the form of an auxiliary integral over an auxiliary parameter τ which, as we shall see later, plays the role of the *proper time* of the particle orbits:

$$\frac{1}{p_E^2 + M^2} = \int_0^\infty d\tau e^{-\tau(p_E^2 + M^2)}. \quad (7.137)$$

Since this way of reexpressing denominators in propagators is extremely useful in quantum field theory, it is referred to, after its author, as *Schwinger's proper-time formalism* [2]. The τ -integral has turned the integral over the denominator into a quadratic exponential function. The exponent can therefore be quadratically completed:

$$e^{ip_E(x-x')_E - \tau p_E^2} \rightarrow e^{-(x-x')_E^2/4\tau - p_E'^2 \tau}, \quad (7.138)$$

with $p_E' = p_E - i(x - x')_E/2\tau$. Since the measure of integration is translationally invariant, and the integrand has become symmetric under four-dimensional rotations, we can replace

$$\int d^4 p_E = \int d^4 p_E' = \pi^2 \int_0^\infty dp_E'^2 p_E'^2, \quad (7.139)$$

and integrate out the four-momentum p_E' , yielding

$$G(x - x') = \frac{1}{16\pi^2} \int_0^\infty \frac{d\tau}{\tau^2} e^{-(x-x')_E^2/4\tau - M^2\tau}. \quad (7.140)$$

The integral is a superposition of nonrelativistic propagators of the type (2.433), with Boltzmann-like weights $e^{-M^2\tau}$, and an additional weight factor τ^{-2} which may be viewed as the effect of an entropy factor $e^S = e^{-2\log \tau}$. This representation has an interesting statistical interpretation. After deriving Eq. (2.433) for a nonrelativistic propagator at imaginary times, we observed that this looks like the probability for a random walk of a fixed length proportional to $\hbar\beta$ to go from $\mathbf{x}$ to $\mathbf{x}'$ in three

dimensions. Here we see that the relativistic propagator looks like a random walk of arbitrary length in four dimensions, with a length distribution ruled mainly by the above Boltzmann factor. This leads to the possibility of describing, by relativistic quantum field theory, ensembles of random lines of arbitrary length. Such lines appear in many physical systems in the form of vortex lines and defect lines [6, 8, 18].

By changing the variable of integration from τ to $\omega = 1/4\tau$, this becomes

$$G(x - x') = \frac{1}{4\pi^2} \int_0^\infty d\omega e^{-(x-x')_E^2 \omega - M^2/4\omega}. \quad (7.141)$$

Now we use the integral formula

$$\int_0^\infty \frac{d\omega}{\omega} \omega^\nu e^{-a\omega - b/4\omega} = 2 \left(\frac{b}{4a} \right)^{\nu/2} K_\nu(\sqrt{ab}), \quad (7.142)$$

where $K_\nu(z)$ is the modified Bessel function,² to find

$$G(x - x') = \frac{M^2}{4\pi^2} \frac{K_1\left(M\sqrt{(x-x')_E^2}\right)}{M\sqrt{(x-x')_E^2}}. \quad (7.143)$$

The D -dimensional generalization of this is calculated in the same way. Equation (7.140) becomes

$$G(x - x') = \frac{1}{(4\pi)^{D/2}} \int_0^\infty \frac{d\tau}{\tau^{D/2}} e^{-(x-x')_E^2/4\tau - M^2\tau}, \quad (7.144)$$

yielding, via (7.142),

$$\begin{aligned} G(x - x') &= \int \frac{d^D q}{(2\pi)^D} \frac{1}{q_E^2 + M^2} e^{iq(x-x')} \\ &= \frac{1}{(2\pi)^{D/2}} \left[\frac{M}{\sqrt{(x-x')_E^2}} \right]^{D/2-1} K_{D/2-1}\left(M\sqrt{(x-x')_E^2}\right). \end{aligned} \quad (7.145)$$

7.2.2 Feynman Propagator in Minkowski Space

Let us now do the calculation in Minkowski space. There the proper-time representation of the propagators (7.66) and (7.90) reads

$$G(x-x') = \int \frac{d^4 p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')} = i \int_0^\infty d\tau \int \frac{d^4 p}{(2\pi)^4} e^{-i[p(x-x') - \tau(p^2 - M^2 + i\eta)]}. \quad (7.146)$$

²I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 3.471.9.

The momentum integrations can be done, after a quadratic completion, with the help of Fresnel's formulas

$$\int \frac{dp^0}{2\pi} e^{ip^{02}a} = \frac{1}{2\sqrt{\pi a/i}}, \quad \int \frac{dp^i}{2\pi} e^{ip^{i2}a} = \frac{1}{2\sqrt{\pi a/i}}. \quad (7.147)$$

In these, it does not matter (as it did in the above Gaussian integrals) that p^{02} and p^{i2} appear with opposite signs in the exponent.

In continuing the evaluation of (7.146), it is necessary to make sure that the integrals over dp^μ and $d\tau$ can be interchanged. The quadratic completion generates a term $e^{-i(x-x')^2/4\tau}$ which is integrable for $\tau \rightarrow 0$ only if we replace $(x-x')^2$ by $(x-x')^2 - i\eta$. Changing again τ to $\omega = 1/4\tau$, we arrive at the integral representation for the Feynman propagator

$$G(x-x') = -\frac{i}{4\pi^2} \int_0^\infty d\omega e^{-i\{[(x-x')^2 - i\eta]\omega + (M^2 - i\eta)/4\omega\}}. \quad (7.148)$$

The two small imaginary parts are necessary to make the integral convergent at both ends. The integral can be done with the help of the formula³

$$\int_0^\infty \frac{d\omega}{\omega} \omega^\nu e^{i(a\omega + b/4\omega)} = 2 \left(\frac{b}{4a} \right)^{\nu/2} i \frac{\pi}{2} e^{i\pi\nu/2} H_\nu^{(1)}(\sqrt{ab}), \quad (7.149)$$

where $H_\nu^{(1)}(z)$ is the Hankel function of the first kind. Upon taking the complex conjugate, using⁴

$$[H_\nu^{(1)}(z)]^* = H_\nu^{(2)}(z^*), \quad (7.150)$$

and replacing a by a^* and b by b^* , we obtain

$$G(x-x') = i \frac{M^2}{8\pi} \frac{H_1^{(2)}(M\sqrt{(x-x')^2})}{M\sqrt{(x-x')^2}}. \quad (7.151)$$

The Hankel functions are combinations of Bessel and Neumann functions

$$H_\nu^{(1,2)}(z) = J_\nu(z) \pm iN_\nu(z). \quad (7.152)$$

In order to check the correctness of this expression, we go to the nonrelativistic limit by letting $c \rightarrow \infty$ in the argument of the Hankel function. Displaying proper CGS-units, for clarity, this becomes

$$\frac{M}{\hbar} \sqrt{(x-x')^2} = \frac{M}{\hbar} \sqrt{c^2(t-t')^2 - (\mathbf{x} - \mathbf{x}')^2} \approx \frac{Mc^2(t-t')}{\hbar} - \frac{1}{2} \frac{M}{\hbar} \frac{(\mathbf{x} - \mathbf{x}')^2}{2(t-t')}. \quad (7.153)$$

³ibid., Formula 3.471.11, together with 8.476.9.

⁴The last two identities are from ibid., Formulas 8.476.8 and 8.476.11.

For large arguments, the Hankel functions behave like

$$H_\nu^{(1,2)}(z) \approx \frac{2}{\pi z} e^{\pm i(z - \nu\pi/2 - \pi/2)}, \quad (7.154)$$

so that (7.151) becomes, for $t > t'$, and taking into account the nonrelativistic limit (4.156) of the fields,

$$G(x - x') \xrightarrow{c \rightarrow \infty} \frac{1}{2M} \frac{1}{\sqrt{2\pi i \hbar (t - t')/M}}^3 \exp \left[\frac{i}{\hbar} \frac{M}{2t} (\mathbf{x} - \mathbf{x}')^2 \right], \quad (7.155)$$

in agreement with the nonrelativistic propagator (2.241).

In the spacelike regime $(x - x')^2 < 0$, we continue $\sqrt{(x - x')^2}$ analytically to $-i\sqrt{-(x - x')^2}$, and $H_1^{(2)}(z) = H_1^{(1)}(-z)$ together with the relation⁵

$$\frac{\pi i}{2} \frac{H_\nu^{(1)}(iz)}{(iz)^\nu} = \frac{K_\nu(z)}{z^\nu}, \quad (7.156)$$

to rewrite (7.151) as

$$G(x - x') = \frac{M}{4\pi^2} \frac{K_1 \left(M \sqrt{-(x - x')^2} \right)}{M \sqrt{-(x - x')^2}}, \quad (x - x')^2 < 0, \quad (7.157)$$

in agreement with (7.143).

It is instructive to study the massless limit $M \rightarrow 0$, in which the asymptotic behavior⁶ $K(z) \rightarrow 1/z$ leads to

$$G(x - x') \rightarrow \frac{1}{4\pi^2} \frac{1}{(x - x')_E^2}. \quad (7.158)$$

To continue this back to Minkowski space where $(x - x')_E^2 = -(x - x')^2$, it is necessary to remember the small negative imaginary part on x^2 which was necessary to make the τ -integral (7.148) converge. The correct massless Green function in Minkowski space is therefore

$$G(x - x') = -\frac{1}{4\pi^2} \frac{1}{(x - x')^2 - i\eta}. \quad (7.159)$$

The same result is obtained from the $M \rightarrow 0$ -limit of the Minkowski space expression (7.151), using the limiting property⁷

$$H_\nu^{(1)}(z) \approx -H_\nu^{(2)}(z) \approx -\frac{i}{\pi} \Gamma(\nu) \frac{1}{(z/2)^\nu}. \quad (7.160)$$

⁵ibid., Formula 8.407.1.

⁶M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Formula 9.6.9.

⁷ibid., Formula 9.1.9.

7.2.3 Retarded and Advanced Propagators

Let us contrast the spacetime behavior of the Feynman propagators (7.151) and (7.159) with that of the *retarded propagator* of classical electrodynamics. A retarded propagator is defined for an arbitrary interacting field $\phi(x)$ by the expectation value

$$G_R(x - x') \equiv \Theta(x^0 - x'^0) \langle 0 | [\phi(x), \phi(x')] | 0 \rangle. \quad (7.161)$$

In general, one defines a commutator function $C(x - x')$ by

$$C(x - x') \equiv \langle 0 | [\phi(x), \phi(x')] | 0 \rangle, \quad (7.162)$$

leading to

$$G_R(x - x') = \Theta(x^0 - x'^0) C(x - x'). \quad (7.163)$$

For a free field $\phi(x)$, the commutator is a c -number, so that the vacuum expectation values can be omitted, and $C(x - x')$ is given by (7.56), leading to a retarded propagator

$$G_R(x - x') = \Theta(x^0 - x'^0) [G^{(+)}(x - x') - G^{(-)}(x - x')]. \quad (7.164)$$

The Heaviside function in front of the commutator function $C(x - x')$ ensures the causality of this propagator. It also has the effect of turning $C(x - x')$, which solves the *homogenous* Klein-Gordon equation, into a solution of the *inhomogenous* equation. In fact, by comparing (7.164) with (7.62) and using the Fourier representations (7.63) of the Heaviside functions, we find, for the retarded propagator, a representation very similar to that of the Feynman propagator in (7.64), except for a reversed $i\eta$ -term in the negative-energy pole:

$$G_R(x - x') = \int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} \left(\frac{i}{E - p^0 + i\eta} - \frac{i}{E + p^0 + i\eta} \right) e^{-iE(x_0 - x'_0) + i\mathbf{p}(\mathbf{x} - \mathbf{x}')}. \quad (7.165)$$

By combining the denominators we now obtain, instead of (7.65),

$$\int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{i}{(E + i\eta)^2 - \mathbf{p}^2 - M^2} e^{-iE(x_0 - x'_0) + i\mathbf{p}(\mathbf{x} - \mathbf{x}')}, \quad (7.166)$$

which may be written as an off-shell integral of the type (7.66):

$$G_R(x - x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p_+^2 - M^2 + i\eta} e^{-ip(x - x')}, \quad (7.167)$$

where the subscript of p_+ indicates that a small $i\eta$ -term has been added to p^0 .

Note the difference in the Fourier representation with respect to that of the commutator function in (7.59). Due to the absence of a Heaviside function, the commutator function solves the *homogenous* Klein-Gordon equation.

It is important to realize that the retarded Green function could be derived from a time-ordered expectation value of second-quantized field operators if we assume

that the Fourier components with the negative frequencies are associated with annihilation operators $d_{-\mathbf{p}}$ rather than creation operators $b_{\mathbf{p}}^\dagger$ of antiparticles. Then the propagator would vanish for $x^0 < x'^0$, implying both poles in the p^0 -plane to lie below the real energy axis.

For symmetry reasons, one also introduces an advanced propagator

$$G_A(x - x') \equiv \Theta(x'^0 - x^0) \langle 0 | [\phi(x), \phi(x')] | 0 \rangle. \quad (7.168)$$

It has the same Fourier representation as $G_R(x - x')$, except that the poles lie both above the real axis:

$$G_A(x - x') = \int \frac{d^4 p}{(2\pi)^4} \frac{i}{p_-^2 - M^2} e^{-ip(x-x')}. \quad (7.169)$$

There will be an application of this Green function in Subsec. 12.12.1.

Let us calculate the spacetime behavior of the retarded propagator. We shall first look at the massless case familiar from classical electrodynamics. For $M = 0$, the integral representation (7.167) reads

$$G_R(x - x') \equiv \int \frac{d^4 p}{(2\pi)^4} e^{-ip(x-x')} \frac{i}{p_+^2}, \quad (7.170)$$

but with the poles in the p^0 -plane at

$$p^0 = p^0 = \pm \omega_{\mathbf{p}} = \pm |\mathbf{p}|, \quad (7.171)$$

both sitting *below* the real axis. This is indicated by writing p_+^2 in the denominator rather than p^2 , the plus sign indicating an infinitesimal $+i\eta$ added to p^0 .

In the Feynman case, the p^0 -integral is evaluated with the decomposition (7.64) and the integral representation (7.63) of the Heaviside function as follows:

$$\begin{aligned} & \int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{1}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{1}{p^0 + \omega_{\mathbf{p}} - i\eta} \right) \\ &= \frac{1}{2\omega_{\mathbf{p}}} [\Theta(x^0 - x'^0) e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} + \Theta(x'^0 - x^0) e^{i\omega_{\mathbf{p}}(x^0-x'^0)}] = \frac{1}{2\omega_{\mathbf{p}}} e^{-i\omega_{\mathbf{p}}|x^0-x'^0|}. \end{aligned} \quad (7.172)$$

In contrast, the retarded expression reads

$$\begin{aligned} & \int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{1}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{1}{p^0 + \omega_{\mathbf{p}} + i\eta} \right) \\ &= \Theta(x^0 - x'^0) \frac{1}{2\omega_{\mathbf{p}}} [e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} - e^{i\omega_{\mathbf{p}}(x^0-x'^0)}]. \end{aligned} \quad (7.173)$$

Thus we may write

$$G(x - x') = \int \frac{d^3 p}{(2\pi)^3 2\omega_{\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} e^{-i\omega_{\mathbf{p}}|x^0-x'^0|}, \quad (7.174)$$

$$G_R(x - x') = \Theta(x^0 - x'^0) \int \frac{d^3 p}{(2\pi)^3 2\omega_{\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} [e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} - e^{i\omega_{\mathbf{p}}(x^0-x'^0)}]. \quad (7.175)$$

In the retarded expression we recognize, behind the Heaviside prefactor $\Theta(x^0 - x'^0)$, the massless limit of the commutator function $C(x, x') = C(x - x')$ of Eq. (7.57), in accordance with the general relation (7.163).

The angular parts of the spatial part of the Fourier integral

$$\int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \quad (7.176)$$

are the same in both cases, producing an integral over $|\mathbf{p}|$:

$$\frac{1}{2\pi R} \int_0^\infty \frac{d|\mathbf{p}|}{\pi} |\mathbf{p}| \sin(|\mathbf{p}|R), \quad (7.177)$$

where $R \equiv |\mathbf{x} - \mathbf{x}'|$. The Feynman propagator has therefore the integral representation

$$G(x - x') = \frac{1}{4\pi R} \int_0^\infty \frac{d|\mathbf{p}|}{\pi} \frac{|\mathbf{p}|}{\omega_{\mathbf{p}}} \sin(|\mathbf{p}|R) e^{-i\omega_{\mathbf{p}}|x^0 - x'^0|}. \quad (7.178)$$

In the massless case where $\omega_{\mathbf{p}} = |\mathbf{p}|$, we can easily perform the $|\mathbf{p}|$ -integration and recover the previous result (7.159).

To calculate the retarded propagator $G_R(x - x') = \Theta(x^0 - x'^0) C(x - x')$ in spacetime, we may focus our attention upon the commutator function, whose integral representation is now

$$C(x - x') = \frac{1}{4\pi R} \int_0^\infty \frac{dp}{\pi} \frac{p}{\omega_{\mathbf{p}}} \sin(pR) [e^{-i\omega_{\mathbf{p}}(x^0 - x'^0)} - e^{i\omega_{\mathbf{p}}(x^0 - x'^0)}]. \quad (7.179)$$

In the massless case where $\omega_{\mathbf{p}} = p$, we decompose the trigonometric function into exponentials, and obtain

$$C(x - x') = -i \frac{1}{4\pi R} \int_{-\infty}^\infty \frac{d\omega}{2\pi} \left\{ e^{-i\omega[(x^0 - x'^0) - R]} - e^{-i\omega[(x^0 - x'^0) + R]} \right\}, \quad (7.180)$$

which is equal to

$$C(x - x') = -i \frac{1}{4\pi R} [\delta(x^0 - x'^0 - R) - \delta(x^0 - x'^0 + R)]. \quad (7.181)$$

It is instructive to verify in this expression the canonical equal-time commutation properties (7.58). For this we multiply $\dot{C}(x)$ by a test function $f(r)$ and calculate, with $r = |\mathbf{x}|$,

$$\int d^3x \dot{C}(x) f(r) = -i \int dr r^2 \frac{1}{r} [\dot{\delta}(x^0 - r) - \dot{\delta}(x^0 + r)]. \quad (7.182)$$

Since $\dot{\delta}(x^0 - r) - \dot{\delta}(x^0 + r) = -(d/dr)[\delta'(x^0 - r) + \delta'(x^0 + r)]$, we can perform a partial integration and find

$$-i \int dr [\delta(x^0 - r) + \delta(x^0 + r)] [rf(r)]' = -i \frac{d}{dx^0} [|x^0| f(|x^0|)]. \quad (7.183)$$

At $x^0 = 0$, this is equal to $-if(0)$ at $x^0 = 0$, as it should.

Using the property of the δ -function (7.61) in spacetime

$$\delta(x^{02} - r^2) = \frac{1}{2r}[\delta(x^0 - r) + \delta(x^0 + r)], \quad (7.184)$$

we can also write the commutator function as

$$C(x - x') = -i\epsilon(x^0 - x'^0) \frac{1}{2\pi} \delta((x - x')^2), \quad (7.185)$$

where $\epsilon(x^0 - x'^0)$ is defined by

$$\epsilon(x^0 - x'^0) \equiv \Theta(x^0 - x'^0) - \Theta(-x^0 + x'^0), \quad (7.186)$$

which changes the sign of the second term in the decomposition (7.184) of $\delta((x - x')^2)$ to the form required in (7.184).

Note that in the form (7.185), the canonical properties (7.58) of the commutator function cannot directly be verified, since $\dot{\epsilon}(x^0 - x'^0) = 2\delta(x^0 - x'^0)$ is too singular to be evaluated at equal times. In fact, products of distributions are in general undefined, and their use is forbidden in mathematics.⁸ We must read $\epsilon(x^0)\delta(x^2)$ as the difference of distributions

$$\epsilon(x^0)\delta(x^2) \equiv \frac{1}{2r}[\delta(x^0 - r) - \delta(x^0 + r)] \quad (7.187)$$

to deduce its consequences. Then with (7.185), the retarded propagator (7.163) becomes

$$\begin{aligned} G_R(x - x') &= -i\Theta(x^0 - x'^0) \frac{1}{4\pi R} [\delta(x^0 - x'^0 - R) - \delta(x^0 - x'^0 + R)] \\ &= -i\Theta(x^0 - x'^0) \frac{1}{2\pi} \delta((x - x')^2). \end{aligned} \quad (7.188)$$

The Heaviside function allows only positive $x^0 - x'^0$, so that only the first δ -function in (7.188) contributes, and we obtain the well-known expression of classical electrodynamics:

$$G_R(x - x') = -i\Theta(x^0 - x'^0) \frac{1}{4\pi R} \delta(x^0 - x'^0 - R). \quad (7.189)$$

This propagator exists only for a causal time order $x^0 > x'^0$, for which it is equal to the Coulomb potential between points which can be connected by a light signal.

The retarded propagator $G_R(x, x')$ describes the massless scalar field $\phi(x)$ caused by a local spacetime event $i\delta^{(4)}(x')$. For a general source $j(x')$, it serves to solve the inhomogeneous field equation

$$-\partial^2 \phi(x) = j(x) \quad (7.190)$$

⁸An extension of the theory of distributions that includes also their products is developed in the textbook H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, World Scientific, Singapore 2009 (klnrt.de/b5).

by superposition:

$$\phi(x) = -i \int d^4x' G_R(x, x') j(x'). \quad (7.191)$$

Inserting (7.189), and separating the integral into time and space parts, the time x'_0 can be integrated out and the result becomes

$$\phi(\mathbf{x}, t) = - \int d^3x' \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|} j(\mathbf{x}', t_R), \quad (7.192)$$

where

$$t_R = t - |\mathbf{x} - \mathbf{x}'| \quad (7.193)$$

is the time at which the source has emitted the field which arrives at the spacetime point x . Relation (7.192) is the basis for the derivation of the *Liénard-Wiechert potential*, which is recapitulated in Appendix 7B.

7.2.4 Comparison of Singular Functions

Let us compare the spacetime behavior (7.188), (7.189) of the retarded propagator with that of the massless Feynman propagator. The denominator in (7.159) can be decomposed into partial fractions, and we find a form very close to (7.188):

$$G(x - x') = -\frac{1}{8\pi^2 R} \left[\frac{1}{|x^0 - x'^0| - R - i\eta} - \frac{1}{|x^0 - x'^0| + R - i\eta} \right]. \quad (7.194)$$

Feynman has found it useful to denote the function $1/(t - i\eta)$ by $i\pi\delta_+(t)$. This has a Fourier representation which differs from that of a Dirac δ -function by containing only positive frequencies:

$$\delta_+(t) \equiv \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(t-i\eta)}. \quad (7.195)$$

The integral converges at large frequencies only due to the $-i\eta$ -term, yielding

$$\delta_+(t) = -\frac{1}{\pi} \frac{i}{t - i\eta}. \quad (7.196)$$

The pole term can be decomposed as⁹

$$\frac{1}{t - i\eta} = \frac{i\eta}{t^2 + \eta^2} + \frac{t}{t^2 + \eta^2} = i\pi\delta(t) + \frac{\mathcal{P}}{t}. \quad (7.197)$$

Recall that the decomposition concerns distributions which make sense only if they are used inside integrals as multipliers of smooth functions. The symbol $\mathcal{P}$ in the

⁹This is often referred to as *Sochocki's formula*. It is the beginning of an expansion in powers of $\eta > 0$: $1/(x \pm i\eta) = \mathcal{P}/x \mp i\pi\delta(x) + \eta[\pi\delta'(x) \pm id_x\mathcal{P}/x] + \mathcal{O}(\eta^2)$.

second term means that the integral has to be calculated with the *principal-value* prescription.¹⁰ For the function $\delta_+(t)$, the decomposition reads

$$\delta_+(t) = \delta(t) - \frac{i}{\pi} \frac{\mathcal{P}}{t}. \quad (7.198)$$

An important property of this function is that it satisfies a relation like $\delta(t)$ in (7.184):

$$\delta_+(t^2 - r^2) = \frac{1}{2r} [\delta_+(t - r) - \delta_+(t + r)]. \quad (7.199)$$

Below we shall also need the complex conjugate of the function $\delta_+(t)$:

$$\delta_-(t) = \frac{1}{\pi} \frac{i}{t + i\eta} = [\delta_+(t)]^*. \quad (7.200)$$

From (7.197) we see that the two functions are related by

$$\delta_+(t) + \delta_-(t) = 2\delta(t). \quad (7.201)$$

Because of (7.199), the Feynman propagator (7.194) can be rewritten as

$$G(x - x') = -\frac{1}{8\pi^2 R} [\delta_+(|x^0 - x'^0| - R) - \delta_+(|x^0 - x'^0| + R)] = -\frac{i}{4\pi} \delta_+((x - x')^2). \quad (7.202)$$

These expressions look very similar to those for the retarded propagator in Eqs. (7.188) and (7.189).

It is instructive to see what becomes of the δ_+ -function in Feynman propagators in the presence of a particle mass. According to (7.148), a mass term modifies the integrand in

$$\delta_+((x - x')^2) = \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(x-x')^2}, \quad (7.203)$$

(in which we omit the $-i\eta$ term, for brevity) from $e^{-i\omega(x-x')^2}$ to $e^{-i\omega(x-x')^2 - iM^2/4\omega}$. We may therefore define a massive version of $\delta_+((x - x')^2)$ by

$$\delta_+^M((x - x')^2) = \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(x-x')^2 - iM^2/2\omega} = -\frac{M^2}{2} \frac{H_1^{(2)}(M\sqrt{(x-x')^2})}{M\sqrt{(x-x')^2}}. \quad (7.204)$$

A similar generalization of the function $\delta((x - x')^2)$ in (7.185) to $\delta^M((x - x')^2)$ may be found by evaluating the commutator function $C(x - x')$ in Eq. (7.185) at a nonzero mass M . Its Fourier representation was given in Eq. (7.179) and may be written as

$$C(x - x') = -\frac{i}{2\pi^2} \int_0^\infty \frac{d|\mathbf{p}| |\mathbf{p}|^2}{\sqrt{|\mathbf{p}|^2 + M^2}} \frac{\sin(|\mathbf{p}|R)}{|\mathbf{p}|R} \sin[p^0(x^0 - x'^0)]. \quad (7.205)$$

¹⁰Due to the entirely different context, no confusion is possible with the second-quantized parity operator $\mathcal{P}$ introduced in (7.96).

This can be expressed as a derivative

$$C(x - x') = -\frac{i}{4\pi} \frac{1}{r} \frac{d}{dr} F(r, x^0 - x'^0) \quad (7.206)$$

of the function

$$F(r, t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dp}{\sqrt{p^2 + M^2}} \cos(pR) \sin \sqrt{p^2 + M^2} t. \quad (7.207)$$

The integral yields [2]:

$$F(r, t) = \begin{cases} J_0(M\sqrt{t^2 - r^2}) & \text{for } t > r, \\ 0 & \text{for } t \in (-r, r), \\ -J_0(M\sqrt{t^2 - r^2}) & \text{for } t < -r, \end{cases} \quad (7.208)$$

where $J_\mu(z)$ are Bessel functions. By carrying out the differentiation in (7.206), using $J'_0(z) = -J_1(z)$, we may write

$$C(x - x') = -i\epsilon(x^0 - x'^0) \delta^M((x - x')^2), \quad (7.209)$$

with

$$\delta^M(x^2) = \delta(x^2) - \Theta(x^2) \frac{M^2}{2} \frac{J_1(M\sqrt{x^2})}{M\sqrt{x^2}}. \quad (7.210)$$

The function $\Theta(x^2)$ enforces the vanishing of the commutator at spacelike distances, a necessity for the causality of the theory. Using (7.210), we can write the retarded propagator $G_R(x - x') = \Theta(x^0 - x'^0) C(x - x')$ as

$$G_R(x - x') = -i\Theta(x^0 - x'^0) \frac{1}{2\pi} \delta^M((x - x')^2). \quad (7.211)$$

In the massless limit, the second term in (7.210) disappears since $J_1(z) \approx z$ for small z , and (7.211) reduces to (7.188).

Summarizing, we may list the Fourier transforms of the various propagators as follows:

$$\begin{aligned} \text{Feynman propagator : } & \frac{i}{p^2 - M^2 + i\eta} = \pi\delta_-(p^2 - M^2) = \pi\delta_-(p^0^2 - \omega_{\mathbf{p}}^2); \\ & = \frac{\pi}{2\omega_{\mathbf{p}}} [\delta_-(p^0 - \omega_{\mathbf{p}}) + \delta_+(p^0 + \omega_{\mathbf{p}})]; \\ \text{retarded propagator : } & \frac{i}{p_+^2 - M^2} = \frac{\pi}{2\omega_{\mathbf{p}}} [\delta_-(p^0 - \omega_{\mathbf{p}}) - \delta_-(p^0 + \omega_{\mathbf{p}})]; \\ \text{advanced propagator : } & \frac{i}{p_-^2 - M^2} = -\frac{\pi}{2\omega_{\mathbf{p}}} [\delta_+(p^0 - \omega_{\mathbf{p}}) - \delta_+(p^0 + \omega_{\mathbf{p}})]; \\ \text{commutator : } & 2\pi\epsilon(p^0)\delta(p^2 - M^2) = 2\pi\epsilon(p^0)\delta(p^0^2 - \omega_{\mathbf{p}}^2) \\ & = \frac{\pi}{\omega_{\mathbf{p}}} [\delta_-(p^0 - \omega_{\mathbf{p}}) - \delta_+(p^0 + \omega_{\mathbf{p}})]. \end{aligned} \quad (7.212)$$

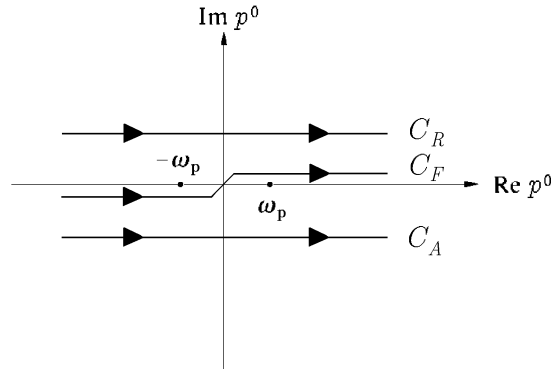


FIGURE 7.3 Integration contours in the complex p^0 -plane of the Fourier integral for various propagators: C_F for the Feynman propagator, C_R for the retarded propagator, and C_A for the advanced propagator.

The corresponding integration contours in the complex energy plane of the representations of the spacetime propagators are indicated in Fig. 7.3. Some exercise with these functions is given in Appendix 7C.

We end this section by pointing out an important physical property of the euclidean Feynman propagator. When generalizing the proper-time representation of $G(x - x')$ to D spacetime dimensions, it reads

$$G(x - x') = \int_0^\infty d\tau \frac{1}{\sqrt{4\pi\tau}^D} e^{-(x-x')_E^2/4\tau - M^2\tau}. \quad (7.213)$$

This reduces to (7.140) for $D = 4$. The integrand can be interpreted as the probability¹¹ that a random world line of length $L = 2D\tau/a$, which is stiff over a length scale $a = 2D$, has the end-to-end distance $\sqrt{(x - x')^2}$. The world line can have any shape. Each configuration is weighted with a Boltzmann probability $e^{-M^2\tau}$ depending on the various lengths. In recent years this worldline interpretation of the Feynman propagator has been very fruitful by giving rise to a new type of quantum field theory, the so-called *disorder field theory* [6]. This theory permits us to study phase transitions of a variety of different physical systems in a unified way. It is dual to Landau's famous theory of phase transitions in which an *order parameter* plays an essential role. In the dual disorder descriptions, the phase transitions have in common that they can be interpreted as a consequence of a sudden proliferation of line-like excitations. This is caused by an overwhelming configuration entropy which sets in at a temperature at which the configurational entropy outweighs the Boltzmann suppression due to the energy of the line-like excitations, the latter being proportional to the length of the excitations. Examples are polymers in solutions, vortex lines in superfluids, defect lines in crystals, etc. Whereas the traditional field

¹¹H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, World Scientific Publishing Co., Singapore 1995, Second extended edition, Sections 5.84 and 15.7.

theoretic description of phase transitions due to Landau is based on the introduction of an *order parameter* and its spacetime version, an *order field*, the new description is based on a *disorder field* describing random fluctuations of line-like excitations. As a result of this different way of looking at phase transitions one obtains a field theoretic formulation of the statistical mechanics of line ensembles, that yields a simple explanation of the phase transitions in superfluids and solids.

7.3 Collapse of Relativistic Wave Function

As earlier in the nonrelativistic discussion on p. 120, a four-field Green function can be used to illustrate the relativistic version of the notorious phenomenon of the *collapse of the wave function* in quantum mechanics [5]. If we create a particle at some spacetime point $x' = (x'_0, \mathbf{x}')$, we generate a Klein-Gordon wave function that covers the forward light cone of this point x' . If we annihilate the particle at some different spacetime point $x'' = (x''_0, \mathbf{x}'')$, the wave function disappears from spacetime. Let us see how this happens about in the quantum field formalism. The creation and later annihilation process give rise to a Klein-Gordon field

$$\langle \varphi(x) \varphi^\dagger(x') \rangle = \sum_{\mathbf{p}} \frac{1}{2V\omega_{\mathbf{p}}} e^{-ip(x-x')}. \quad (7.214)$$

If we measure the particle density at a spacetime x'' point that lies only slightly later than the later spacetime point t by inserting the current operator (7.128) in the above Green function, we find

$$\begin{aligned} G(x'', x, x') &= \langle 0 | \rho(x'') \varphi(x) \varphi^\dagger(x') | 0 \rangle \\ &= -\langle 0 | i\varphi^\dagger(x'') \overleftrightarrow{\partial}_0 \varphi(x'') \varphi(x) \varphi^\dagger(x') | 0 \rangle. \end{aligned} \quad (7.215)$$

The second and the fourth field operators yield a Green function $\Theta(x''_0 - x'_0) G(x'' - x')$. This is multiplied by the Green function of the first and the third field operators which is $\Theta(x - x'') G(x'' - x')$, and is thus equal to zero since $x''_0 > x_0$. Thus proves that by the time $x'_0 > x_0$, the wave function created at the initial spacetime point x' has completely collapsed. More interesting is the situation if we perform an analogous study for a state $|\varphi(x'_1) \varphi(x'_2)\rangle$ that contains two particles. Here we look at the Green function

$$\begin{aligned} G(x'', x_1, x'_1, x_2, x'_2) &= \langle 0 | \rho(x'') \varphi(x_1) \varphi(x_2) \varphi^\dagger(x'_1) \varphi^\dagger(x'_2) | 0 \rangle \\ &= -\langle 0 | i\varphi^\dagger(x'') \overleftrightarrow{\partial}_0 \varphi(x'') \varphi(x_1) \varphi(x_2) \varphi^\dagger(x'_1) \varphi^\dagger(x'_2) | 0 \rangle. \end{aligned} \quad (7.216)$$

Depending on the various positions of x'' with respect to x_1 and x_2 , we can observe the consequences of putting counter for one particle of the two-particle wave function, i.e., from which we learn of the collapse of a one-particle content of the two-particle wave function.¹²

¹²K.E. Hellwig and K. Kraus, Phys. Rev. D **1**, 566 (1970).

7.4 Free Dirac Field

We now turn to the quantization of the Dirac field obeying the field equation (4.500):

$$(i\gamma^\mu \partial_\mu - M)\psi(x) = 0. \quad (7.217)$$

Their plane-wave solutions were given in Subsec. 4.13.1, and just as in the case of a scalar field, we shall introduce creation and annihilation operators for particles associated with these solutions.

The classical Lagrangian density is [recall (4.501)]:

$$\mathcal{L}(x) = \bar{\psi}(x)i\gamma^\mu \partial_\mu \psi(x) - M\bar{\psi}(x)\psi(x). \quad (7.218)$$

7.4.1 Field Quantization

The canonical momentum of the $\psi(x)$ field is

$$\pi(x) = \frac{\partial \mathcal{L}(x)}{\partial [\partial^0 \psi(x)]} = i\bar{\psi}(x)\gamma^0 = i\psi^\dagger(x). \quad (7.219)$$

Up to the factor i , this is equal to the complex-conjugate field $\psi^\dagger$, as in the non-relativistic equation (7.5.1). Note that the field $\bar{\psi}$ has no conjugate momentum, since

$$\frac{\partial \mathcal{L}(x)}{\partial [\partial^0 \bar{\psi}(x)]} = 0. \quad (7.220)$$

This zero is a mere artifact of the use of complex field variables. It is unrelated to a more severe problem in Section 7.5.1, where the canonical momentum of a component of the real electromagnetic vector field vanishes as a consequence of gauge invariance.

If $\psi(\mathbf{x}, t)$ were a Bose field, its canonical commutation rule would read

$$[\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.221)$$

However, since electrons must obey Fermi statistics to produce the periodic system of elements, the fields have to satisfy anticommutation rules

$$\{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)\} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.222)$$

Recall that in the nonrelativistic case, this modification of the commutation rules was dictated by the Pauli principle and the implied antisymmetric electronic wave functions. To ensure this, the relativistic theory can be correctly quantized *only* by anticommutation rules. Commutation rules (7.221) are *incompatible* either with microcausality or the positivity of the energy. This will be shown in Section 7.10.

We now expand the field $\psi(x)$ into the complete set of classical plane-wave solutions (4.662). In a large but finite volume V , the expansion reads

$$\psi(x) = \sum_{\mathbf{p}, s_3} \left[f_{\mathbf{p} s_3}(x) a_{\mathbf{p}, s_3} + f_{\mathbf{p} s_3}^c(x) b_{\mathbf{p}, s_3}^\dagger \right], \quad (7.223)$$

or more explicitly:

$$\psi(x) = \sum_{\mathbf{p}, s_3} \frac{1}{\sqrt{V p^0/M}} \left[e^{-ipx} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ipx} v(\mathbf{p}, s_3) b_{\mathbf{p}, s_3}^\dagger \right]. \quad (7.224)$$

As in the scalar equation (7.12), we have associated the expansion coefficients of the plane waves e^{ipx} with a creation operator $b_{\mathbf{p}, s_3}^\dagger$ rather than an annihilation operator $d_{-\mathbf{p}, -s_3}^\dagger$. For reasons similar to those explained after Eqs. (7.75) and (7.87), the sign is reversed in both $\mathbf{p}$ and s_3 .

Expansion (7.224) is inverted and solved for $a_{\mathbf{p}, s_3}$ and $b_{\mathbf{p}, s_3}^\dagger$ by applying the orthogonality relations (4.665) for the bispinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ to the spatial Fourier transform

$$\int d^3x e^{-i\mathbf{p}\mathbf{x}} \psi(x) = \sum_{\mathbf{p}, s_3} \frac{\sqrt{V}}{\sqrt{p^0/M}} \left[e^{-ip^0x^0} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ip^0x^0} v(-\mathbf{p}, s_3) b_{-\mathbf{p}, s_3}^\dagger \right]. \quad (7.225)$$

The results are

$$\begin{aligned} a_{\mathbf{p}, s_3} &= e^{ip^0x^0} \frac{1}{\sqrt{V p^0/M}} u^\dagger(\mathbf{p}, s_3) \int d^3x e^{-i\mathbf{p}\mathbf{x}} \psi(x), \\ b_{\mathbf{p}, s_3}^\dagger &= e^{-ip^0x^0} \frac{1}{\sqrt{V p^0/M}} v^\dagger(\mathbf{p}, s_3) \int d^3x e^{i\mathbf{p}\mathbf{x}} \psi(x), \end{aligned} \quad (7.226)$$

these being the analogs of the scalar equations (7.76). The same results can, of course, be obtained from (7.223) with the help of the scalar products (4.664), in terms of which Eqs. (7.226) are simply

$$a_{\mathbf{p}, s_3} = (f_{\mathbf{p}, s_3}, \psi)_t, \quad b_{\mathbf{p}, s_3}^\dagger = (f_{\mathbf{p}, s_3}^c, \psi)_t, \quad (7.227)$$

as in the scalar equations (7.19).

From (7.226) we derive that all anticommutators between $a_{\mathbf{p}, s_3}$, $a_{\mathbf{p}', s'_3}^\dagger$, $b_{\mathbf{p}, s_3}$, $b_{\mathbf{p}', s'_3}^\dagger$ vanish, except for

$$\{a_{\mathbf{p}, s_3}, a_{\mathbf{p}', s'_3}^\dagger\} = \sqrt{\frac{M}{p^0} \frac{M}{p'^0}} u^\dagger(\mathbf{p}, s_3) u(\mathbf{p}', s'_3) \delta_{\mathbf{p}, \mathbf{p}'} = \delta_{\mathbf{p}, \mathbf{p}'} \delta_{s_3, s'_3}, \quad (7.228)$$

$$\{b_{\mathbf{p}, s_3}, b_{\mathbf{p}', s'_3}^\dagger\} = \sqrt{\frac{M}{p^0} \frac{M}{p'^0}} v^\dagger(\mathbf{p}, s_3) v(\mathbf{p}', s'_3) \delta_{\mathbf{p}, \mathbf{p}'} = \delta_{\mathbf{p}, \mathbf{p}'} \delta_{s_3, s'_3}. \quad (7.229)$$

The single-particle states

$$|\mathbf{p}, s_3\rangle = a_{\mathbf{p}, s_3}^\dagger |0\rangle \quad (7.230)$$

have the wave functions

$$\begin{aligned} \langle 0 | \psi(x) | \mathbf{p}, s_3 \rangle &= \frac{1}{\sqrt{V p^0/M}} e^{-ipx} u(\mathbf{p}, s_3) = \bar{f}_{\mathbf{p}, s_3}(x) \\ \langle \mathbf{p}, s_3 | \bar{\psi}(x) | 0 \rangle &= \frac{1}{\sqrt{V p^0/M}} e^{ipx} \bar{u}(\mathbf{p}, s_3) = \bar{f}_{\mathbf{p}, s_3}(x). \end{aligned} \quad (7.231)$$

The similar antiparticle states

$$|\bar{\mathbf{p}}, s_3\rangle = b_{\mathbf{p}, s_3}^\dagger |0\rangle, \quad (7.232)$$

have the matrix elements

$$\begin{aligned} \langle \bar{\mathbf{p}}, s_3 | \psi(x) | 0 \rangle &= \frac{1}{\sqrt{V p^0 / M}} e^{ipx} v(\mathbf{p}, s_3) = f_{\mathbf{p}, s_3}^c(x), \\ \langle 0 | \bar{\psi}(x) | \bar{\mathbf{p}}, s_3 \rangle &= \frac{1}{\sqrt{V p^0 / M}} e^{-ipx} \bar{u}(\mathbf{p}, s_3) = \bar{f}_{\mathbf{p}, s_3}^c(x). \end{aligned} \quad (7.233)$$

As in the scalar field expansion (7.75), the negative-frequency solution $v(\mathbf{p}, s_3)e^{ipx}$ of the Dirac equation is associated with a creation operator $b_{\mathbf{p}, s_3}^\dagger$ of an antiparticle rather than a second annihilation operator $d_{-\mathbf{p}, -s_3}$. This ensures that the antiparticle state $|\bar{\mathbf{p}}, s_3\rangle$ has the same exponential form e^{-ipx} as that of $|\mathbf{p}, s_3\rangle$, both exhibiting the same time dependence $e^{-ip^0 t}$ with a positive energy $p^0 = \omega_{\mathbf{p}}$. The other assignment would have given a negative energy.

In an infinite volume, a more convenient field expansion makes use of the plane-wave solutions (4.666). It uses covariant creation and annihilation operators as in (7.16) to expand:

$$\psi(x) = \int \frac{d^3 p}{(2\pi)^3 p^0 / M} \sum_{s_3} \left[e^{-ipx} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ipx} v(\mathbf{p}, s_3) b_{\mathbf{p}, s_3}^\dagger \right]. \quad (7.234)$$

The commutation rules between $a_{\mathbf{p}, s_3}$, $a_{\mathbf{p}, s_3}^\dagger$, $b_{\mathbf{p}, s_3}$, and $b_{\mathbf{p}, s_3}^\dagger$ are the same as in (7.228) and (7.229), but with a replacement of the Kronecker symbols by their invariant continuum version similar to (7.20):

$$\delta_{\mathbf{p}, \mathbf{p}'} \rightarrow \frac{p^0}{M} \delta^{(3)}(\mathbf{p} - \mathbf{p}') = \frac{p^0}{M} (2\pi\hbar)^D \delta^{(3)}(\mathbf{p} - \mathbf{p}'). \quad (7.235)$$

Note that this fermionic normalization is different from the bosonic one in (7.20), where the factor in front of the δ -function was $2p^0$. This is a standard convention throughout the literature.

In an infinite volume, we may again introduce single-particle states

$$|\mathbf{p}, s_3\rangle = a_{\mathbf{p}, s_3}^\dagger |0\rangle, \quad |\bar{\mathbf{p}}, s_3\rangle = b_{\mathbf{p}, s_3}^\dagger |0\rangle, \quad (7.236)$$

with the vacuum $|0\rangle$ defined by $a_{\mathbf{p}, s_3}|0\rangle = 0$ and $b_{\mathbf{p}, s_3}|0\rangle = 0$. These states will satisfy the orthogonality relations

$$(\mathbf{p}', s'_3 | \mathbf{p}, s_3) = \frac{p^0}{M} \delta^{(3)}(\mathbf{p}' - \mathbf{p}) \delta_{s'_3, s_3}, \quad (\bar{\mathbf{p}}', s'_3 | \bar{\mathbf{p}}, s_3) = \frac{p^0}{M} \delta^{(3)}(\mathbf{p}' - \mathbf{p}) \delta_{s'_3, s_3}, \quad (7.237)$$

in accordance with the replacement (7.235) [and in contrast to the normalization (7.27) for scalar particles]. They have the wave functions

$$\begin{aligned} \langle 0 | \psi(x) | \mathbf{p}, s_3 \rangle &= e^{-ipx} u(\mathbf{p}, s_3) = f_{\mathbf{p}, s_3}(x), & (\mathbf{p}, s_3 | \bar{\psi}(x) | 0) &= e^{ipx} \bar{u}(\mathbf{p}, s_3) = \bar{f}_{\mathbf{p}, s_3}(x), \\ (\bar{\mathbf{p}}, s_3 | \psi(x) | 0) &= e^{ipx} v(\mathbf{p}, s_3) = f_{\mathbf{p}, s_3}^c(x), & \langle 0 | \bar{\psi}(x) | \bar{\mathbf{p}}, s_3 \rangle &= e^{-ipx} \bar{v}(\mathbf{p}, s_3) = \bar{f}_{\mathbf{p}, s_3}^c(x). \end{aligned} \quad (7.238)$$

We end this section by stating also the explicit form of the quantized field of massless left-handed neutrinos and their antiparticles, the right-handed antineutrinos:

$$\psi^\nu(x) = \frac{1 - \gamma_5}{2} \psi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}} \left[e^{-ipx} u_L(\mathbf{p}) a_{\mathbf{p}, -\frac{1}{2}} + e^{ipx} v_R(\mathbf{p}) b_{\mathbf{p}, \frac{1}{2}}^\dagger \right], \quad (7.239)$$

where the operators $a_{\mathbf{p}, -\frac{1}{2}}^\dagger$ and $b_{\mathbf{p}, \frac{1}{2}}^\dagger$ carry helicity labels $\mp \frac{1}{2}$, and $p^0 = |\mathbf{p}|$. The massless helicity bispinors are those of Eqs. (4.726) and (4.727). Remember the normalization (4.725):

$$\begin{aligned} u_L^\dagger(\mathbf{p}) u_L(\mathbf{p}) &= 2p^0, & u_R^\dagger(\mathbf{p}) u_R(\mathbf{p}) &= 2p^0, \\ v_L^\dagger(\mathbf{p}) v_L(\mathbf{p}) &= 2p^0, & v_R^\dagger(\mathbf{p}) v_R(\mathbf{p}) &= 2p^0, \end{aligned} \quad (7.240)$$

which is the reason for the factor $1/\sqrt{2Vp^0}$ in the expansion (7.239) [as in the expansions (7.12) and (7.75) for the scalar mesons].

7.4.2 Energy of Free Dirac Particles

We now turn to the energy of the free quantized Dirac field. The energy density is given by the Legendre transform of the Lagrangian density

$$\begin{aligned} \mathcal{H}(x) &= \pi(x) \dot{\psi}(x) - \mathcal{L}(x) \\ &= i\psi^\dagger(x) \dot{\psi}(x) - \mathcal{L}(x) \\ &= \bar{\psi}(x) i\gamma^i \partial^i \psi(x) + M\bar{\psi}(x) \psi(x). \end{aligned} \quad (7.241)$$

Inserting the expansion (7.224) and performing the spatial integral [recall the step from (7.30) to (7.31)], the double sum over momenta reduces to a single sum, and we obtain the second-quantized Hamilton operator

$$\begin{aligned} H = \sum_{\mathbf{p}, s_3, s'_3} \frac{M}{p^0} &\left[a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s'_3} \bar{u}(\mathbf{p}, s_3) (\gamma^i p^i + M) u(\mathbf{p}, s'_3) \right. \\ &+ b_{\mathbf{p}, s_3} b_{\mathbf{p}, s'_3}^\dagger \bar{v}(\mathbf{p}, s_3) (-\gamma^i p^i + M) v(\mathbf{p}, s'_3) \\ &+ a_{\mathbf{p}, s_3}^\dagger b_{-\mathbf{p}, s'_3}^\dagger \bar{u}(\mathbf{p}, s_3) (\gamma^i p^i + M) v(-\mathbf{p}, s'_3) e^{2ip^0 t} \\ &\left. + b_{-\mathbf{p}, s_3} a_{\mathbf{p}, s'_3} \bar{v}(-\mathbf{p}, s_3) (\gamma^i p^i + M) u(\mathbf{p}, s'_3) e^{2ip^0 t} \right]. \end{aligned} \quad (7.242)$$

We now use the Dirac equation, according to which

$$\begin{aligned} (\gamma^i p^i + M) u(\mathbf{p}, s_3) &= \gamma^0 p^0 u(\mathbf{p}, s_3), \\ (-\gamma^i p^i + M) v(\mathbf{p}, s_3) &= -\gamma^0 p^0 v(\mathbf{p}, s_3), \end{aligned} \quad (7.243)$$

and the orthogonality relations (4.696)–(4.699), and simplify (7.243) to

$$H = \sum_{\mathbf{p}, s_3} p^0 \left(a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s_3} - b_{\mathbf{p}, s_3} b_{\mathbf{p}, s_3}^\dagger \right). \quad (7.244)$$

With the help of the anticommutation rule (7.229), this may be rewritten as

$$H = \sum_{\mathbf{p}, s_3} p^0 \left(a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s_3} + b_{\mathbf{p}, s_3}^\dagger b_{\mathbf{p}, s_3} \right) - \sum_{\mathbf{p}, s_3} p^0. \quad (7.245)$$

The total energy adds up all single-particle energies. In contrast to the second-quantized scalar field, the vacuum has now a negatively infinite energy due to the zero-point oscillations, as announced in the discussion of Eq. (7.37).

Note that if we had used here the annihilation operators of negative energy states $d_{-\mathbf{p}, -s_3}$ instead of the creation operators $b_{\mathbf{p}, s_3}^\dagger$, then the energy would have read

$$H = \sum_{\mathbf{p}, s_3} p^0 \left(a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s_3} - d_{\mathbf{p}, s_3}^\dagger d_{\mathbf{p}, s_3} \right), \quad (7.246)$$

so that the particles created by $d_{\mathbf{p}, s_3}^\dagger$ would again have had negative energies. By going over from $d_{-\mathbf{p}, -s_3}$ to $b_{\mathbf{p}, s_3}^\dagger$, we have transformed missing negative energy states into states of antiparticles, thereby obtaining a positive sign for the energy of an antiparticle. This happens, however, at the expense of having a negatively infinite zero-point energy of the vacuum. This also explains why the spin orientation s_3 changes sign under the above replacement. A missing particle with spin down behaves like a particle with spin up.

Actually, the above statements about the exchange $d_{\mathbf{p}, s_3} \rightarrow b_{\mathbf{p}, s_3}^\dagger$ are correct only as far as the sum of all momentum states and spin indices s_3 in (7.246) is concerned. For a single state, we also have to consider the momentum operator and the spin.

The situation is the same as in the free-electron approximation to the electrons in a metal. At zero temperature, the electrons are in the ground state, forming a Fermi sea in which all single-particle levels below a Fermi energy E_F are occupied. If all energies are measured from that energy, all occupied levels have a negative energy, and the ground state has a large negative value. If an electron is kicked out from one of the negative-energy states, an electron-hole pair is observed, both particle and hole carrying a positive energy with respect to the undisturbed Fermi liquid. The hole appears with a positive charge relative to the Fermi sea.

Note also that unlike the Bose case, the exchange $d_{-\mathbf{p}, -s_3} \rightarrow b_{\mathbf{p}, s_3}^\dagger$ maintains the correct sign of canonical anticommutation rules (7.229). In fact, the negative sign of the term $-d_{\mathbf{p}, s_3}^\dagger d_{\mathbf{p}, s_3}$ in the Hamilton operator (7.246) is somewhat less devastating than in the Bose case. It can actually be avoided by a mere redefinition of the vacuum as the state in which all momenta are occupied by a $d_{\mathbf{p}, s_3}^\dagger$ particle:

$$|0\rangle_{\text{new}} = \prod_{\mathbf{p}, s_3} d_{\mathbf{p}, s_3}^\dagger |0\rangle. \quad (7.247)$$

This state has now the same negative infinite energy

$$E_{0 \text{ new}} \equiv {}_{\text{new}}\langle 0 | H | 0 \rangle_{\text{new}} = - \sum_{\mathbf{p}, s_3} p^0, \quad (7.248)$$

found in the correct quantization. Counting from this ground state energy, all other states have positive energies, obtained either by adding a particle with the

operator $a_{\mathbf{p},s_3}^\dagger$ or by removing a particle with $d_{-\mathbf{p},-s_3}$. Of course, this description is just a reflection of the fact that if creation and annihilation operators satisfy anticommutation rules $-d_{\mathbf{p},s_3}^\dagger d_{\mathbf{p},s_3} = d_{\mathbf{p},s_3} d_{\mathbf{p},s_3}^\dagger - 1$, a reinterpretation of the operators $d_{-\mathbf{p},-s_3} \rightarrow b_{\mathbf{p},s_3}^\dagger$ and $d_{-\mathbf{p},-s_3}^\dagger \rightarrow b_{\mathbf{p},s_3}$ makes the product $d_{\mathbf{p},s_3} d_{\mathbf{p},s_3}^\dagger$ a positive operator. For commutators, the same reinterpretation is impossible since $-d_{\mathbf{p},s_3}^\dagger d_{\mathbf{p},s_3}$ can have *any* negative eigenvalue and it is impossible to introduce a new “zero level” that would make all energy differences positive!

It was the major discovery of Dirac that the annihilation of a negative-energy particle may be viewed as a creation of a positive-energy particle with the same mass and spin, but with reversed directions of momentum and spin. Dirac called it the *antiparticle*. When dealing with electrons, the antiparticle is a *positron*. Dirac imagined all negative energy states in the world as being filled, forming a sea of negative energy states, just as the above-described Fermi sea in metals. The annihilation of a negative-energy particle in the sea would create a hole which would appear to the observer as a particle of positive energy with the opposite charge.

As in the scalar case of Eqs. (7.32)–(7.36), it is often possible to simply drop this infinite energy of the vacuum by introducing a normal product $:\mathcal{H}:$. As before, the double dots mean: Order all operators such that all creators stand to the left of all annihilators. But in contrast to the boson case, every transmutation of two Fermi operators, done to achieve the normal order, is now accompanied by a phase factor -1 .

7.4.3 Lorentz Transformation Properties of Particle States

The behavior of the bispinors $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$ under Lorentz transformations determines the behavior of the creation and annihilation operators of particles and antiparticles, and thus of the particle states created by them, in particular the single-particle states (7.230) and (7.232). Under a Lorentz transformation Λ , the field operator $\psi(x)$ transforms according to the law (4.521):

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda)\psi(\Lambda^{-1}x) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}\psi(\Lambda^{-1}x), \quad (7.249)$$

On the right-hand side, we now insert the expansion (7.234), so that

$$D(\Lambda)\psi(\Lambda^{-1}x) = \int \frac{d^3p}{(2\pi)^3 p^0/M} \sum_{s_3, s'_3} \left[e^{-ip'x} u(\mathbf{p}', s'_3) W_{s'_3, s_3}(p', \Lambda, p) a_{\mathbf{p}, s_3} + e^{ip'x} v(\mathbf{p}', s'_3) W_{s'_3, s_3}^*(p', \Lambda, p) b_{\mathbf{p}, s_3}^\dagger \right],$$

where we have set $p' \equiv \Lambda p$, and used the fact that $p\Lambda^{-1}x = p'x$. In order to derive the transformation laws for the creation and annihilation operators, we rewrite this expansion in the same form as the original (7.234), expressing it now in terms of primed momenta and spins:

$$D(\Lambda)\psi(\Lambda^{-1}x) = \int \frac{d^3p'}{(2\pi)^3 p'^0/M} \sum_{s_3, s'_3} \left[e^{-ip'x} u(\mathbf{p}', s'_3) a'_{\mathbf{p}', s'_3} + e^{ip'x} v(\mathbf{p}', s'_3) b_{\mathbf{p}', s'_3}^\dagger \right]. \quad (7.250)$$

Because of the Lorentz invariance of the integration measure in momentum space observed in (4.184), we can replace in (7.250)

$$\int \frac{d^3p}{(2\pi)^3 p^0/M} \rightarrow \int \frac{d^3p}{(2\pi)^3 p'^0/M}. \quad (7.251)$$

Comparing now the coefficients, we find the transformation laws

$$\begin{aligned} a_{\mathbf{p}', s'_3} &\xrightarrow{\Lambda} a'_{\mathbf{p}', s'_3} = \sum_{s_3=-1/2}^{1/2} W_{s'_3, s_3}(p', \Lambda, p) a_{\mathbf{p}, s_3}, \\ b_{\mathbf{p}', s'_3}^\dagger &\xrightarrow{\Lambda} b'_{\mathbf{p}', s'_3}^\dagger = \sum_{s_3=-1/2}^{1/2} W_{s'_3, s_3}^*(p', \Lambda, p) b_{\mathbf{p}, s_3}^\dagger. \end{aligned} \quad (7.252)$$

In contrast to the Lorentz transformations (7.249) of the field, the creation and annihilation operators are transformed *unitarily* under the Lorentz group. The right-hand sides define a unitary representation of the Lorentz transformations Λ :

$$\begin{aligned} a'_{\mathbf{p}', s'_3} &= \mathcal{U}^{-1}(\Lambda) a_{\mathbf{p}', s'_3} \mathcal{U}(\Lambda) = \sum_{s_3=-1/2}^{1/2} W_{s'_3, s_3}(p', \Lambda, p) a_{\mathbf{p}, s_3}, \\ b'_{\mathbf{p}', s'_3}^\dagger &= \mathcal{U}^{-1}(\Lambda) b_{\mathbf{p}', s'_3}^\dagger \mathcal{U}(\Lambda) = \sum_{s_3=-1/2}^{1/2} W_{s'_3, s_3}^*(p', \Lambda, p) b_{\mathbf{p}, s_3}^\dagger, \end{aligned} \quad (7.253)$$

with similar relations for $a_{\mathbf{p}, s_3}^\dagger$ and $b_{\mathbf{p}, s_3}$. For the single-particle states (7.236), this implies the transformation laws:

$$\begin{aligned} \mathcal{U}(\Lambda) |\mathbf{p}, s_3\rangle &= \mathcal{U}(\Lambda) a_{\mathbf{p}, s_3}^\dagger \mathcal{U}^{-1}(\Lambda) |0\rangle = \sum_{s'_3=-1/2}^{1/2} |\mathbf{p}', s'_3\rangle W_{s'_3, s_3}(p', \Lambda, p), \\ \mathcal{U}(\Lambda) |\bar{\mathbf{p}}, s_3\rangle &= \mathcal{U}(\Lambda) b_{\mathbf{p}, s_3}^\dagger \mathcal{U}^{-1}(\Lambda) |0\rangle = \sum_{s'_3=-1/2}^{1/2} |\bar{\mathbf{p}}', s'_3\rangle W_{s'_3, s_3}(p', \Lambda, p), \end{aligned} \quad (7.254)$$

where we have used the Lorentz-invariance of the vacuum state

$$\mathcal{U}(\Lambda) |0\rangle = |0\rangle. \quad (7.255)$$

We are now ready to understand the reason for introducing the matrix c in the bispinors $v(\mathbf{p}, s_3)$ of Eq. (4.684), and thus the sign reversal of the spin orientation. In (4.742) we found that the canonical spin indices of $v(\mathbf{p}, s_3)$ transformed under rotations by the complex-conjugate 2×2 Wigner matrices with respect to those of $u(\mathbf{p}, s_3)$. This implies that the Wigner rotations mixing the spin components of the operators $a_{\mathbf{p}, s_3}$ and $b_{\mathbf{p}, s_3}^\dagger$ are complex conjugate to each other. As a consequence, $b_{\mathbf{p}, s_3}^\dagger$ transforms in the same way as $a_{\mathbf{p}, s_3}^\dagger$, so that antiparticles behave in precisely the same way as particles under Lorentz transformations.

For massless particles in the helicity representation, the creation and annihilation operators transform under Lorentz transformations merely by a phase factor, as discussed at the end of Section 4.15.3.

Under translations by a four-vector a^μ , the particle and antiparticle states $|\mathbf{p}, s_3\rangle = a_{\mathbf{p}, s_3}^\dagger |0\rangle$ and $|\bar{\mathbf{p}}, s_3\rangle = b_{\mathbf{p}, s_3}^\dagger |0\rangle$ transform rather trivially. Since they have a definite momentum, they receive merely a phase factor e^{ipa} . This follows directly from applying the transformation law (4.524) on the Dirac field operator:

$$\psi(x) \longrightarrow \psi'(x) = \psi(x - a). \quad (7.256)$$

Inserting the operator expansion (7.234) into the right-hand side, we see that the creation and annihilation operators transform as follows:

$$\begin{aligned} a_{\mathbf{p}, s_3} &\longrightarrow a'_{\mathbf{p}, s_3} = e^{ipa} a_{\mathbf{p}, s_3}, \\ b_{\mathbf{p}, s_3}^\dagger &\longrightarrow b'^\dagger_{\mathbf{p}, s_3} = e^{-ipa} b_{\mathbf{p}, s_3}^\dagger. \end{aligned} \quad (7.257)$$

These transformation laws define a unitary operator of translations $\mathcal{U}(a)$:

$$\begin{aligned} a'_{\mathbf{p}, s_3} &= \mathcal{U}^{-1}(a) a_{\mathbf{p}, s_3} \mathcal{U}(a) = e^{ipa} a_{\mathbf{p}, s_3}, \\ b'^\dagger_{\mathbf{p}, s_3} &= \mathcal{U}^{-1}(a) b_{\mathbf{p}, s_3}^\dagger \mathcal{U}(a) = e^{-ipa} b_{\mathbf{p}, s_3}^\dagger. \end{aligned} \quad (7.258)$$

On the single-particle states, the operator $\mathcal{U}(a)$ has the effect

$$\begin{aligned} \mathcal{U}(a)|\mathbf{p}, s_3\rangle &= \mathcal{U}(a) a_{\mathbf{p}, s_3}^\dagger \mathcal{U}^{-1}(a) |0\rangle = |\mathbf{p}, s_3\rangle e^{ipa}, \\ \mathcal{U}(a)|\bar{\mathbf{p}}, s_3\rangle &= \mathcal{U}(a) b_{\mathbf{p}, s_3}^\dagger \mathcal{U}^{-1}(\Lambda) |0\rangle = |\bar{\mathbf{p}}, s_3\rangle e^{ipa}. \end{aligned} \quad (7.259)$$

One can immediately write down an explicit expression for this operator:

$$\mathcal{U}(a) = e^{iaP}, \quad (7.260)$$

where P^0 is the Hamilton operator (7.245), rewritten in the infinite-volume form as

$$P^0 \equiv H = \int \frac{d^3p}{(2\pi)^3 p^0 / M} \left(a_{\mathbf{p}, s_3}^\dagger p^0 a_{\mathbf{p}, s_3} + b_{\mathbf{p}, s_3}^\dagger p^0 b_{\mathbf{p}, s_3} - p^0 \frac{p^0}{M} \delta^{(3)}(\mathbf{0}) \right). \quad (7.261)$$

The last term is a formal infinite-volume expression for the finite-volume vacuum energy

$$P_{\text{vac}}^0 = - \int \frac{d^3p V}{(2\pi)^3} p^0, \quad (7.262)$$

as we see from the Fourier representation of $\delta^{(3)}(\mathbf{p}) = \int d^3x e^{i\mathbf{p}\mathbf{x}}$ which is equal to V for $\mathbf{p} = 0$. The operator of total momentum reads

$$\mathbf{P} \equiv \int \frac{d^3p}{(2\pi)^3 p^0 / M} \left(a_{\mathbf{p}, s_3}^\dagger \mathbf{p} a_{\mathbf{p}, s_3} + b_{\mathbf{p}, s_3}^\dagger \mathbf{p} b_{\mathbf{p}, s_3} \right). \quad (7.263)$$

Together, they form the operator of total four-momentum $P^\mu = (P^0, \mathbf{P})$ which satisfies the commutation rules with the particle creation and annihilation operators

$$[P^\mu, a_{\mathbf{p}, s_3}^\dagger] = p^\mu a_{\mathbf{p}, s_3}^\dagger, \quad [P^\mu, b_{\mathbf{p}, s_3}^\dagger] = p^\mu b_{\mathbf{p}, s_3}^\dagger. \quad (7.264)$$

These express the fact that by adding a particle of energy and momentum p^μ to the system, the total energy-momentum P^μ is increased by p^μ .

By combining Lorentz transformations and translations as in (4.526), we cover the entire Poincaré group, and the single-particle states form an irreducible representation space of this group. The invariants of the representation are the mass $M = \sqrt{p^2}$ and the spin s . Thus the complete specification of a representation state is

$$|\mathbf{p}, s_3[M, s]\rangle. \quad (7.265)$$

The Hilbert space of two-particle states $|\mathbf{p}, s_3[M, s]; \mathbf{p}', s'_3[M', s']\rangle$ gives rise to a reducible representation of the Poincaré group. The reducibility is obvious from the fact that if both particles are at rest, the state $|\mathbf{0}, s_3[M, s]; \mathbf{0}', s'_3[M', s']\rangle$ is simply a product of two rotational states of spins s and s' , and decomposes into irreducible representations of the rotation group with spins $S = |s - s'|, |s - s'| + 1, \dots, s + s'$. If the two particles carry momenta, the combined state will also have all possible orbital angular momenta. In the center-of-mass frame of the two particles, the momenta are of equal size and point in opposite directions. The states are then characterized by the direction of one of the momenta, say $\hat{\mathbf{p}}$, and may be written as $|\hat{\mathbf{p}}, s_3, s'_3\rangle$. They satisfy the completeness relation

$$\sum_{s_3=-s}^s \sum_{s'_3=-s'}^{s'} \int_0^\pi d\theta \int_0^{2\pi} d\varphi |\hat{\mathbf{p}}, s_3, s'_3\rangle \langle \hat{\mathbf{p}}, s_3, s'_3| = 1, \quad (7.266)$$

where θ and φ are the spherical angles of the direction $\hat{\mathbf{p}}$.

In the absence of spin, it is then simple to find the irreducible contents of the rotation group. We merely expand the state $|\hat{\mathbf{p}}\rangle$ in partial waves:

$$|\hat{\mathbf{p}}\rangle = \sum_{l,m} |l, m\rangle \langle l, m | \hat{\mathbf{p}} \rangle \equiv \sum_{l,m} |l, m\rangle Y_{lm}(\theta, \phi), \quad (7.267)$$

with the spherical harmonics $Y_{l,m}(\theta, \phi)$. The states $|j, m\rangle$ are orthonormal and complete in this Hilbert space:

$$\langle j, m | j', m' \rangle = \delta_{j,j'} \delta_{m,m'}, \quad \sum_{j,m} |j, m\rangle \langle j, m| = 1. \quad (7.268)$$

In the presence of spins s, s' , the decomposition is simplest if the spin orientations are specified in the helicity basis. Then the two-particle states possess an azimuthal angular momentum of size $h - h'$ around the direction $\hat{\mathbf{p}}$, and may be written as $|\hat{\mathbf{p}}, h - h'\rangle$. These have the same rotation properties as the wave functions of a

spinning top with an azimuthal angular momentum $h - h'$ around the body axis. The latter functions are well known — they are just the representation functions

$$D_{mm'}^j(\alpha, \beta, \gamma) = e^{-i(m\alpha + m'\gamma)} d_{mm'}^j(\beta) \quad (7.269)$$

of rotations of angular momentum j introduced in Eq. (4.865). These serve as wave functions of a spinning top with angular momentum j and magnetic quantum number m , and with an azimuthal component m' of angular momentum around the body axis. They are the basis states of irreducible representations of the rotation group in the center-of-mass frame. Thus, extending (7.267), we can expand

$$\begin{aligned} |\hat{\mathbf{p}}, h - h'\rangle &= \sum_{j,m} |j, m, h - h'\rangle \{j, m, h - h' | \hat{\mathbf{p}}\} \\ &\equiv \sum_{j,m} |j, m, h - h'\rangle \sqrt{\frac{2j+1}{4\pi}} D_{mh-h'}^j(\varphi, \theta, 0), \end{aligned} \quad (7.270)$$

with an orthonormal and complete set of states $|j, m, h - h'\rangle$ at a fixed $h - h'$. The normalization factor is determined to comply with the orthonormality property (4.885) of the rotation functions.

Now we boost this expansion from the center-of-mass frame back to the initial frame in which the total momentum is $\mathbf{P} = \mathbf{p} + \mathbf{p}'$, the energy $P^0 = p^0 + p'^0$, and the mass $\mu = \sqrt{P^2}$. The direction of $\mathbf{P}$ may be chosen as a quantization axis for the angular momentum j . Then the quantum number m is equal to the helicity of the combined state. The angular momentum j in the rest frame determines the spin of the combined state. The resulting Clebsch-Gordan-like expansion of the two-particle state into irreducible representations of the Poincaré group is [10]

$$\begin{aligned} |\mathbf{p}, s_3[M, s]; \mathbf{p}', s'_3[M', s']\rangle &= \sum_{j,m} \int_{(M+M')^2}^{\infty} \frac{d\mu}{2\pi} \int \frac{d^3P}{(2\pi)^3 P^0/\mu} |\mathbf{P}, m[\mu, j]\eta\rangle \\ &\times \langle \mathbf{P}, m[\mu, j]\eta | \mathbf{p}, s_3[M, s]; \mathbf{p}', s'_3[M', s'] \rangle, \end{aligned} \quad (7.271)$$

with the expansion coefficients

$$\begin{aligned} \langle \mathbf{P}, m[\mu, j]\eta | \mathbf{p}, h[M, s]; \mathbf{p}', h'[M', s'] \rangle &= \delta^{(4)}(P - p - p') \mathcal{N}(\mu; M, M') \\ &\times \frac{2j+1}{4\pi} D_{mh-h'}^j(\varphi, \theta, 0), \end{aligned} \quad (7.272)$$

where $\mathcal{N}(\mu; M, M')$ is some normalization factor. The product representation is not simply reducible. It requires distinguishing the different irreducible *biparticle states* according to their spin S . For this purpose, a degeneracy label η is introduced. It may be taken as the pair of helicity indices (h, h') of the individual particles which the biparticle is composed of. However, to describe different processes most efficiently, other linear combinations may be more convenient. One may, for example, combine first the individual spins to a total intermediate spin S . After this one combines the states with spin S with the orbital angular momentum L (in the center-of-mass

frame) to states with a total angular momentum j of the biparticle (in that frame). This corresponds to the LS -coupling scheme in atomic physics. Explicitly, these states are

$$|\mathbf{P}, m [\mu, j] (LS)\rangle = \langle j, h-h' | L, 0; S, h-h' \rangle \langle S, h-h' | s, h; s', -h' \rangle |\mathbf{P}, m [\mu, j] (h, h')\rangle. \quad (7.273)$$

A sum over all h, h' is implied. Since the quantization axis is the direction of $\mathbf{p}$ in the center-of-mass frame, the orbital angular momentum has no L_3 -component.

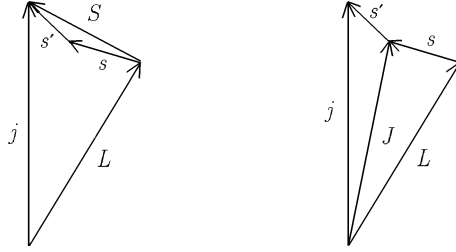


FIGURE 7.4 Different coupling schemes for two-particle states of total angular momentum j and helicity m . The first is the LS -coupling, the second the JL -coupling scheme.

Another possibility of coupling the two particles corresponds to the multipole radiation in electromagnetism. Here one of the particles, say $[M, s]$, is singled out to carry off radiation, which is analyzed according to its total angular momentum J composed of L and s . This total angular momentum is coupled with the other spin s' to the combined total angular momentum j of the biparticle. Here the states are

$$|\mathbf{P}, m [\mu, j] (JL)\rangle = \langle J, h | s, h; L, 0 \rangle \langle j, h-h' | J, h; s', -h' \rangle |\mathbf{P}, m [\mu, j] (h, h')\rangle. \quad (7.274)$$

As in (7.273), a sum over all h, h' is implied. The (LS) - and (JL) -states are related to each other by *Racah's recoupling coefficients*.¹³

The integral over μ can be performed after decomposing the δ -function that ensures the conservation of energy and momentum as

$$\delta^{(4)}(P - p - p') = \delta^{(3)}(\mathbf{P} - \mathbf{p} - \mathbf{p}') \delta\left(\mu - \sqrt{(p + p')^2}\right) \frac{P^0}{\mu}. \quad (7.275)$$

A suitable normalization of the irreducible states is

$$\langle \mathbf{P}, m [\mu, j] \eta | \mathbf{P}', m' [\mu', j'] \eta' \rangle = \delta^{(3)}(\mathbf{P} - \mathbf{P}') \delta(\mu - \mu') \delta_{j,j'} \delta_{m,m'} \delta_{\eta,\eta'}. \quad (7.276)$$

For more details on this subject see Notes and References.

¹³For the general recoupling theory of angular momenta see Chapter VI of the textbook by Edmonds, cited in Notes and References of Chapter 4.

Propagator of Free Dirac Particles

Let us now use the quantized field to calculate the propagator of the free Dirac field. Thus we form the vacuum expectation value of the time ordered product

$$S(x, x') = \langle 0 | T \psi(x) \bar{\psi}(x') | 0 \rangle. \quad (7.277)$$

For, if we use the explicit decomposition

$$T \psi(x) \bar{\psi}(x') = \Theta(x_0 - x'_0) \psi(x) \bar{\psi}(x') - \Theta(x'_0 - x_0) \bar{\psi}(x') \psi(x), \quad (7.278)$$

and apply the Dirac equation (4.661), we obtain

$$\begin{aligned} (i\gamma^\mu \partial_\mu - M) T \psi(x) \bar{\psi}(x') \\ = T(i\gamma^\mu \partial_\mu - M) \psi(x) \bar{\psi}(x') + i\delta(x_0 - x'_0) \{ \gamma_0 \psi(x), \bar{\psi}(x') \}. \end{aligned} \quad (7.279)$$

The right-hand side reduces indeed to $i\delta^{(4)}(x - x')$, due to the Dirac equation (7.217) and the canonical commutation relation (7.222).

Let us now insert the free-field expansion (7.224) into (7.277) and calculate, in analogy to (7.47),

$$\begin{aligned} S_{\alpha\beta}(x, x') &= S_{\alpha\beta}(x - x') \\ &= \Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{p}, s_3; \mathbf{p}', s'_3} \frac{M}{\sqrt{p^0 p'^0}} e^{i(p x - p' x')} u_\alpha(\mathbf{p}, s'_3) \bar{u}_\beta(\mathbf{p}', s'_3) \langle 0 | a_{\mathbf{p}, s_3} a_{\mathbf{p}', s'_3}^\dagger | 0 \rangle \\ &\quad - \Theta(x'_0 - x_0) \frac{1}{V} \sum_{\mathbf{p}, s_3; \mathbf{p}', s'_3} \frac{M}{\sqrt{p^0 p'^0}} e^{i(p x - p' x')} v_\alpha(\mathbf{p}, s_3) \bar{v}_\beta(\mathbf{p}', s'_3) \langle 0 | b_{\mathbf{p}', s'_3} b_{\mathbf{p}, s_3}^\dagger | 0 \rangle \\ &= \Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{p}, s_3} \frac{M}{p^0} e^{-ip(x-x')} \sum_{s_3} u_\alpha(\mathbf{p}, s_3) \bar{u}_\beta(\mathbf{p}, s_3) \\ &\quad - \Theta(x'_0 - x_0) \frac{1}{V} \sum_{\mathbf{p}, s_3} \frac{M}{p^0} e^{ip(x-x')} \sum_{s_3} v_\alpha(\mathbf{p}, s_3) \bar{v}_\beta(\mathbf{p}, s_3). \end{aligned} \quad (7.280)$$

We now recall the polarization sums (4.702) and (4.703), and obtain

$$\begin{aligned} S_{\alpha\beta}(x - x') &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{-ip(x-x')} (\not{p} + M) \\ &\quad + \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{ip(x-x')} (-\not{p} + M). \end{aligned} \quad (7.281)$$

Let us mention here that this type of decomposition can be found for particles of any spin. In (4.705) we introduced the polarization sum

$$P(p) = \sum_{s_3} u(\mathbf{p}, s_3) \bar{u}(\mathbf{p}, s_3), \quad \bar{P}(p) = \sum_{s_3} v(\mathbf{p}, s_3) \bar{v}(\mathbf{p}, s_3) = -P(-p). \quad (7.282)$$

In terms of these, the propagator has the general form

$$\begin{aligned} S_{\alpha\beta}(x-x') &= \Theta(x_0-x'_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{-ip(x-x')} P(p) \\ &+ \Theta(x'_0-x_0) \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{ip(x-x')} P(-p). \end{aligned} \quad (7.283)$$

This structure is found for particles of any spin, in particular also for integer-valued ones. If the statistics is chosen properly, the inverted signs in relation (4.706) between the polarization sums of particles and antiparticles is cancelled by the sign change in the definition of the time-ordered product for bosons and fermions. This will be discussed in more detail in Section 7.10.

In an infinite volume, the momentum sums are replaced by integrals and yield the invariant functions $G^{(+)}(x-x')$, $G^{(-)}(x-x')$ [recall (7.48) and (7.55)]. The sum containing a momentum factor $\not{p}$ may be calculated by taking it outside in the form of a spacetime derivative, i.e., by writing

$$\frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{\mp ip(x-x')} (\pm \not{p} + M) = (\pm i\not{\partial} + M) G^{(\pm)}(x-x'). \quad (7.284)$$

Note that the zeroth component inside the sum comes from the polarization sum over spinors and their energies lie all *on the mass shell*, so that the Green functions $G^{(+)}(x-x')$ and $G^{(-)}(x-x')$ contain only wave functions with on-shell energies. We therefore find the propagator

$$S_{\alpha\beta}(x-x') = \Theta(x_0-x'_0) (i\not{\partial} + M) G^{(+)}(x-x') + \Theta(x'_0-x_0) (i\not{\partial} + M) G^{(-)}(x-x'). \quad (7.285)$$

This expression can be simplified further by moving the derivatives to the left of the Heaviside function. This gives

$$\begin{aligned} S_{\alpha\beta}(x-x') &= (i\not{\partial} + M) \left[\Theta(x_0-x'_0) G^{(+)}(x-x') + \Theta(x'_0-x_0) G^{(-)}(x-x') \right] \\ &- i\gamma^0 \delta(x_0-x'_0) \left[G^{(+)}(x-x') - G^{(-)}(x-x') \right]. \end{aligned} \quad (7.286)$$

The second term happens to vanish because of the property

$$G^{(+)}(\mathbf{x}, 0) = G^{(-)}(\mathbf{x}, 0). \quad (7.287)$$

The final result is therefore the simple expression

$$S_{\alpha\beta}(x-x') = (i\not{\partial} + M) G(x-x'), \quad (7.288)$$

i.e., the propagator of the Dirac field reduces to that of the scalar field multiplied by the differential operator $i\not{\partial} + M$. Inserting on the right-hand side the Fourier representation (7.66) of the scalar propagator, we find for Dirac particles the representation

$$S_{\alpha\beta}(x-x') = \int \frac{d^4p}{(2\pi)^4} (\not{p} + M) \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')}. \quad (7.289)$$

This has to be contrasted with the Fourier representation of the intermediate expression (7.285). If the Heaviside functions are expressed as in Eq. (7.62), we see that (7.285) can be written as

$$S_{\alpha\beta}(x-x') = \gamma^0 \int \frac{d^4p}{(2\pi)^4} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{\omega_{\mathbf{p}}}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{-\omega_{\mathbf{p}}}{p^0 + \omega_{\mathbf{p}} - i\eta} \right) e^{-ip(x-x')}. \quad (7.290)$$

The difference between (7.290) and (7.289) is an integral

$$- \int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{p^0 - \omega_{\mathbf{p}}}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{p^0 + \omega_{\mathbf{p}}}{p^0 + \omega_{\mathbf{p}} - i\eta} \right). \quad (7.291)$$

Here the two distributions in the integrand are of the form $x/(x \pm i\eta)$, so that they cancel each other and (7.291) vanishes.

The integrand in (7.289) can be rewritten in a more compact way using the product formula

$$(\not{p} - M)(\not{p} + M) = p^2 - M^2. \quad (7.292)$$

This leads to the Fourier representation of the Dirac propagator

$$S_{\alpha\beta}(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{\not{p} - M + i\eta} e^{-ip(x-x')}. \quad (7.293)$$

It is worth noting that while in Eq. (7.281) the particle energy p^0 in $\not{p}$ lies on the mass shell, being equal to $\sqrt{\mathbf{p}^2 + M^2}$, those in the integral (7.289) lie off-shell. They are integrated over the entire p^0 -axis and have no relation to the spatial momenta $\mathbf{p}$.

As in the case of the scalar fields [see Eqs. (7.364)], the free-particle propagator is equal to the Green function of the free-field equation. Indeed, by writing (4.661) as

$$L(i\partial)\psi(x) = 0 \quad (7.294)$$

with the differential operator

$$L(i\partial) = i\partial\!\!\!\!/ - M, \quad (7.295)$$

we see that the propagator is the Fourier transform of the inverse of $L(p)$:

$$S(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{L(p)} e^{-ip(x-x')}. \quad (7.296)$$

It obviously satisfies the inhomogeneous Dirac equation

$$(i\gamma^\mu \partial_\mu - M)S(x, x') = i\delta^{(4)}(x - x'). \quad (7.297)$$

For completeness, we also write down the commutator function of Dirac fields. From the expansion (7.224) and the canonical commutation rules (7.228) and (7.229), we find directly

$$[\psi(x), \bar{\psi}(x')] \equiv C_{\alpha\beta}(x - x') \quad (7.298)$$

with the commutator function

$$\begin{aligned} C_{\alpha\beta}(x-x') &= \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{-ip(x-x')} (\not{p} + M) - \frac{1}{2V} \sum_{\mathbf{p}} \frac{1}{p^0} e^{ip(x-x')} (-\not{p} + M) \\ &= (i\not{\partial} + M)C(x-x'). \end{aligned} \quad (7.299)$$

7.4.4 Behavior under Discrete Symmetries

Let us conclude this section by studying the behavior of spin- $\frac{1}{2}$ particles under the discrete symmetries P , C , T .

Space Inversion

The space reflection

$$\psi(x) \xrightarrow{P} \psi'(x) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi(\tilde{x}) = \eta_P \gamma_0 \psi(\tilde{x}) \quad (7.300)$$

is achieved by defining the unitary parity operator $\mathcal{P}$ on the creation and annihilation operators as follows:

$$\begin{aligned} \mathcal{P} a_{\mathbf{p},s_3}^\dagger \mathcal{P}^{-1} &\equiv a'^\dagger(\mathbf{p}, s_3) = \eta_P a^\dagger(-\mathbf{p}, s_3), \\ \mathcal{P} b_{\mathbf{p},s_3}^\dagger \mathcal{P}^{-1} &\equiv b'^\dagger(\mathbf{p}, s_3) = -\eta_P b^\dagger(-\mathbf{p}, s_3). \end{aligned} \quad (7.301)$$

The opposite sign in front of $b_{\mathbf{p},s_3}^\dagger$ is necessary since the spinors behave under parity as follows:

$$\begin{aligned} \gamma^0 u(\mathbf{p}, s_3) &= u(-\mathbf{p}, s_3), \\ \gamma^0 v(\mathbf{p}, s_3) &= -v(-\mathbf{p}, s_3). \end{aligned} \quad (7.302)$$

This follows directly from the explicit representation (4.674) and (4.684):

$$\begin{aligned} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ \sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi(s_3), \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi^c(s_3) &= -\frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s_3). \end{aligned} \quad (7.303)$$

It is easy to verify that with (7.301) and (7.302), the second-quantized field $\psi(x)$ with the expansion (7.224) transforms as it should:

$$\mathcal{P}\psi(x)\mathcal{P}^{-1} = \psi'_P(x) = \eta_P \gamma^0 \psi(\tilde{x}). \quad (7.304)$$

The opposite phase factors of $a^\dagger(\mathbf{p}, s_3)$ and $b^\dagger(\mathbf{p}, s_3)$ under space inversion imply that in contrast to two identical scalar particles the bound state of a Dirac particle

with its antiparticle in a relative orbital angular momentum l carries an extra minus sign, i.e., it has a parity

$$\eta_P = (-)^{l+1}. \quad (7.305)$$

Therefore, the ground state of a positronium atom, which is an s -wave bound state of an electron and a positron, represents a pseudoscalar composite particle whose spins are coupled to zero. For the two different Dirac particles, the combined parity (7.305) carries an extra factor consisting of the two individual parties: $\eta_{P_1}\eta_{P_2}$.

Charge Conjugation

Charge conjugation transforms particles into antiparticles. We therefore define this operation on the creation and annihilation operators of the Dirac particles by

$$\begin{aligned} \mathcal{C}a_{\mathbf{p},s_3}^\dagger \mathcal{C}^{-1} &= a_{\mathbf{p},s_3}'^\dagger = \eta_C b_{\mathbf{p},s_3}^\dagger, \\ \mathcal{C}b_{\mathbf{p},s_3}^\dagger \mathcal{C}^{-1} &= b_{\mathbf{p},s_3}'^\dagger = \eta_C a_{\mathbf{p},s_3}^\dagger. \end{aligned} \quad (7.306)$$

To find out how this operation changes the Dirac field operator, we observe that the charge conjugation matrix C introduced in Eq. (4.603) has the property of changing $\bar{u}^T(\mathbf{p}, s_3)$ into $v(\mathbf{p}, s_3)$, and $\bar{v}^T(\mathbf{p}, s_3)$ into $u(\mathbf{p}, s_3)$:

$$v(\mathbf{p}, s_3) = C\bar{u}^T(\mathbf{p}, s_3), \quad u(\mathbf{p}, s_3) = C\bar{v}^T(\mathbf{p}, s_3). \quad (7.307)$$

The first property was proven in (4.680). The second is proven similarly. As a consequence, the operations (7.306) have the following effect upon the second-quantized field $\psi(x)$:

$$\mathcal{C}\psi(x)\mathcal{C}^{-1} = \psi_C'(x) = \eta_C C\bar{\psi}^T(x). \quad (7.308)$$

Let us now check the transformation property of the second-quantized Dirac current $j^\mu(x)$ under charge conjugation. In the first-quantized form we have found in Eq. (4.617) that the current remains invariant. After field quantization however, there is a minus sign arising from the need to interchange the order of the Dirac field operators when bringing the transformed current $\psi^T(x)\gamma^{\mu T}\bar{\psi}^T(x)$ in Eq. (4.618) back to the original operator ordering $\bar{\psi}(x)\gamma^\mu\psi(x)$ in the current $j^\mu(x)$. Thus we obtain the second-quantized transformation law

$$j^\mu(x) \xrightarrow{C} j^{\mu'}(x) = -j^\mu(x), \quad (7.309)$$

rather than (4.617). This is the law listed in Table 4.12.8.

A bound state of a particle and its antiparticle such as the positronium in a relative angular momentum l , with the spins coupled to S , has the charge parity

$$\eta_C = (-1)^{l+S}. \quad (7.310)$$

In order to see this we form the state

$$|\psi_{lm}^{SS_3}\rangle = \int_0^\infty dp R_l(p) \int d^2\hat{\mathbf{p}} Y_{lm}(\hat{\mathbf{p}}) a_{\mathbf{p},s_3}^\dagger b_{-\mathbf{p},s_3'}^\dagger |0\rangle \langle S, S_3 | s, s_3; s, s_3' \rangle, \quad (7.311)$$

where $\langle S, S_3 | s, s_3; s, s'_3 \rangle$ are the Clebsch-Gordan coefficients coupling the two spins to a total spin S with a third component S_3 [recall Table 4.2].

Under charge conjugation, the product $a_{\mathbf{p}, s_3}^\dagger b_{-\mathbf{p}, s'}^\dagger$ goes over into $b_{\mathbf{p}, s_3}^\dagger a_{-\mathbf{p}, s'_3}^\dagger$. In order to bring this back to the original state we have to interchange the order of the two operators and the spin indices s_3 and s'_3 , and invert $\mathbf{p}$ into $-\mathbf{p}$. The first gives a minus sign, the second a $(-)^l$ sign, and the third a $(-)^{(S-2s_3)}$ sign, since

$$\langle S, S_3 | s, s_3; s', s'_3 \rangle = (-)^{S-s-s'} \langle S, S_3 | s', s'_3; s, s_3 \rangle. \quad (7.312)$$

Altogether, this gives $(-)^{l+S}$.

Time Reversal

Under time reversal, the Dirac equation is invariant under the transformation (4.620):

$$\psi(x) \xrightarrow{T} \psi'_T(x) = D(T) \psi^*(x_T), \quad (7.313)$$

with the 4×4 -representation matrix $D(T)$ of Eq. (4.629):

$$D(T) = \eta_T C \gamma_5. \quad (7.314)$$

The second-quantized version of this transformation of the Dirac field operators reads

$$\psi(x) \xrightarrow{T} \mathcal{T}^{-1} \psi(x) \mathcal{T} = \psi'_T(x) = D(T) \psi(-\tilde{x}). \quad (7.315)$$

The antilinearity of $\mathcal{T}$ generates the complex conjugation of the classical Dirac field in (7.313). Indeed, inserting the expansion (7.224) according to creation and annihilation operators into $\mathcal{T}^{-1} \psi(x) \mathcal{T}$, the antilinearity leads to complex-conjugate spinor wave functions:

$$\begin{aligned} \mathcal{T}^{-1} \psi(x) \mathcal{T} &= \sum_{\mathbf{p}, s_3} \frac{1}{\sqrt{V p^0 / M}} \left[e^{ipx} u^*(\mathbf{p}, s_3) \mathcal{T}^{-1} a_{\mathbf{p}, s_3} \mathcal{T} + e^{-ipx} v^*(\mathbf{p}, s_3) \mathcal{T}^{-1} b_{\mathbf{p}, s_3}^\dagger \mathcal{T} \right] \\ &= D(T) \psi(-\tilde{x}). \end{aligned} \quad (7.316)$$

Expanding likewise the field operator $\psi(-\tilde{x})$ on the right-hand side, and comparing the Fourier coefficients, we find the equations

$$\begin{aligned} u^*(-\mathbf{p}, s_3) \mathcal{T}^{-1} a_{-\mathbf{p}, s_3} \mathcal{T} &= D(T) u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3}, \\ v^*(-\mathbf{p}, s_3) \mathcal{T}^{-1} b_{-\mathbf{p}, s_3}^\dagger \mathcal{T} &= D(T) v(\mathbf{p}, s_3) b_{\mathbf{p}, s_3}^\dagger. \end{aligned} \quad (7.317)$$

To calculate the expressions on the right-hand sides we go to the chiral representations (4.674), where

$$D(T) = \eta_T C \gamma_5 = \begin{pmatrix} c & 0 \\ 0 & c \end{pmatrix}, \quad (7.318)$$

and we see that

$$\begin{aligned} C\gamma_5 \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} c\sqrt{\frac{p\sigma}{M}} \\ c\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3), \\ C\gamma_5 \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi^c(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} c\sqrt{\frac{p\sigma}{M}} \\ -c\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi^c(s_3). \end{aligned} \quad (7.319)$$

We now proceed as in the treatment of Eq. (4.681), using relation (4.683) to find

$$\begin{aligned} C\gamma_5 \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ \sqrt{\frac{p\sigma}{M}} \end{pmatrix}^* \chi(-s_3)(-1)^{s-s_3}, \\ C\gamma_5 \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix}^* \chi(-s_3)(-1)^{s-s_3}, \end{aligned} \quad (7.320)$$

and therefore

$$\begin{aligned} C\gamma_5 u(\mathbf{p}, s_3) &= u^*(-\mathbf{p}, -s_3)(-1)^{s-s_3}, \\ C\gamma_5 v(\mathbf{p}, s_3) &= v^*(-\mathbf{p}, -s_3)(-1)^{s-s_3}. \end{aligned} \quad (7.321)$$

Comparing now the two sides of Eqs. (7.316), we obtain the transformation laws for the creation and annihilation operators

$$\begin{aligned} \mathcal{T} a_{\mathbf{p}, s_3}^\dagger \mathcal{T}^{-1} &\equiv a_{\mathbf{p}, s_3}'^\dagger = \eta_T a_{\mathbf{p}, s_3}'^\dagger c_{s_3' s_3} = \eta_T (-1)^{s-s_3} a_{-\mathbf{p}, -s_3}^\dagger, \\ \mathcal{T} b_{\mathbf{p}, s_3}^\dagger \mathcal{T}^{-1} &\equiv b_{\mathbf{p}, s_3}'^\dagger = \eta_T b_{\mathbf{p}, s_3}'^\dagger c_{s_3' s_3} = \eta_T (-1)^{s-s_3} b_{-\mathbf{p}, -s_3}^\dagger. \end{aligned} \quad (7.322)$$

The occurrence of the c -matrix accounts for the fact that the time-reversed state has the opposite internal rotational motion, with the phases adjusted so that the rotation properties of the transformed state remain correct.

The operator $\mathcal{T}$ is antilinear and antiunitary. This has the effect that just as the wave functions of the Schrödinger theory, the Dirac wave function of a particle of momentum $\mathbf{p}$

$$f_{\mathbf{p}}(x) = u(\mathbf{p}, s_3) e^{-ipx} \quad (7.323)$$

receives a complex conjugation under time reversal:

$$f_{\mathbf{p}, s_3}(x) \xrightarrow{T} f_{\mathbf{p}, s_3 T}(x) = D(T) f_{\mathbf{p}, s_3}^*(x_T) = D(T) u^*(\mathbf{p}, s_3) e^{-i\tilde{p}x}. \quad (7.324)$$

The time-reversed wave function on the right-hand side satisfies again the Dirac equation

$$(i\cancel{\partial} - M) f_{\mathbf{p}, s_3 T}(x) = 0. \quad (7.325)$$

In momentum space this reads

$$(\cancel{p} - M) D(T) u^*(-\mathbf{p}, s_3) = 0. \quad (7.326)$$

It follows directly from (4.625) and a complex conjugation. A similar consideration holds for a wave function

$$f_{\mathbf{p},s_3}^c(x) = v(\mathbf{p}, s_3) e^{ipx}, \quad (7.327)$$

where

$$(\not{p} + M)D(T)v^*(-\mathbf{p}, s_3) = 0. \quad (7.328)$$

As discussed previously on p. 314, parity is maximally violated. One may therefore wonder why the neutron, which may be described by a Dirac spinor as far as its Lorentz transformation properties are concerned, has an extremely small electric dipole moment. At present, one has found only an upper bound for this:

$$d_{\text{el}} < 16 \times 10^{-25} \text{ e} \cdot \text{cm}. \quad (7.329)$$

It was Landau who first pointed out that this can be understood as being a consequence of the extremely small violation of time reversal invariance. The electric dipole moment is a vector operator $\mathbf{d} = e \mathbf{x}$ where $\mathbf{x}$ is the distance between the positive and negative centers of charge in the particle. This operator is obviously invariant under time reversal. Now, for a neutron at rest, $\mathbf{d}$ must be proportional to the only other vector operator available, which is the spin operator $\boldsymbol{\sigma}$, i.e.,

$$\mathbf{d} = \text{const.} \times \boldsymbol{\sigma}. \quad (7.330)$$

But under time reversal, the right-hand side changes its sign, whereas the left-hand side does not. The constant must therefore be zero.¹⁴

Time reversal invariance ensures that a two-particle scattering amplitude for the process

$$1 + 2 \rightarrow 3 + 4 \quad (7.331)$$

is the same as for the reversed process

$$3 + 4 \rightarrow 1 + 2. \quad (7.332)$$

This will be discussed later in Section 9.7, after having developed a scattering theory. Also other consequences of time reversal invariance can be found there.

7.5 Free Photon Field

Let us now discuss the quantization of the electromagnetic field. The classical Lagrangian density is, according to (4.237),

$$\mathcal{L}(x) = \frac{1}{2}[\mathbf{E}^2(x) - \mathbf{B}^2(x)] = -\frac{1}{4}F_{\mu\nu}^2(x), \quad (7.333)$$

where $\mathbf{E}(x)$ and $\mathbf{B}(x)$ are electric and magnetic fields, and the Euler-Lagrange equations are

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial [\partial_\mu A^\nu]} = \frac{\partial \mathcal{L}}{\partial A^\nu}, \quad (7.334)$$

i.e.,

$$(g_{\mu\nu} \partial^2 - \partial_\nu \partial_\mu) A^\nu(x) = 0. \quad (7.335)$$

¹⁴This argument is due to L.D. Landau, Nucl. Phys. 3, 127 (1957).

7.5.1 Field Quantization

The spatial components $A^i(x)$ ($i = 1, 2, 3$) have the canonical momenta

$$\pi_i(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^i(x)} = -F_{0i}(x) = -E^i(x), \quad (7.336)$$

which are just the electric field components. The zeroth component $A^0(x)$, however, poses a problem. Its canonical momentum vanishes identically

$$\pi_0(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^0(x)} = 0, \quad (7.337)$$

since the action does not depend on the time derivative of $A^0(x)$. This property of the canonical momentum is a so-called *primary constraint* in Dirac's classification scheme of Hamiltonian systems.¹⁵ As a consequence, the Euler-Lagrange equation for $A^0(x)$:

$$\partial_i \frac{\partial \mathcal{L}}{\partial [\partial_i A^0]} = \frac{\partial \mathcal{L}}{\partial A^0}, \quad (7.338)$$

is merely an equation of constraint

$$-\nabla \cdot \mathbf{E}(\mathbf{x}, t) = 0, \quad (7.339)$$

which is Coulomb's law for free fields, the first of the field equations (4.247). This is a so-called *secondary constraint* in Dirac's nomenclature. In the presence of a charge density $\rho(\mathbf{x}, t)$, the right hand side is equal to $-\rho(\mathbf{x}, t)$.

We have encountered a vanishing field momentum before in the nonhermitian formulation of the complex nonrelativistic and scalar field theories. There, however, this was an artifact of the complex formulation of the canonical formalism [recall the remarks after Eqs. (7.5.1) and (7.220)]. In contrast to the present situation, the field was fully dynamical.

Let us return to electromagnetism and calculate the Hamiltonian density:

$$\mathcal{H} = \sum_{i=1}^3 \pi_i \dot{A}^i - \mathcal{L} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) + \mathbf{E} \cdot \nabla A^0. \quad (7.340)$$

In the Hamiltonian $H = \int d^3x \mathcal{H}$, the last term can be integrated by parts and we find, after neglecting a surface term $\int d^3x \nabla \cdot (\mathbf{E} A^0)(\mathbf{x}, t)$ and enforcing Coulomb's law (7.339), that the total energy is simply

$$H = \frac{1}{2} \int d^3x (\mathbf{E}^2 + \mathbf{B}^2). \quad (7.341)$$

¹⁵P.A.M. Dirac, *The Principles of Quantum Mechanics*, Oxford University Press, Oxford, Third Edition, 1947, p.114.

We now attempt to convert the canonical fields $A^i(\mathbf{x}, t)$ and $E^i(\mathbf{x}, t)$ into field operators by enforcing canonical commutation rules. There is, however, an immediate obstacle to this caused by Coulomb's law. Proceeding naively, we would impose the equal-time commutators

$$[A^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = 0, \quad (7.342)$$

$$[\pi_i(\mathbf{x}, t), \pi_j(\mathbf{x}', t)] = 0, \quad (7.343)$$

$$[\pi_i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -[E^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] \stackrel{?}{=} -i\delta^{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.344)$$

But the third equation (7.344) is incompatible with Coulomb's law (7.339). The reason for this is clear: We have seen above that the zeroth component of the vector potential $A^0(\mathbf{x}, t)$ is not even an operator. As a consequence, Coulomb's law written out as

$$\nabla^2 A^0(\mathbf{x}, t) = -\partial^0 \nabla \cdot \mathbf{A}(\mathbf{x}, t), \quad (7.345)$$

implies that $\nabla \cdot \mathbf{A}(x)$ cannot be an operator either. As such it must commute with both canonical field operators $A^i(\mathbf{x}, t)$ and $E^i(\mathbf{x}, t)$. The commutation with $A^i(\mathbf{x}, t)$ follows directly from the first relation (7.342). In order to enforce also the commutation with $E^i(\mathbf{x}, t)$, we must correct the canonical commutation rules (7.344) between $E^i(\mathbf{x}, t)$ and $A^j(\mathbf{x}', t)$. We require instead that

$$[\pi_i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -[E^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -i\delta_T^{ij}(\mathbf{x} - \mathbf{x}'), \quad (7.346)$$

where $\delta_T^{ij}(\mathbf{x} - \mathbf{x}')$ is the *transverse* δ -function:

$$\delta_T^{ij}(\mathbf{x} - \mathbf{x}') \equiv \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \left(\delta^{ij} - \frac{k^i k^j}{\mathbf{k}^2} \right). \quad (7.347)$$

This guarantees the vanishing commutation rule

$$[E^i(\mathbf{x}, t), \nabla \cdot \mathbf{A}(\mathbf{x}', t)] = 0, \quad (7.348)$$

which ensures that $\nabla \cdot \mathbf{A}(\mathbf{x}', t)$ is a *c*-number field, and so is $A^0(\mathbf{x}', t)$ via (7.345), thus complying with Coulomb's law (7.345).

In the second-quantized theory, the fields $A^0(\mathbf{x}, t)$ and $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$ play a rather inert role. Both are determined by an equation of motion. The reason for this lies in the gauge invariance of the action, which makes the theory independent of the choice of $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$, or $A^0(\mathbf{x}, t)$. In Section 4.6.2 we have learned that we are free to choose the Coulomb gauge in which $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$ vanishes identically, so that by (7.345) also $A^0(\mathbf{x}, t) \equiv 0$.

In the Coulomb gauge, the canonical field momenta of the vector potential (7.336) are simply their time derivatives:

$$\pi_i(\mathbf{x}, t) = -E^i(\mathbf{x}, t) = \dot{A}^i(\mathbf{x}, t), \quad (7.349)$$

just as for scalar fields [see (7.1)].

We are now ready to expand each component of the vector potential into plane waves, just as previously the scalar field:

$$A^\mu(x) = \sum_{\mathbf{k}, \lambda} \frac{1}{\sqrt{2V k^0}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, \lambda) a_{\mathbf{k}, \lambda} + \epsilon^{\mu*}(\mathbf{k}, \lambda) a_{\mathbf{k}, \lambda}^\dagger \right]. \quad (7.350)$$

Here $\epsilon^\mu(\mathbf{k}, \lambda)$ are four-dimensional polarization vectors (4.319), (4.331) labeled by the helicities $\lambda = \pm 1$. They contain the transverse spatial polarization vectors

$$\boldsymbol{\epsilon}(\mathbf{k}, \pm 1) = \mp \frac{1}{\sqrt{2}} \begin{pmatrix} \cos \theta \cos \phi \mp i \sin \phi \\ \cos \theta \sin \phi \pm i \sin \phi \\ -\sin \theta \end{pmatrix} \quad (7.351)$$

as $\epsilon^\nu(\mathbf{k}, \lambda) \equiv (0, \boldsymbol{\epsilon}(\mathbf{k}, \lambda))$. The four-dimensional polarization vectors satisfy the orthonormality condition (4.337), and possess the polarization sums (4.340) and (4.345).

Let us quantize the vector field (7.350). In order to impose the canonical commutation rules upon the creation and annihilation operators, we invert the field expansion (7.350), as in the scalar equation (7.14), and find:¹⁶

$$\begin{Bmatrix} a_{\mathbf{k}, \lambda} \\ a_{\mathbf{k}, \lambda}^\dagger \end{Bmatrix} = e^{\pm i k^0 x^0} \frac{1}{\sqrt{2V k^0}} \begin{Bmatrix} \boldsymbol{\epsilon}^*(\mathbf{k}, \lambda) \\ \boldsymbol{\epsilon}(\mathbf{k}, \lambda) \end{Bmatrix} \int d^3x e^{\mp i \mathbf{k} \cdot \mathbf{x}} \left[\pm i \dot{\mathbf{A}}(\mathbf{x}, t) + k^0 \mathbf{A}(\mathbf{x}, t) \right]. \quad (7.352)$$

Using now the commutators (7.346), we find

$$[a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}] = 0, \quad [a_{\mathbf{k}, \lambda}^\dagger, a_{\mathbf{k}', \lambda'}^\dagger] = 0, \quad (7.353)$$

and

$$\begin{aligned} [a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}^\dagger] &= \frac{\sqrt{k^0 k'^0}}{2V} \left(\frac{1}{k^0} + \frac{1}{k'^0} \right) e^{i(k^0 - k'^0)x^0} \\ &\quad \times \int d^3x d^3x' e^{-i(\mathbf{k} \cdot \mathbf{x} - \mathbf{k}' \cdot \mathbf{x}')} \epsilon_i^*(\mathbf{k}, \lambda) \epsilon_j(\mathbf{k}', \lambda') \delta_T^{ij}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (7.354)$$

Inserting the finite-volume version of the Fourier representation (7.347) of the transverse δ -function (7.347), the spatial integrations can be done with the result

$$\epsilon_i^*(\mathbf{k}, \lambda) \epsilon_j(\mathbf{k}', \lambda') \delta_{\mathbf{k}, \mathbf{k}'} \left(\delta^{ij} - k^i k^j / \mathbf{k}^2 \right).$$

Due to the transversality condition (4.314), this reduces to

$$\epsilon_i^*(\mathbf{k}, \lambda) \epsilon_j(\mathbf{k}', \lambda') \delta^{ij} \delta_{\mathbf{k}, \mathbf{k}'}.$$

Using the orthonormality relation (4.333), we therefore obtain

$$[a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}^\dagger] = \delta_{\lambda \lambda'} \delta_{\mathbf{k}, \mathbf{k}'}. \quad (7.355)$$

Thus we have found the usual commutation rules for the creation and annihilation operators of the two transversely polarized photons existing for each momentum $\mathbf{k}$.

¹⁶The reader is invited to express this in terms of a scalar product in analogy with (7.13).

Energy of Free Photons

We can easily express the field energy (7.341) in terms of the field operators. In the Coulomb gauge with $\nabla \cdot \mathbf{A}(\mathbf{x}, t) = 0$, and $\mathbf{E}(\mathbf{x}, t) = -\dot{\mathbf{A}}(\mathbf{x}, t)$, the field energy simplifies to

$$H = \int d^3x \frac{1}{2} \left(\partial_0 A^i \partial_0 A^i + \nabla A^i \cdot \nabla A^i \right). \quad (7.356)$$

This is a sum over the field energies of the three components $A^i(\mathbf{x}, t)$, each of them being of the same form as in Eq. (7.29) for a scalar field of zero mass. The subsequent calculation is therefore the same as the one in that equation. Inserting the field expansion (7.350), we find the Hamilton operator

$$H = \sum_{\mathbf{k}, \lambda=\pm 1} k^0 \left(a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda} + \frac{1}{2} \right), \quad (7.357)$$

which contains the vacuum energy

$$E_0 \equiv \langle 0 | H | 0 \rangle = \frac{1}{2} \sum_{\mathbf{k}, \lambda=\pm 1} k^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}}, \quad (7.358)$$

due to the zero-point oscillations. It consists of the sum of all energies $\omega_{\mathbf{k}}$.

Propagator of Free Photons

Let us now calculate the Feynman propagator of the photon field, defined by the vacuum expectation value

$$G^{\mu\nu}(x, x') \equiv \langle 0 | T A^\mu(x) A^\nu(x') | 0 \rangle. \quad (7.359)$$

Inserting the field expansion (7.350), we calculate the vacuum expectation separately for $t > t'$ and $t < t'$ as in (7.47), and find

$$\begin{aligned} G^{\mu\nu}(x, x') &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{\omega_{\mathbf{k}}} e^{-ik(x-x')} \sum_{\lambda} \epsilon^\mu(\mathbf{k}, \lambda) \epsilon^{\nu*}(\mathbf{k}, \lambda) \\ &+ \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{\omega_{\mathbf{k}}} e^{ik(x-x')} \sum_{\lambda} \epsilon^{\mu*}(\mathbf{k}, \lambda) \epsilon^\nu(\mathbf{k}, \lambda). \end{aligned} \quad (7.360)$$

The Heaviside functions are represented as in Eqs. (7.63). The polarization sums in the two terms are real and therefore the same, both being given by the projection matrices $P_T^{\mu\nu}(\mathbf{k})$ or $P_T^{\mu\nu}(k)$ of Eqs. (4.340) or (4.345), respectively. Since these are independent of k^0 , we may proceed as in the derivation of (7.64) from (7.47), thus arriving at a propagator in an infinite spatial volume:

$$G^{\mu\nu}(x - x') = \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-x')} \frac{i}{k^2 + i\eta} P_T^{\mu\nu}(k). \quad (7.361)$$

The independence of $P_T^{\mu\nu}(k)$ on k^0 permits us to assume k^0 in the η -dependent expression (4.345) to be off mass shell, with k^μ covering the entire four-dimensional

momentum space in the integral (7.361). Alternatively, it may be assumed to be equal to the $\mathbf{k}$ -dependent mass-shell values $\omega_{\mathbf{k}}$, i.e., we may use the polarization sum $P_T^{\mu\nu}(\omega_{\mathbf{k}}, \mathbf{k})$ rather than (4.345). The latter is, however, an unconventional option, since the off-shell form is more convenient for deducing the consequences of gauge invariance in the presence of charged particles [see the discussion after (12.101)].

In any case, the free-photon propagator is a Green function of the field equations. Neglecting surface terms, we rewrite the action associated with the Lagrangian density (7.333), after a partial integration, as

$$\mathcal{A} = \frac{1}{2} \int d^4x A^\mu(x) (g_{\mu\nu} \partial^2 - \partial_\mu \partial_\nu) A^\nu(x). \quad (7.362)$$

It corresponds to a Lagrangian density

$$\mathcal{L}(x) = \frac{1}{2} A^\mu(x) L_{\mu\nu}(i\partial) A^\nu(x), \quad (7.363)$$

with the differential operator

$$L_{\mu\nu}(i\partial) \equiv g_{\mu\nu} \partial^2 - \partial_\mu \partial_\nu. \quad (7.364)$$

The Euler-Lagrange equation (7.335) can then be written as

$$L_{\mu\nu}(i\partial) A^\nu(x) = 0. \quad (7.365)$$

Ordinarily, we would define a Green function by the inhomogenous differential equation

$$L_{\mu\nu}(i\partial) G^{\nu\lambda}(x - x') = i \delta_\mu^\lambda \delta^{(4)}(x - x'). \quad (7.366)$$

Here, however, this equation cannot be solved since the Fourier transform of the differential operator $L_{\mu\nu}(i\partial)$ is the 4×4 -matrix

$$L_{\mu\nu}(k) = -g_{\mu\nu} k^2 + k_\mu k_\nu, \quad (7.367)$$

and this possesses an eigenvector with eigenvalue zero, the vector k^ν . Thus $L_{\mu\nu}(k)$ cannot have an inverse, and Eq. (7.366) cannot have a solution. Instead, the nonzero spatial components of the propagator (7.361) satisfy the transverse equation

$$L_{ij}(i\partial) G^{jk}(x - x') = -i \delta_T^{ik}(\mathbf{x} - \mathbf{x}') \delta(x^0 - x'^0), \quad (7.368)$$

and the transversality condition

$$\partial_i G^{ij}(x - x') = 0. \quad (7.369)$$

Let us also calculate the commutator from the Feynman propagator according to the rules (7.212). It is most conveniently expressed in terms of the explicitly k^0 -independent projection matrix (4.340) as

$$[A^\mu(x), A^\nu(x')] = \int \frac{d^4k}{(2\pi)^4} \epsilon(k^0) \delta(k^2) e^{-ik(x-x')} P_T^{\mu\nu}(\mathbf{k}). \quad (7.370)$$

Since the polarization sum depends only on the spatial momenta, it can be taken out of the integral replacing k_i by $-i\partial_i$, yielding

$$[A^\mu(x), A^\nu(x')] = \left[-g^{\mu\nu} + \left(\frac{1}{0} \middle| \frac{0}{-\partial^i \partial^j / \partial^2} \right)^{\mu\nu} \right] C(x - x'). \quad (7.371)$$

Here $C(x - x')$ is the commutator function of the scalar field defined in (7.56) with Fourier representations (7.57), (7.206), and (7.179). Taking the time derivative of one of the fields and using the property $\dot{C}(x - x') = -i\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ for $x^0 = x'^0$ which follows from Eq. (7.58), we find the canonical equal-time commutator

$$[\dot{A}^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)] = -i \left[-g^{\mu\nu} + \left(\frac{1}{0} \middle| \frac{0}{-\partial^i \partial^j / \partial^2} \right)^{\mu\nu} \right] \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.372)$$

Recall that this was the starting point (7.346) of the quantization procedure in the Coulomb gauge with $\mathbf{E}(\mathbf{x}, t) = -\dot{\mathbf{A}}(\mathbf{x}, t)$.

It is instructive to see how the quantization proceeds in the presence of a source term, where the action (7.362) reads

$$\mathcal{A} = \frac{1}{2} \int d^4x A^\mu(x) (g_{\mu\nu} \partial^2 - \partial_\mu \partial_\nu) A^\nu(x) - \int d^4x A^\mu(x) j_\mu(x). \quad (7.373)$$

Going to the individual components A^0 and $\mathbf{A} = (A^1, A^2, A^3)$ as in (4.249), this reads

$$\begin{aligned} \mathcal{A} = \int d^4x \left\{ \frac{1}{2} [A^0(x) (-\nabla^2) A^0(x) - 2A^0(x) \partial_0 \nabla^i A^i(x) \right. \\ \left. - \mathbf{A}(x) (\partial_0^2 - \nabla^2) \mathbf{A}(x) - A^i(x) \nabla^i \nabla^i(x)] - \rho(x) A^0(x) + \mathbf{j}(x) \mathbf{A}(x) \right\}. \end{aligned} \quad (7.374)$$

As we have observed in (4.249), the Coulomb gauge (4.274) ensures that the field equation for A^0 has no time derivative and can be solved by the instantaneous Coulomb potential of the charge density $\rho(x)$ by Eq. (4.273). The field equation for the spatial components, however, is hyperbolic and amounts to Ampère's law:

$$(\partial_0^2 - \nabla^2) \mathbf{A}(x) = \mathbf{j}(x). \quad (7.375)$$

This is solved in Eq. (5.21) with the help of the retarded Coulomb potential.

7.5.2 Covariant Field Quantization

There exists an alternative formalism in which the photon propagator is manifestly covariant. This can, however, be achieved only at the expense of extending the Hilbert space by a nonphysical sector from which the physical subspace is obtained by certain operator conditions. Such an approach can be followed consistently if the interaction does not mix physical states with unphysical ones. As a function of time,

physical states must remain physical, i.e., the physical subspace must be invariant under the dynamics of the system.

Gauge transformations modify only the unphysical states. It will turn out that half of them have a negative or zero norm and do not allow for a probabilistic interpretation. This, however, does not cause any problems since the physical subspace is positive-definite and dynamically invariant. On this space, the second-quantized time evolution operator $U = e^{-iHt}$ is unitary and the completeness sums between physical observables can be restricted to physical states.

The covariant quantization method is based on a modified Lagrangian in which $A^0(x)$ plays no longer a special role, so that every field component $A^\mu(x)$ possesses a canonically conjugate momentum. For this purpose one introduces an auxiliary field $D(x)$, and adds to the original Lagrangian a so-called *gauge-fixing term*¹⁷

$$\mathcal{L}(x) \rightarrow \mathcal{L}'(x) = \mathcal{L}(x) + \mathcal{L}_{\text{GF}}(x), \quad (7.376)$$

which is defined by

$$\mathcal{L}_{\text{GF}}(x) \equiv -D(x)\partial^\mu A_\mu(x) + \frac{\alpha}{2}D^2(x), \quad \alpha \geq 0. \quad (7.377)$$

Now, it is this auxiliary field $D(x)$, which has no canonical momentum:

$$\pi_D(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{D}(x)} \equiv 0, \quad (7.378)$$

so that the Euler-Lagrange equation for $D(x)$ is not a proper equation of motion, but merely a constraint:

$$\alpha D(x) = \partial_\mu A^\mu(x). \quad (7.379)$$

In contrast to the earlier treatment, all four components of the vector potential $A^\mu(x)$ are here dynamical fields and obey a proper equation of motion:

$$\partial^\mu F_{\mu\nu}(x) = \partial^2 A^\mu(x) - \partial^\mu \partial_\nu A^\nu(x) = -\partial_\nu D(x). \quad (7.380)$$

Together with the constraint (7.379), we can write these field equations as

$$\partial^2 A^\mu(x) - \left(1 - \frac{1}{\alpha}\right) \partial^\mu \partial_\nu A^\nu(x) = 0. \quad (7.381)$$

From these we may derive, by one more differentiation, a field equation for $D(x)$:

$$\partial^2 D(x) = 0, \quad (7.382)$$

which shows that $D(x)$ is a massless Klein-Gordon field.

If we want to use the new extended Lagrangian for the description of electromagnetism, where the field equations are $\partial^\mu F_{\mu\nu} = 0$, we have to make sure that $D(x)$ is,

¹⁷This modification was proposed by E. Fermi, Rev. Mod. Phys. 4, 125 (1932).

at the end, identically zero at all times. With $D(x)$ satisfying the free Klein Gordon equation (7.382), this is guaranteed if $D(x)$ satisfies the initial conditions

$$D(\mathbf{x}, t) \equiv 0, \quad t = t_0, \quad (7.383)$$

$$\dot{D}(\mathbf{x}, t) \equiv 0, \quad t = t_0. \quad (7.384)$$

In other words, if the auxiliary field is zero and does not move at some initial time t_0 , for example at $t_0 \rightarrow -\infty$, it will vanish everywhere at all times. With these initial conditions we can replace the original Lagrangian density by the extended version $\mathcal{L}'(x)$. This has the desired property that all field components $A^\mu(x)$ possess a proper canonically conjugate momentum:

$$\pi_\mu(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^\mu(x)} = -F_{0\mu}(x) - g_{0\mu}D(x). \quad (7.385)$$

Thus, while the spatial field components $A^i(x)$ have the electric fields $-E^i(x)$ as their canonical momenta as before, the new auxiliary field $-D(x)$ plays the role of a canonical momentum to the time component $A^0(x)$. We can now quantize the fields $A^\mu(x)$ and the associate field momenta $(-D(x), -E^i(x))$ by the canonical equal-time commutation rules:

$$\begin{aligned} [A^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)] &= 0, & [E^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] &= i\delta^{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [D(\mathbf{x}, t), A^i(\mathbf{x}', t)] &= 0, & [D(\mathbf{x}, t), A^0(\mathbf{x}', t)] &= i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [E^i(\mathbf{x}, t), E^j(\mathbf{x}', t)] &= 0, & [D(\mathbf{x}, t), E^i(\mathbf{x}', t)] &= 0, \\ [E^i(\mathbf{x}, t), A^0(\mathbf{x}', t)] &= 0, & [D(\mathbf{x}, t), D(\mathbf{x}', t)] &= 0. \end{aligned} \quad (7.386)$$

The Hamiltonian density associated with the Lagrangian density $\mathcal{L}'(x)$ is

$$\mathcal{H}' = \pi_\mu \dot{A}^\mu - \mathcal{L} = -\mathbf{E} \cdot \dot{\mathbf{A}} - D\dot{A}^0 - \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2) + D\partial^\mu A_\mu - \frac{\alpha}{2}D^2. \quad (7.387)$$

Expressing the electric field in terms of the vector potential, $E^i = -F^{0i} = -\dot{A}^i - \partial_i A^0$, this becomes

$$\mathcal{H}' = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) + \mathbf{E} \cdot \nabla A^0 + D\nabla \cdot \mathbf{A} - \frac{\alpha}{2}D^2. \quad (7.388)$$

For a vanishing field $D(x)$, this is the same Hamiltonian density as before in (7.340).

Let us now quantize this theory in terms of particle creation and annihilation operators.

Feynman Gauge $\alpha = 1$

The field equations (7.381) become simplest if we take the special case $\alpha = 1$ called the *Feynman gauge*. Then (7.381) reduces to

$$-\partial^2 A^\mu(x) = 0, \quad (7.389)$$

so that the four components $A^\mu(x)$ simply obey four massless Klein-Gordon equations. The fields can then be expanded into plane-wave solutions as

$$A^\mu(x) = \sum_{\mathbf{k}, \nu=0}^3 \frac{1}{2Vk^0} \left[e^{-ikx} \epsilon^\mu(\nu) a_{\mathbf{k}, \nu} + e^{ikx} \epsilon^{\mu*}(\nu) a_{\mathbf{k}, \nu}^\dagger \right], \quad (7.390)$$

where $\epsilon^\mu(\nu)$ are now *four* momentum-independent polarization vectors

$$\epsilon^\mu(\nu) = g^{\mu\nu}, \quad (7.391)$$

satisfying the orthogonality and completeness relations

$$\epsilon^{\mu*}(\nu) \epsilon_\mu(\nu') = g_{\nu\nu'}, \quad (7.392)$$

$$\sum_{\nu\nu'} g^{\nu\nu'} \epsilon^{\mu'}(\nu) \epsilon^{\nu*}(\nu') = g^{\mu\mu'}. \quad (7.393)$$

Inverting the field expansion, we obtain

$$\begin{Bmatrix} a_{\mathbf{k}, \nu} \\ a_{\mathbf{k}, \nu}^\dagger \end{Bmatrix} = e^{\pm ik^0 x^0} \sum_{\nu'=0}^3 g^{\nu\nu'} \frac{1}{\sqrt{2Vk^0}} \begin{Bmatrix} \epsilon_\mu^*(\nu') \\ \epsilon_\mu(\nu') \end{Bmatrix} \int d^3x e^{\pm i\mathbf{k}\mathbf{x}} \left[\pm i \dot{A}^\mu(x) + k^0 A^\mu(x) \right]. \quad (7.394)$$

Here we use the canonical commutation rules. From Eqs. (7.386) we see that $A^\mu(\mathbf{x}, t)$ and $A^\nu(\mathbf{x}, t)$ commute with each other at equal times:

$$[A^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)] = 0. \quad (7.395)$$

Expressing the canonical momentum (7.385) in terms of the vector potential, $\pi_i(x) = -F_{0i}(x) = -E^i(x) = \dot{A}^i(x) + \partial_i A^0(x)$, the canonical commutator $[\pi_i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -i\delta^{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ implies

$$[\dot{A}^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -i\delta_{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}') - \partial_i[A^0(\mathbf{x}, t), A^j(\mathbf{x}', t)]. \quad (7.396)$$

Now we use (7.395) to see that

$$[\dot{A}^i(\mathbf{x}, t), A^j(\mathbf{x}', t)] = -i\delta^{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.397)$$

In contrast to (7.346), the right-hand side is not restricted to the transverse δ -function.

To find the commutation relations for $A^0(\mathbf{x}, t)$, we take the canonical commutator

$$[D(\mathbf{x}, t), A^0(\mathbf{x}', t)] = i\delta^{(3)}(\mathbf{x} - \mathbf{x}') \quad (7.398)$$

and express D in the Feynman gauge as $\partial^\mu A_\mu = \partial_0 A^0 + \partial_i A^i$ [recalling (7.379)]. The commutators of $A^i(x)$ with $A^0(x)$ vanish so that (7.398) amounts to

$$[\dot{A}^0(\mathbf{x}, t), A^0(\mathbf{x}', t)] = i\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.399)$$

We now use the fact that the commutators of $D(\mathbf{x}, t)$ with the spatial components $A^i(\mathbf{x}', t)$ vanish, due to the third of the canonical commutation rules (7.386). Then the identity (7.379) leads to

$$[\dot{A}^0(\mathbf{x}, t), A^i(\mathbf{x}', t)] = 0. \quad (7.400)$$

Similarly we derive

$$[\dot{A}^i(\mathbf{x}, t), A^0(\mathbf{x}', t)] = 0. \quad (7.401)$$

This follows from the canonical commutator $[E^i(\mathbf{x}, t), A^0(\mathbf{x}', t)] = 0$ after expressing again $E^i = -\dot{A}^i + \partial^i A^0$, or more directly by differentiating the commutator $[A^i(\mathbf{x}, t), A^0(\mathbf{x}', t)] = 0$ with respect to t .

For the commutators between the time derivatives of the fields, we find similarly:

$$\begin{aligned} [\dot{A}^i(\mathbf{x}, t), \dot{A}^j(\mathbf{x}', t)] &= [E^i, E^j] + \{[E^i, \partial_j A^0] - (ij)\} + [\partial_i A^0, \partial_j A^0] = 0, \\ [\dot{A}^0(\mathbf{x}, t), \dot{A}^i(\mathbf{x}', t)] &= [D - \partial_j A^j, -E^i - \partial_i A^0] = 0, \\ [\dot{A}^0(\mathbf{x}, t), \dot{A}^0(\mathbf{x}', t)] &= [D - \partial_j A^j, D - \partial_j A^j] = 0. \end{aligned} \quad (7.402)$$

On the right-hand sides, the equal-time arguments $\mathbf{x}, t$ and $\mathbf{x}', t$ have been omitted for brevity.

Summarizing, the commutators between the field components $A^\nu(\mathbf{x}', t)$ and their time derivatives are given by the manifestly covariant expressions

$$\begin{aligned} [\dot{A}^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)] &= ig^{\mu\nu} \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [A^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)] &= 0, \\ [\dot{A}^\mu(\mathbf{x}, t), \dot{A}^\nu(\mathbf{x}', t)] &= 0. \end{aligned} \quad (7.403)$$

They have the same form as if $A^\mu(\mathbf{x}, t)$ were four independent Klein-Gordon fields, except for the fact that the sign in the commutator between the temporal components of $\dot{A}^\mu(\mathbf{x}, t)$ is opposite to that between the spatial components. This will be the source of considerable complications in the subsequent discussion.

Using the covariant commutation rules (7.403), we find from (7.394) the commutation rules for the creation and annihilation operators:

$$\begin{aligned} [a_{\mathbf{k}, \nu}, a_{\mathbf{k}', \nu'}] &= [a_{\mathbf{k}, \nu}^\dagger, a_{\mathbf{k}', \nu'}^\dagger] = 0, \\ [a_{\mathbf{k}, \nu}, a_{\mathbf{k}', \nu'}^\dagger] &= -\delta_{\mathbf{k}, \mathbf{k}'} g_{\nu \nu'}. \end{aligned} \quad (7.404)$$

It is useful to introduce the contravariant creation and annihilation operators

$$a_{\mathbf{k}}^{\mu\dagger} \equiv \sum_{\nu=0}^3 \epsilon^{\mu*}(\nu) a_{\mathbf{k}, \nu}^\dagger, \quad a_{\mathbf{k}}^\mu \equiv \sum_{\nu=0}^3 \epsilon^\mu(\nu) a_{\mathbf{k}, \nu}. \quad (7.405)$$

They satisfy the commutation rules

$$\begin{aligned} [a_{\mathbf{k}}^\mu, a_{\mathbf{k}'}^\nu] &= [a_{\mathbf{k}}^{\mu\dagger}, a_{\mathbf{k}'}^{\nu\dagger}] = 0, \\ [a_{\mathbf{k}}^\mu, a_{\mathbf{k}'}^{\nu\dagger}] &= -\delta_{\mathbf{k}, \mathbf{k}'} g^{\mu\nu}. \end{aligned} \quad (7.406)$$

The opposite sign of the commutator $[\dot{A}^0(\mathbf{x}, t), A^0(\mathbf{x}', t)]$ shows up in the commutators (7.404) and (7.406) between creation and annihilation operators with the polarization labels $\mu = 0$ or $\nu = 0$. This has the unpleasant consequence that the states created by the operators $a_{\mathbf{k}}^{0\dagger} = a_{\mathbf{k},0}^\dagger$ have a negative norm:

$$\langle 0|a_{\mathbf{k}}^0 a_{\mathbf{k}}^{0\dagger}|0\rangle \equiv \langle 0|[a_{\mathbf{k}}^0, a_{\mathbf{k}}^{0\dagger}]0\rangle = -\langle 0|0\rangle = -1. \quad (7.407)$$

Such states cannot be physical. By applying any odd number of these creation operators to the vacuum, one obtains an infinite set of unphysical states.

Another infinite set of unphysical states is

$$|\tilde{0}\rangle_n \equiv (a_{\mathbf{k}}^{0\dagger} \pm a_{\mathbf{k}}^{3\dagger})^n |0\rangle, \quad n > 1. \quad (7.408)$$

These have a vanishing norm, as follows from the fact that $a_{\mathbf{k}}^{0\dagger} \pm a_{\mathbf{k}}^{3\dagger}$ commutes with its Hermitian conjugate. The label 3 can of course be exchanged by 1 or 2.

Fermi-Dirac Subsidiary Condition

At first sight, this seems to make the usual probabilistic interpretation of quantum mechanical amplitudes impossible. However, as announced in the beginning, this problem can be circumvented. According to Eqs. (7.380)–(7.384), the classical equations of motion are satisfied correctly only if the auxiliary field $D(x)$ vanishes at some initial time, together with its velocity $\dot{D}(x)$. In the quantized theory we have to postulate an equivalent operator property. Exactly the same condition cannot be imposed upon the second-quantized field operator version of $D(x)$. That would be too stringent, since it would contradict the canonical quantization rule

$$[D(\mathbf{x}, t), A^0(\mathbf{x}', t)] = i\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.409)$$

We must require that the equation $D(\mathbf{x}, t) = 0$ is true only when applied to physical states. Thus we postulate that only those states in the Hilbert space are physical which satisfy the subsidiary conditions

$$D(\mathbf{x}, t)|\psi_{\text{phys}}\rangle = 0, \quad \dot{D}(\mathbf{x}, t)|\psi_{\text{phys}}\rangle = 0 \quad (7.410)$$

at some fixed initial time t . Because of the equation of motion (7.382) for $D(x)$, this is equivalent to requiring at all times:

$$D(\mathbf{x}, t)|\psi_{\text{phys}}\rangle \equiv 0. \quad (7.411)$$

This is called the *Fermi-Dirac condition*.¹⁸

In order to discuss its consequences it is useful to introduce the “vectors”

$$\hat{k}_s^\mu \equiv k^\mu/k^0, \quad \hat{k}_l^\mu \equiv \tilde{k}^\mu/2k^0, \quad \text{with} \quad k \equiv (k^0, \mathbf{k}), \quad \tilde{k} \equiv (k^0, -\mathbf{k}), \quad (7.412)$$

¹⁸E. Fermi, *Rev. Mod. Phys.* **4**, 87, (1932); P.A.M. Dirac, *Lectures in Quantum Field Theory*, Academic Press, New York, 1966; W. Heisenberg and W. Pauli, *Z. Phys.* **59**, 168 (1930).

with $k^0 = |\mathbf{k}|$ on the light cone. The quotation marks are used in the same sense as in Section 4.9.6, where we introduced the “vector” (4.420). Due to the normalization factors, both $\hat{k}_s^\mu$ and $\hat{k}_l^\mu$ do *not* transform like vectors under Lorentz transformations. Nevertheless, they do have Lorentz-invariant scalar products when multiplied with each other:

$$\hat{k}_s \hat{k}_s = 0, \quad \hat{k}_l \hat{k}_l = 0, \quad \hat{k}_s \hat{k}_l = 1. \quad (7.413)$$

By analogy with Eqs. (7.619) and (4.420), we shall span the four-dimensional vector space here by supplementing the transverse polarization vectors (7.619), (4.420) by the four-component objects

$$\epsilon^\mu(\mathbf{k}, s) = \hat{k}_s^\mu, \quad \epsilon^\mu(\mathbf{k}, \bar{s}) = \hat{k}_{\bar{s}}^\mu. \quad (7.414)$$

These agree with the earlier-introduced scalar and antiscalar polarization vectors (7.619) and (4.420) in Section 4.9.6, except for a different normalization which will be more convenient in the sequel. We shall use the same symbols for these new objects. Since there is only little danger of confusion, this will help avoiding a proliferation of symbols. Together with the transverse polarization vectors (4.331), the four “vectors” satisfy the orthogonality relation

$$\epsilon_{\mu*}(\mathbf{k}, \sigma) \epsilon^\mu(\mathbf{k}, \sigma') = g_{\sigma\sigma'}, \quad (7.415)$$

where the index σ runs through $+1, -1, s, \bar{s}$, and $g_{\sigma\sigma'}$ is the metric

$$g_{\sigma\sigma'} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}_{\sigma\sigma'}. \quad (7.416)$$

The completeness relation reads, in a slight modification of (4.421),

$$\sum_{\sigma=\pm 1, s, \bar{s}} \epsilon^\mu(\mathbf{k}, \sigma) \epsilon^{\nu*}(\mathbf{k}, \sigma') g^{\sigma\sigma'} = g^{\mu\nu}. \quad (7.417)$$

Multiplying the field expansion (7.390) with the left-hand side of this relation, and defining creation and annihilation operators with polarization label $\sigma = \pm 1, s, \bar{s}$ by

$$a_{\mathbf{k}, \sigma} = \epsilon_\mu^*(\sigma) \sum_{\nu=0}^3 \epsilon_\mu(\nu) a_{\mathbf{k}, \nu}, \quad a_{\mathbf{k}, \sigma}^\dagger = \epsilon_\mu(\sigma) \sum_{\nu=0}^3 \epsilon_{\mu*}(\nu) a_{\mathbf{k}, \nu}^\dagger, \quad (7.418)$$

we obtain the new field expansion

$$A^\mu(x) = \sum_{\mathbf{k}} \frac{1}{2V k^0} \sum_{\sigma=\pm 1, s, \bar{s}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, \sigma) a_{\mathbf{k}, \sigma} + e^{ikx} \epsilon^{\mu*}(\mathbf{k}, \sigma) a_{\mathbf{k}, \sigma}^\dagger \right]. \quad (7.419)$$

This expansion may be inverted by equations like (7.394), expressing the new creation and annihilation operators $a_{\mathbf{k}, \sigma}^\dagger$ and $a_{\mathbf{k}, \sigma}$ in terms of the fields $A^\mu(x)$ and

$\dot{A}^\mu(x)$. The result looks precisely the same as in (7.394), except that the metric $g^{\nu\nu'}$ is replaced by $g^{\sigma\sigma'}$ of (7.416), and the polarization vectors $\epsilon^\mu(\nu')$ by $\epsilon^\mu(\mathbf{k}, \sigma')$.

For the two transverse polarization labels $\sigma = \pm 1$, the new creation and annihilation operators coincide with those introduced during the earlier noncovariant quantization in expansion (7.350), i.e., the operators $a_{\mathbf{k},\sigma}^\dagger$ are equal to $a_{\mathbf{k},\lambda}^\dagger$ for polarization labels $\sigma = \lambda = \pm 1$. In addition, the new expansion (7.419) contains the creation and annihilation operators:

$$a_{\mathbf{k},s} = \hat{k}_s^\mu \sum_{\nu=0}^3 \epsilon_\mu(\nu) a_{\mathbf{k},\nu}, \quad a_{\mathbf{k},s}^\dagger = \hat{k}_s^\mu \sum_{\nu=0}^3 \epsilon_\mu^*(\nu) a_{\mathbf{k},\nu}^\dagger, \quad (7.420)$$

$$a_{\mathbf{k},\bar{s}} = \hat{k}_{\bar{s}}^\mu \sum_{\nu=0}^3 \epsilon_\mu(\nu) a_{\mathbf{k},\nu}, \quad a_{\mathbf{k},\bar{s}}^\dagger = \hat{k}_{\bar{s}}^\mu \sum_{\nu=0}^3 \epsilon_\mu^*(\nu) a_{\mathbf{k},\nu}^\dagger. \quad (7.421)$$

For the spatial momenta $\mathbf{k}$ pointing in the z -direction, these are

$$\begin{aligned} a_{\mathbf{k},s} &= a_{\mathbf{k}}^0 - a_{\mathbf{k}}^3, & a_{\mathbf{k},s}^\dagger &= a_{\mathbf{k}}^{0\dagger} - a_{\mathbf{k}}^{3\dagger}, \\ a_{\mathbf{k},\bar{s}} &= a_{\mathbf{k}}^0 + a_{\mathbf{k}}^3, & a_{\mathbf{k},\bar{s}}^\dagger &= a_{\mathbf{k}}^{0\dagger} + a_{\mathbf{k}}^{3\dagger}. \end{aligned} \quad (7.422)$$

Note that the previous physical polarization sum (7.403) may be written as

$$P_{\text{phys}}^{\mu\nu}(\mathbf{k}) = \sum_{\sigma=\pm 1} \epsilon^\mu(\mathbf{k}, \sigma) \epsilon^\nu(\mathbf{k}, \sigma) = -g^{\mu\nu} + \hat{k}_s^\mu \hat{k}_{\bar{s}}^\nu + \hat{k}_{\bar{s}}^\mu \hat{k}_s^\nu. \quad (7.423)$$

The commutation rules for the new creation and annihilation operators are

$$\begin{aligned} [a_{\mathbf{k},\sigma}, a_{\mathbf{k}',\sigma'}] &= [a_{\mathbf{k},\sigma}^\dagger, a_{\mathbf{k}',\sigma'}^\dagger] = 0, \\ [a_{\mathbf{k},\sigma}, a_{\mathbf{k},\sigma'}^\dagger] &= -g_{\sigma\sigma'} \delta_{\mathbf{k},\mathbf{k}'}. \end{aligned} \quad (7.424)$$

By Fourier-transforming the field $D(x)$, we see that the Fermi-Dirac condition can be rewritten as

$$a_{\mathbf{k},s} |\psi_{\text{phys}}\rangle = 0, \quad (7.425)$$

$$a_{\mathbf{k},s}^\dagger |\psi_{\text{phys}}\rangle = 0, \quad (7.426)$$

i.e., the physical vacuum is annihilated by both the scalar creation *and* by the annihilation operators.

Let us calculate the energy of the free-photon system. For this we integrate the Hamiltonian density (7.388) over all space, insert $D(x) = \dot{A}^0(x) + \partial_i A^i(x)$, $\mathbf{E}(x) = -\dot{\mathbf{A}} - \nabla A^0$, $\mathbf{B}(x) = \nabla \times \mathbf{A}(\mathbf{x})$, and perform some partial integrations, neglecting surface terms, to obtain for $\alpha = 1$ the simple expression

$$H' = \int d^3x \frac{1}{2} (-\dot{A}^\mu \dot{A}_\mu - \nabla A^\mu \nabla A_\mu). \quad (7.427)$$

This is precisely the sum of four independent Klein-Gordon energies [compare with (7.30) and contrast this with (7.356)], one for each spacetime component $A^\mu(x)$.

Due to relativistic invariance, however, the energy of the component $A^0(x)$ has an opposite sign which is related to the above-observed opposite sign in the commutation relations (7.404) and (7.406) for the $\nu = 0$ and $\mu = 0$ polarizations of the creation and annihilation operators.

Inserting now the expansion (7.390) of the field $A^\mu(x)$ in terms of creation and annihilation operators, we obtain by the same calculation which led to Eqs. (7.87) and (7.357):

$$H' = \sum_{\mathbf{k}} \frac{k^0}{2} [-a_{\mathbf{k},\nu}^\dagger a_{\mathbf{k},\nu'} - a_{\mathbf{k},\nu} a_{\mathbf{k},\nu'}^\dagger] g^{\nu\nu'} = \sum_{\mathbf{k}} \frac{k^0}{2} [-a_{\mathbf{k},\mu}^\dagger a_{\mathbf{k}}^\mu - a_{\mathbf{k}}^\mu a_{\mathbf{k},\mu}^\dagger]. \quad (7.428)$$

This operator corresponds to an infinite set of four-dimensional oscillators, one for every spatial momentum and polarization state. Due to the indefinite metric $g^{\nu\nu'}$, the Hilbert space is not of the usual type, and the subsidiary conditions (7.425) and (7.426) are necessary to extract physically consistent results.

The expansion (7.419) in terms of transverse, scalar, and longitudinal creation and annihilation operators yields the Hamiltonian (7.428) in the form

$$H' = \sum_{\mathbf{k}} \frac{k^0}{2} \left[\sum_{\sigma=\pm 1} (a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + a_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger) - a_{\mathbf{k},s} a_{\mathbf{k},\bar{s}}^\dagger - a_{\mathbf{k},\bar{s}} a_{\mathbf{k},s}^\dagger - a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},s} - a_{\mathbf{k},s}^\dagger a_{\mathbf{k},\bar{s}} \right]. \quad (7.429)$$

Let us bring this operator to *normal order*, i.e., to normal order with respect to the physical vacuum. For the transverse modes we move the annihilation operators to the right of the creation operators, as usual. For the modes s and l , the physical normal order has the operators $a_{\mathbf{k},s}$ and $a_{\mathbf{k},s}^\dagger$ on the right. This allows immediate use of the subsidiary conditions (7.425) and (7.426) for the physical vacuum. Using the two commutation rules

$$\begin{aligned} [a_{\mathbf{k},\bar{s}}, a_{\mathbf{k}',s}^\dagger] &= -\delta_{\mathbf{k},\mathbf{k}'}, \\ [a_{\mathbf{k},\bar{s}}^\dagger, a_{\mathbf{k}',s}] &= \delta_{\mathbf{k},\mathbf{k}'}, \end{aligned} \quad (7.430)$$

the Hamiltonian takes the form:

$$H' = \sum_{\mathbf{k}} k^0 \left[\sum_{\sigma=\pm 1} \left(a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + \frac{1}{2} \right) - a_{\mathbf{k},\bar{s}} a_{\mathbf{k},s}^\dagger - a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},s} \right]. \quad (7.431)$$

Note that the ordering of the s and l components produces no constant term due to the opposite signs on the right-hand sides of the commutation rules (7.430). The Dirac conditions (7.425) and (7.426) have the consequence that the last two terms vanish for *all* physical states. Thus the Hamilton operator contains only the energies of transverse photons and can be replaced by

$$H'_{\text{phys}} = \sum_{\mathbf{k}} \frac{k^0}{2} \sum_{\sigma=\pm 1} (a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + a_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger). \quad (7.432)$$

Finally, we bring also the transverse creation and annihilation operators to a normal order to obtain

$$H'_{\text{phys}} = \sum_{\mathbf{k}} k^0 \sum_{\sigma=\pm 1} \left(a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + \frac{1}{2} \right). \quad (7.433)$$

The second term gives the vacuum energy:

$$E_0 \equiv \langle 0 | H' | 0 \rangle = \frac{1}{2} \sum_{\mathbf{k}} k^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}}. \quad (7.434)$$

In contrast to all other particles, this divergent expression has immediate experimental consequences in the laboratory — it is observable as the so-called *Casimir effect*, to be discussed in Section 7.12.

The photon number operator is obtained by dropping the factor $k^0/2$ in the normally ordered part of the Hamiltonian (7.429):

$$N = \sum_{\mathbf{k}} \left[\left(\sum_{\sigma=\pm 1} a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} \right) - a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},s} - a_{\mathbf{k},s}^\dagger a_{\mathbf{k},\bar{s}} \right]. \quad (7.435)$$

With the Dirac conditions (7.425) and (7.426), the last two terms can be omitted between physical states, so that only the transverse photons are counted:

$$N = \sum_{\mathbf{k}} \sum_{\sigma=\pm 1} \left(a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} \right). \quad (7.436)$$

Its action on the physical subspace is completely analogous to that of H' .

Physical Hilbert Space

In the above calculations of the energies we have assumed that the physical vacuum $|0_{\text{phys}}\rangle$ has a unit norm. This, however, cannot be true. A simple argument shows that the Fermi-Dirac condition (7.411) is inconsistent with the canonical commutation rule (7.398). For this one considers the diagonal element

$$\langle 0_{\text{phys}} | [D(\mathbf{x}, t), A^0(\mathbf{x}', t)] | 0_{\text{phys}} \rangle = i\delta^{(3)}(\mathbf{x} - \mathbf{x}') \langle 0_{\text{phys}} | 0_{\text{phys}} \rangle. \quad (7.437)$$

Writing out the commutator and taking $D(\mathbf{x}, t)$ out of the expectation values, the left-hand side apparently vanishes whereas the right-hand side is obviously nonzero. However, this problem is not fatal for the quantization approach. It occurs and can be solved in ordinary quantum mechanics. Consider the canonical commutator $[p, x] = -i$ between localized states $|x\rangle$:

$$\langle x | [p, x] | x \rangle \stackrel{\text{not}}{=} -i \langle x | x \rangle. \quad (7.438)$$

The left-hand side gives zero, the right-hand side infinity, so the Heisenberg uncertainty principle seems violated. The puzzle is resolved by the fact that Eq. (7.438)

is meaningless since the states $|x\rangle$ are not normalizable. They satisfy the orthogonality condition with a δ -function $\langle x'|x\rangle = \delta(x' - x)$, in which the right-hand side is a distribution. The equation must be multiplied by a smooth test function of x or x' to turn into a finite equation, as in the treatment of Eq. (7.43). Similarly, we can derive from the canonical commutator the equation

$$\langle x'|[p, x]|x\rangle = -i\langle x'|x\rangle. \quad (7.439)$$

This is zero for $x \neq x'$, and gives correct finite results after such a smearing procedure.

Another way to escape the contradiction is by abandoning the use of completely localized states $|x\rangle$ and working only with approximately localized states, for example the lattice states $|x^n\rangle$ with the proper orthogonality relations (1.138) and completeness relations (1.143). Another possibility is to use a sequence of wave packets in the form of narrow Gaussians

$$\langle x'|x\rangle^\eta = \frac{1}{\sqrt{\pi\eta}} e^{-(x'-x)^2/2\eta}, \quad (7.440)$$

which becomes more and more localized for $\eta \rightarrow 0$.

The same subtleties exist for the commutation rule (7.398). The physical states in the Hilbert space are improper states. To see how this comes about let us go to the position representation of the Hamilton operator (7.428) which reads

$$H = \sum_{\mathbf{k}} \frac{k^0}{2} \left[\left(\frac{\partial}{\partial \chi_{\mathbf{k}}} \right)^2 - \chi_{\mathbf{k}}^2 \right], \quad (7.441)$$

where

$$\chi_{\mathbf{k}}^2 = \chi_{\mathbf{k}}^{0^2} - \chi_{\mathbf{k}}^{1^2} - \chi_{\mathbf{k}}^{2^2} - \chi_{\mathbf{k}}^{3^2}. \quad (7.442)$$

The ground state is given by the product of harmonic wave functions

$$\langle \chi|0\rangle = \prod_{\mathbf{k}} \frac{1}{\pi^{1/4}} e^{\chi_{\mathbf{k}}^2/2}. \quad (7.443)$$

The excited states are obtained by applying to this the creation operators

$$a_{\mathbf{k}}^{\mu\dagger} = \frac{1}{\sqrt{2}} \left(\chi_{\mathbf{k}}^\mu + g^{\mu\nu} \frac{\partial}{\partial \chi_{\mathbf{k}}^\nu} \right). \quad (7.444)$$

Due to the positive sign of $\chi_{\mathbf{k}}^{0^2}$ in the ground state (7.443), this procedure does not produce a traditional oscillator Hilbert space with the scalar product

$$\langle \psi'|\psi\rangle = \prod_{\mathbf{k},\mu} \left[\int d\chi_{\mathbf{k}}^\mu \right] \langle \psi'|\chi\rangle \langle \chi|\psi\rangle. \quad (7.445)$$

However, this is not a serious problem, since it can be resolved by rotating the contour of integration in $\chi_{\mathbf{k}}^0$ in the complex $\chi_{\mathbf{k}}^0$ -plane by 90° , so that it runs along the imaginary $\chi_{\mathbf{k}}^0$ -axis.

We now impose the subsidiary conditions (7.425) and (7.426) upon this Hilbert space. To simplify the discussion we shall consider only the problematic modes with polarization labels 0 and 3 at a fixed momentum $\mathbf{k}$ in the z -direction, so that the momentum labels can be suppressed,

Then the conditions (7.425) and (7.426) take the simple form

$$(a^0 - a^3)|\psi_{\text{phys}}\rangle = 0 \quad (7.446)$$

and

$$(a^{0\dagger} - a^{3\dagger})|\psi_{\text{phys}}\rangle = 0. \quad (7.447)$$

In the position representation, these conditions amount to

$$\left(\frac{\partial}{\partial\chi^0} + \frac{\partial}{\partial\chi^3}\right)\langle\chi|\psi_{\text{phys}}\rangle = 0, \quad (7.448)$$

$$(\chi_0 - \chi_3)\langle\chi|\psi_{\text{phys}}\rangle = 0. \quad (7.449)$$

The first condition is fulfilled by wave functions which do not depend on $\chi^0 + \chi^3$, the second restricts the dependence on $\chi^0 - \chi^3$ to a δ -function. The wave function of the physical vacuum is therefore (for particles of a fixed momentum running along the z -axis)

$$\langle\chi|0_{\text{phys}}\rangle = \delta(\chi^0 - \chi^3) \frac{1}{\pi^{1/4}} e^{-(\chi^{1^2} + \chi^{2^2})/2}. \quad (7.450)$$

The complete set of physical states is obtained by applying to this any number of creation operators for transverse photons

$$a^{1\dagger} = \frac{1}{\sqrt{2}} \left(\chi^1 - \frac{\partial}{\partial\chi^1} \right), \quad a^{2\dagger} = \frac{1}{\sqrt{2}} \left(\chi^2 - \frac{\partial}{\partial\chi^2} \right). \quad (7.451)$$

The physical vacuum (7.450) displays precisely the unpleasant feature which caused the problems with the quantum mechanical equation (7.438). Due to the presence of the δ -functions the wave function is *not* normalizable. The normalization problem of the wave function $\delta(\chi^0 - \chi^3)$ is completely analogous to that of ordinary plane waves, and we know how to do quantum mechanics with such generalized states. The standard Hilbert space is obtained by superimposing plane waves to wave packets. Normalizable wave packets can be constructed to approximate the positional wave functions $\delta(\chi^0 - \chi^3)$ in various ways. One may, for instance, discretize the field variables χ^μ and work on a lattice in field space. Alternatively one may replace the δ -function in (7.450) by a narrow Gaussian

$$\delta(\chi^0 - \chi^3) \rightarrow \text{const} \times e^{-(\chi^0 - \chi^3)^2/2\eta}, \quad (7.452)$$

with an appropriate normalization factor.

When performing calculations in the physical Hilbert space of the Dirac quantization scheme, we would like to proceed as in the case of Klein-Gordon and Dirac particles, assuming that the scalar product $\langle 0_{\text{phys}} | 0_{\text{phys}} \rangle$ is unity, as we did when evaluating the vacuum energy (7.434) (which was really illegal as we have just learned).

Only with a unit norm of the vacuum state can we find physical expectation values by simply bringing all creation and annihilation operators between the vacuum states to normal order, the desired result being the sum of the c -numbers produced by the commutators. Such a unit norm is achieved by introducing the analogs of the wave packets (7.440), which in this case are normalizable *would-be vacuum states* to be denoted by $|0_{\text{phys}}\rangle^\eta$ which approach the true unnormalizable vacuum state arbitrarily close for $\eta \rightarrow 0$. These would-be vacuum states are most easily constructed algebraically.¹⁹ Considering only the problematic creation and annihilation operators $a^{0\dagger}$, a^0 and $a^{3\dagger}$, a^3 , we define an auxiliary state $|0_{\text{aux}}\rangle$ to be the one that is annihilated by $a^{0\dagger}$ and a^3 :

$$a^{0\dagger}|0_{\text{aux}}\rangle = 0, \quad a^3|0_{\text{aux}}\rangle = 0. \quad (7.453)$$

From this we construct the physical vacuum state as a power series

$$|0_{\text{phys}}\rangle = \sum_{n,m=0}^{\infty} c_{n,m} (a^{3\dagger})^n (a^0)^m |0_{\text{aux}}\rangle. \quad (7.454)$$

The subsidiary conditions (7.425) and (7.426) are now

$$a_s|0_{\text{phys}}\rangle = (a^0 - a^3)|0_{\text{phys}}\rangle = 0, \quad a_s^\dagger|0_{\text{phys}}\rangle = (a^{0\dagger} - a^{3\dagger})|0_{\text{phys}}\rangle = 0. \quad (7.455)$$

These are obviously fulfilled by the *coherent state*:

$$|0_{\text{phys}}\rangle = e^{a^{3\dagger}a^0}|0_{\text{aux}}\rangle. \quad (7.456)$$

To verify this we merely note that a^3 acts on this state like a differential operator $\partial/\partial a^{3\dagger}$ producing a factor a^0 , and the same holds with $a^{3\dagger}$ and a^3 replaced by $a^{0\dagger}$ and a^0 , respectively.

The norm of this state is infinite:

$$\langle 0_{\text{phys}}|0_{\text{phys}}\rangle = \sum_{n,m=0}^{\infty} \frac{1}{n!m!} \langle 0_{\text{aux}}|(a^3)^n (a^{0\dagger})^n (a^{3\dagger})^m (a^0)^m |0_{\text{aux}}\rangle = \sum_{n=0}^{\infty} 1 = \infty. \quad (7.457)$$

We now approximate this physical vacuum by a sequence of normalized states $|0_{\text{phys}}\rangle^\eta$ defined by

$$|0_{\text{phys}}\rangle^\eta \equiv \sqrt{\eta(2-\eta)} e^{(1-\eta)a^{3\dagger}a^0} = \sqrt{\eta(2-\eta)} \sum_{n=0}^{\infty} \frac{1}{n!} [(1-\eta)a^{3\dagger}a^0]^n |0_{\text{aux}}\rangle. \quad (7.458)$$

It is easy to check that these have a unit norm:

$${}^\eta \langle 0_{\text{phys}}|0_{\text{phys}}\rangle^\eta = \eta(2-\eta) \sum_{n=0}^{\infty} (1-\eta)^{2n} = 1. \quad (7.459)$$

¹⁹R. Utiyama, T. Imamura, S. Sunakawa, and T. Dodo, Progr. Theor. Phys. 6, 587 (1951).

On this sequence of states, the subsidiary conditions (7.455) are not exactly satisfied. Using the above derivative rules, we see that

$$\begin{aligned} a^3 |0_{\text{phys}}\rangle^\eta &= \frac{\partial}{\partial a^{3\dagger}} |0_{\text{phys}}\rangle^\eta = (1 - \eta) a^0 |0_{\text{phys}}\rangle^\eta, \\ a^{0\dagger} |0_{\text{phys}}\rangle^\eta &= \frac{\partial}{\partial a^0} |0_{\text{phys}}\rangle^\eta = (1 - \eta) a^{3\dagger} |0_{\text{phys}}\rangle^\eta, \end{aligned} \quad (7.460)$$

corresponding to the approximate subsidiary conditions

$$\begin{aligned} a_s |0_{\text{phys}}\rangle^\eta &= \eta a^0 |0_{\text{phys}}\rangle^\eta, \\ a_s^\dagger |0_{\text{phys}}\rangle^\eta &= \eta a^{3\dagger} |0_{\text{phys}}\rangle^\eta. \end{aligned} \quad (7.461)$$

Let us calculate the norm of the states on the right-hand side. Using the power series expansion (7.458), we find

$$\begin{aligned} {}^\eta \langle 0_{\text{phys}} | a^3 a^{3\dagger} | 0_{\text{phys}} \rangle^\eta &= \eta(2 - \eta) \sum_{n,m=0}^{\infty} \frac{1}{n!m!} \langle 0_{\text{aux}} | (1 - \eta)^n (a^3)^n (a^{0\dagger})^n a^3 a^{3\dagger} (1 - \eta)^m (a^{3\dagger})^m (a^0)^m | 0_{\text{aux}} \rangle \\ &= \eta(2 - \eta) \sum_{n=0}^{\infty} (n + 1) (1 - \eta)^{2n}, \end{aligned} \quad (7.462)$$

and thus

$${}^\eta \langle 0_{\text{phys}} | a^3 a^{3\dagger} | 0_{\text{phys}} \rangle^\eta = \frac{1}{\eta(2 - \eta)}. \quad (7.463)$$

Similarly we derive

$${}^\eta \langle 0_{\text{phys}} | a^{0\dagger} a^0 | 0_{\text{phys}} \rangle^\eta = \frac{1}{\eta(2 - \eta)}, \quad (7.464)$$

and via the commutation rules

$$a^0 a^{0\dagger} = -1 + a^{0\dagger} a^0, \quad a^{3\dagger} a^3 = -1 + a^3 a^{3\dagger} \quad (7.465)$$

the expectation values

$${}^\eta \langle 0_{\text{phys}} | a^0 a^{0\dagger} | 0_{\text{phys}} \rangle^\eta = {}^\eta \langle 0_{\text{phys}} | a^{3\dagger} a^3 | 0_{\text{phys}} \rangle^\eta = \frac{(1 - \eta)^2}{\eta(2 - \eta)}. \quad (7.466)$$

These results can actually be obtained directly by trivial algebra from Eqs. (7.461) using the commutation relations (7.465).

Equations (7.463) and (7.464) show that the norm of the states on the right-hand side of Eqs. (7.461) is $\sqrt{\eta/(1 - \eta)}$, the normalized states $|0_{\text{phys}}\rangle^\eta$ satisfy the desired constraints (7.455) in the limit $\eta \rightarrow 0$, thus converging towards the physical vacuum state.

To be consistent, all calculations in the Dirac quantization scheme have to be done in one of the would-be vacuum states $|0_{\text{phys}}\rangle^\eta$, with the limit taken at the end. Only in this way the earlier-observed apparent contradiction in (7.437) can be avoided. In the present context, it is observed when taking the expectation value of the commutation relation $[a_{\bar{s}}, a_s^\dagger] = -1$:

$$\langle 0_{\text{phys}} | a_{\bar{s}} a_s^\dagger | 0_{\text{phys}} \rangle - \langle 0_{\text{phys}} | a_s^\dagger a_{\bar{s}} | 0_{\text{phys}} \rangle = -\langle 0_{\text{phys}} | 0_{\text{phys}} \rangle. \quad (7.467)$$

Since $a_s^\dagger$ annihilates the physical vacuum to its right and to its left, the left-hand side should be zero, contradicting the right-hand side. For the normalized finite- η would-be vacuum, on the other hand, the equation becomes

$${}^\eta \langle 0_{\text{phys}} | a_{\bar{s}} a_s^\dagger | 0_{\text{phys}} \rangle^\eta - {}^\eta \langle 0_{\text{phys}} | a_s^\dagger a_{\bar{s}} | 0_{\text{phys}} \rangle^\eta = -1. \quad (7.468)$$

From (7.463)–(7.464), we find

$${}^\eta \langle 0_{\text{phys}} | a_{\bar{s}} a_s^\dagger | 0_{\text{phys}} \rangle^\eta = -1, \quad {}^\eta \langle 0_{\text{phys}} | a_s^\dagger a_{\bar{s}} | 0_{\text{phys}} \rangle^\eta = -1, \quad (7.469)$$

so that (7.468) is a correct equation. Thus, although the states (7.461) have a small norm of order $\sqrt{\eta}$, the products $a_{\bar{s}} a_s^\dagger$ and $a_s^\dagger a_{\bar{s}}$ have a unit expectation value.

We can easily see the reason for this by calculating

$$\begin{aligned} a_{\bar{s}} | 0_{\text{phys}} \rangle^\eta &= (2 - \eta) a^0 | 0_{\text{phys}} \rangle^\eta, \\ a_s^\dagger | 0_{\text{phys}} \rangle^\eta &= (2 - \eta) a^{3\dagger} | 0_{\text{phys}} \rangle^\eta, \end{aligned} \quad (7.470)$$

and by observing that the norm of the states on the right-hand sides is, by (7.463) and (7.464), equal to $(2 - \eta)/\sqrt{\eta(2 - \eta)} = \sqrt{(2 - \eta)/\eta}$, which diverges like $1/\sqrt{\eta}$ for $\eta \rightarrow 0$ [being precisely the inverse of the norm of the states (7.461)]. Thus we can only drop safely expectation values in which a_s or $a_s^\dagger$ act upon the physical vacuum to its right, if there is no operator $a_{\bar{s}}^\dagger$ or $a_{\bar{s}}$ doing the same thing to its left. This could be a problem with respect to the vacuum energy of the unphysical modes in (7.429), which is proportional to

$$- {}^\eta \langle 0_{\text{phys}} | a_s a_{\bar{s}}^\dagger + a_{\bar{s}} a_s^\dagger + a_{\bar{s}}^\dagger a_s + a_s^\dagger a_{\bar{s}} | 0_{\text{phys}} \rangle^\eta. \quad (7.471)$$

Fortunately, this expectation value does vanish, as it should, since by (7.463)–(7.466):

$$\begin{aligned} {}^\eta \langle 0_{\text{phys}} | a_s a_{\bar{s}}^\dagger | 0_{\text{phys}} \rangle^\eta &= {}^\eta \langle 0_{\text{phys}} | a_{\bar{s}} a_s^\dagger | 0_{\text{phys}} \rangle^\eta = 1/2, \\ {}^\eta \langle 0_{\text{phys}} | a_s^\dagger a_{\bar{s}} | 0_{\text{phys}} \rangle^\eta &= {}^\eta \langle 0_{\text{phys}} | a_{\bar{s}}^\dagger a_s | 0_{\text{phys}} \rangle^\eta = -1/2, \end{aligned} \quad (7.472)$$

so that the energy of the unphysical modes in the normalized would-be vacuum state $|0_{\text{phys}}\rangle^\eta$ is indeed zero for all η , and the true vacuum energy in the limit $\eta \rightarrow 0$ contains only the zero-point oscillations of the physical transverse modes.

In this context it is worth emphasizing that the normally ordered operator $a^{0\dagger} a^0 - a^{3\dagger} a^3$ is *not* normally ordered with respect to the physical vacuum $|0_{\text{phys}}\rangle$ and thus

does not yield zero when sandwiched between two such states. This is obvious by rewriting $a^{0\dagger}a^0 - a^{3\dagger}a^3$ as $a_s^\dagger a_s + a_{\bar{s}}^\dagger a_{\bar{s}}$, and the fact that the annihilation operators a_s and $a_{\bar{s}}$ on the right-hand side do *not* annihilate the physical vacuum: $a_{\mathbf{k},s}|0_{\text{phys}}\rangle \neq 0$, $a_{\mathbf{k},\bar{s}}|0_{\text{phys}}\rangle \neq 0$.

In axiomatic quantum field theory, the vacuum is always *postulated* to be a proper discrete state with a unit norm. Without this property, the discussion of symmetry operations in a Hilbert space becomes quite subtle, since infinitesimal transformations can produce finite changes of a state. The Dirac vacuum $|0_{\text{phys}}\rangle$ is not permitted by this postulate, whereas the pseudophysical vacuum $|0_{\text{phys}'}\rangle$ is. There are other problems within axiomatic quantum field theory, however, due to the non-uniqueness of this vacuum, and due to the fact that the vacuum is not separated from all other states by an energy gap, an important additional postulate. That latter postulate is actually unphysical, due to the masslessness of the photon and the existence of many other massless particles in nature. But it is necessary for the derivation of many “rigorous results” in that somewhat esoteric discipline.

Because of the subtleties with the limiting procedure of the vacuum state, it will not be convenient to work with the Dirac quantization scheme. Instead we shall use a simplified procedure due to Gupta and Bleuler, to be introduced below. First, however, we shall complete the present discussion by calculating the photon propagator within the Dirac scheme.

Propagator in Dirac Quantization Scheme

Let us calculate the propagator of the A_μ -field in the Dirac quantization scheme. We take the expansion of the field operator (7.419) and evaluate the expectation value

$$G^{\mu\nu}(x, x') = {}^\eta\langle 0_{\text{phys}} | T A^\mu(x) A^\nu(x') | 0_{\text{phys}} \rangle^\eta, \quad (7.473)$$

in which we take the limit $\eta \rightarrow 0$ at the end. For $x_0 > x'_0$, we obtain a contribution proportional to

$$\Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{-ik(x-x')} \quad (7.474)$$

multiplied by the sum of the expectation values of

$$\epsilon^{\mu*}(\mathbf{k}, +1) \epsilon^\nu(\mathbf{k}, +1) a_{\mathbf{k},+1} a_{\mathbf{k},+1}^\dagger, \quad \epsilon^{\mu*}(\mathbf{k}, -1) \epsilon^\nu(\mathbf{k}, -1) a_{\mathbf{k},-1} a_{\mathbf{k},-1}^\dagger, \quad (7.475)$$

and

$$\epsilon^{\mu*}(\mathbf{k}, \bar{s}) \epsilon^\nu(\mathbf{k}, s) a_{\mathbf{k},s} a_{\mathbf{k},\bar{s}}^\dagger, \quad \epsilon^{\mu*}(\mathbf{k}, s) \epsilon^\nu(\mathbf{k}, \bar{s}) a_{\mathbf{k},\bar{s}} a_{\mathbf{k},s}^\dagger, \quad (7.476)$$

and a contribution proportional to

$$\Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{ik(x-x')} \quad (7.477)$$

multiplied by the sum of the expectation values of

$$\epsilon^\mu(\mathbf{k}, +1)\epsilon^{\nu*}(\mathbf{k}, +1)a_{\mathbf{k},+1}^\dagger a_{\mathbf{k},+1}, \quad \epsilon^\mu(\mathbf{k}, -1)\epsilon^{\nu*}(\mathbf{k}, -1)a_{\mathbf{k},-1}^\dagger a_{\mathbf{k},-1}, \quad (7.478)$$

and

$$\epsilon^\mu(\mathbf{k}, \bar{s})\epsilon^{\nu*}(\mathbf{k}, s)a_{\mathbf{k},s}^\dagger a_{\mathbf{k},\bar{s}}, \quad \epsilon^\mu(\mathbf{k}, s)\epsilon^{\nu*}(\mathbf{k}, \bar{s})a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},s}. \quad (7.479)$$

The first two terms containing transverse photons produce a polarization sum

$$\epsilon^{\mu*}(\mathbf{k}, +1)\epsilon^\nu(\mathbf{k}, +1) + \epsilon^{\mu*}(\mathbf{k}, -1)\epsilon^\nu(\mathbf{k}, -1). \quad (7.480)$$

The expectation values of the normally ordered transverse photon terms (7.478) vanish. The remaining terms in (7.476) and (7.479) are evaluated with the help of the matrix elements (7.472) of opposite signs. They cancel each other, due to the evenness of $\epsilon^\mu(\mathbf{k}, s)\epsilon^{\nu*}(\mathbf{k}, \bar{s}) = k^{02} - k^{32}$ as functions of k^μ . Such a function, appearing as a factor inside the momentum sums (7.474) and (7.477), guarantees their equality and ensures the cancellation of the contributions from (7.476) and (7.479).

For $x_0 < x'_0$, we obtain once more the same expression with spacetime and Lorentz indices interchanged: $x \leftrightarrow x'$, $\mu \leftrightarrow \nu$.

The propagator becomes therefore

$$\begin{aligned} G^{\mu\nu}(x, x') &= \eta \langle 0_{\text{phys}} | T A^\mu(x) A^\nu(x') | 0_{\text{phys}} \rangle^\eta \\ &= \Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{-ik(x-x')} \sum_{\nu=1}^2 \epsilon^{\mu*}(\mathbf{k}, \nu) \epsilon^\nu(\mathbf{k}, \nu) \\ &+ \Theta(x'_0 - x_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{ik(x-x')} \sum_{\nu=1}^2 \epsilon^{\mu*}(\mathbf{k}, \nu) \epsilon^\nu(\mathbf{k}, \nu). \end{aligned} \quad (7.481)$$

This is the same propagator as in Eq. (7.361), where it was obtained in the manifestly noncovariant quantization scheme, in which only the physical degrees of freedom of the vector potential were made operators. Thus, although the field operators have been quantized with the covariant commutation relations (7.386), the selection procedure of the physical states has produced the same noncovariant propagator.

It is worth pointing out the difference between the propagator (7.361) and the retarded propagator used in classical electrodynamics. The classical one is given by the same Fourier integral as $G(x - x')$:

$$G_R(x - x') \equiv \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-x')} \frac{i}{k^2}, \quad (7.482)$$

except that the poles at $k^0 \equiv \pm\omega = |\mathbf{k}|$ are both placed *below* the real axis. The quantum-field-theoretic k^0 -integral

$$\begin{aligned} &\int \frac{dk^0}{2\pi} e^{-ik^0(x^0-x'^0)} \frac{i}{2|\mathbf{k}|} \left(\frac{1}{k^0 - |\mathbf{k}| + i\eta} - \frac{1}{k^0 + |\mathbf{k}| - i\eta} \right) \\ &= \frac{1}{2\omega} [\Theta(x^0 - x'^0) e^{-i\omega(x^0-x'^0)} + \Theta(x'^0 - x^0) e^{i\omega(x^0-x'^0)}] = \frac{1}{2\omega} e^{-i\omega|x^0-x'^0|} \end{aligned} \quad (7.483)$$

with ω on the light cone, $\omega = |\mathbf{k}|$, has to be compared with the retarded expression

$$\begin{aligned} \int \frac{dk^0}{2\pi} e^{-ik^0(x^0-x'^0)} \frac{i}{2|\mathbf{k}|} \left(\frac{1}{k^0 - |\mathbf{k}| + i\eta} - \frac{1}{k^0 + |\mathbf{k}| + i\eta} \right) \\ = \Theta(x^0 - x'^0) \frac{1}{2\omega} (e^{-i\omega(x^0-x'^0)} - e^{i\omega(x^0-x'^0)}) = -2i\Theta(x^0 - x'^0) \frac{1}{2\omega} \sin[\omega(x^0 - x'^0)]. \end{aligned} \quad (7.484)$$

The angular part of the spatial integral

$$\int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\mathbf{x}} \quad (7.485)$$

can be done in either case in the same way leading to

$$\frac{1}{2\pi^2 R} \int_0^\infty d\omega \sin(\omega R). \quad (7.486)$$

Thus we find

$$G_R(x - x') = i\Theta(x^0 - x'^0) \int_{-\infty}^\infty d\omega \{e^{-i\omega[(x^0-x'^0)-R]} - e^{-i\omega[(x^0-x'^0)+R]}\}. \quad (7.487)$$

Since R and $x^0 - x'^0$ are both positive, the result is

$$G_R(x - x') = i\Theta(x^0 - x'^0) \frac{1}{4\pi R} \delta(x^0 - x'^0 - R). \quad (7.488)$$

The retarded propagator exists only for causal times $x^0 > x'^0$ and it is equal to the Coulomb potential if the end points can be connected by a light signal. In contrast to this, the propagator of the quantized electromagnetic field, in which the creation operator of antiparticles accompanies the negative energy solutions of the wave equation, is

$$G(x - x') = i \frac{1}{4\pi R} \delta_+(|x^0 - x'^0| - R) + i \frac{1}{4\pi R} \delta_+(-|x^0 - x'^0| - R), \quad (7.489)$$

where

$$\delta_+(t) = \int \frac{d\omega}{\pi} e^{-i\omega t} \quad (7.490)$$

is equal to twice the positive-frequency part of the Fourier decomposition of the δ -function. With the help of an infinitesimal imaginary part in the time argument, the integral can be done by closing the contour in the upper or lower half-plane, and the results of both contours can be expressed as

$$\delta_+(t) = \frac{1}{\pi i} \frac{1}{t - i\eta}. \quad (7.491)$$

This, in turn, can be decomposed as follows:

$$\delta_+(t) = \frac{1}{\pi i} \left(\frac{i\eta}{t^2 + \eta^2} + \frac{t}{t + \eta^2} \right) = \delta(t) + \frac{1}{\pi i} \frac{\mathcal{P}}{t}. \quad (7.492)$$

The second term selects the principal value in any integral involving $\delta_+(t)$.

Incidentally, both $\delta_+(t)$ and $\delta(t)$ satisfy

$$\delta(t^2 - R^2) = \frac{1}{2R}[\delta(t - R) + \delta(t + R)]. \quad (7.493)$$

As a consequence, the propagator $G(x - x')$ in (7.489) can also be written as

$$G(x - x') = i \frac{1}{2\pi} \delta_+((x - x')^2), \quad (7.494)$$

to be compared with the retarded propagator of (7.488):

$$G_R(x - x') = \Theta(x^0 - x'^0) i \frac{1}{2\pi} \delta((x - x')^2). \quad (7.495)$$

In configuration space, the massive propagators are quite simply related to the massless ones. One simply writes the δ -functions $\delta((x - x')^2)$ and $\delta_+((x - x')^2)$ in $G_R(x - x')$ and $G(x - x')$ as Fourier integrals

$$\delta((x - x')^2) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\omega i(x - x')^2}, \quad \delta_+((x - x')^2) = \int_0^{\infty} \frac{d\omega}{\pi} e^{\omega i(x - x')^2} \quad (7.496)$$

and replaces $e^{-i\omega(x - x')^2}$ by $e^{-i\omega(x - x')^2 - \frac{M^2}{2\omega}}$ as in (7.141). With the additional term in the exponent, the ω -integrals yield Bessel functions:

$$\delta(x^2) \rightarrow \delta(x^2) + \Theta(x^2) \frac{M^2}{2} \frac{J_1(M\sqrt{x^2})}{M\sqrt{x^2}}, \quad (7.497)$$

$$\delta_+(x^2) \rightarrow \delta(x^2) + \mathcal{P} \frac{M^2}{2} \frac{J_1(M\sqrt{x^2}) - iN_1(M\sqrt{x^2})}{M\sqrt{x^2}}. \quad (7.498)$$

For $M \rightarrow 0$, we use the limiting behavior $J_1(z) \rightarrow z/2$, $N_1(z) \rightarrow -2/\pi z$ and see that the mass term disappears in the first equation, whereas in the second term it becomes $\mathcal{P}/\pi i x^2$.

According to the wave equation (7.381), the polarization vectors have to satisfy

$$k^2 \epsilon^\mu(\mathbf{k}, \nu) - \left(1 - \frac{1}{\alpha}\right) k^\mu k_\nu \epsilon^\nu(\mathbf{k}, \nu) = 0. \quad (7.499)$$

The propagator of the fields A^μ in momentum space is obtained by inverting the inhomogeneous version of this equation: Correspondingly, the polarization vectors in the field expansion (7.390) will now, instead of (7.392)–(7.393), satisfy the completeness and orthogonality relations

$$\sum_{\nu\nu'} g^{\nu\nu'} \epsilon^\mu(\mathbf{k}, \nu) \epsilon^{\mu'*}(\mathbf{k}, \nu') = g^{\mu\mu'} - (1 - \alpha) \frac{k^\mu k^{\mu'}}{k^2}, \quad (7.500)$$

$$\left[g^{\mu\mu'} - (1 - \alpha) \frac{k^\mu k^{\mu'}}{k^2} \right] \epsilon_{\mu*}(\mathbf{k}, \nu) \epsilon_{\mu'}(\mathbf{k}, \nu') = g^{\nu\nu'}. \quad (7.501)$$

7.5.3 Gupta-Bleuler Subsidiary Condition

One may wonder whether it is possible to avoid the awesome limiting procedure $\eta \rightarrow 0$ and find a way of working with an ordinary vacuum state. This is indeed possible if one is only interested in physical matrix elements containing at least one particle. Such matrix elements can be calculated using only the condition (7.425), while discarding the condition (7.426). Thus, we select what we shall call *pseudo-physical states* by requiring only

$$a_{\mathbf{k},s}|\psi_{\text{“phys”}}\rangle = 0. \quad (7.502)$$

The restriction to this condition is the basis of the *Gupta-Bleuler approach* to quantum electrodynamics [11]. Take, for instance, the number operator (7.435) and insert it between two pseudo-physical states selected in this way. It yields

$$\begin{aligned} \langle \psi'_{\text{“phys”}} | N | \psi_{\text{“phys”}} \rangle &= \langle \psi'_{\text{“phys”}} | a_{\mathbf{k},+1}^\dagger a_{\mathbf{k},+1} + a_{\mathbf{k},-1}^\dagger a_{\mathbf{k},-1} | \psi_{\text{“phys”}} \rangle \\ &- \langle \psi'_{\text{“phys”}} | [a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s} + a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},\bar{s}}] | \psi_{\text{“phys”}} \rangle. \end{aligned} \quad (7.503)$$

The second line vanishes due to the condition (7.448) and its Hermitian adjoint. Thus the number operator counts only the number of transverse photons.

The same mechanism ensures correct particle energies. With the help of the first commutation rule in (7.430), we bring the Hamilton operator (7.431) to the normally ordered form in the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$:

$$H' = \sum_{\mathbf{k}} k^0 \left[\sum_{\sigma=\pm 1} \left(a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + \frac{1}{2} \right) + 1 - a_{\mathbf{k},s}^\dagger a_{\mathbf{k},\bar{s}} - a_{\mathbf{k},\bar{s}}^\dagger a_{\mathbf{k},s} \right]. \quad (7.504)$$

The last two terms vanish because of the Gupta-Bleuler condition (7.502). Thus the Hamilton operator counts only the energies of the transverse photons.

So why did we have to impose the second Dirac condition (7.426) at all? It is needed to ensure only one property of the theory: the correct vacuum energy. In the Gupta-Bleuler approach this energy comes out wrong by a factor two, showing that the unphysical degrees of freedom have not been completely eliminated. The normal ordering of the Hamilton operator (7.431) with respect to the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$ has produced an extra vacuum energy

$$E_0^{\text{extra}} = \sum_{\mathbf{k}} k^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}}, \quad (7.505)$$

which previously did not appear because of the second Dirac condition (7.426). It is the vacuum energy of two unphysical degrees of freedom for each momentum $\mathbf{k}$. This wrong vacuum energy may also be seen directly by bringing the Hamilton operator (7.428) to normal order using the commutation rule (7.406), yielding

$$H = \sum_{\mathbf{k}} k^0 \left(-a_{\mathbf{k},\mu}^{\mu\dagger} a_{\mathbf{k},\mu} + \frac{1}{2} \right), \quad (7.506)$$

the second term showing the vacuum energy of *four* polarization degrees of freedom, rather than just the physical ones.

A heuristic remedy to the wrong vacuum energy in the Gupta-Bleuler formalism will be discussed below, to be followed by a more satisfactory one in Section 14.16.

Photon Propagator in Gupta-Bleuler Approach

We now calculate the propagator of the A_μ -field in the Gupta-Bleuler quantization scheme, which is given by the expectation value in the pseudo-physical vacuum state

$$G^{\mu\nu}(x, x') = \langle 0_{\text{“phys”}} | T A^\mu(x) A^\nu(x') | 0_{\text{“phys”}} \rangle. \quad (7.507)$$

Expanding the vector field A^μ as in (7.419), and inserting it into (7.507), we obtain for $x_0 > x'_0$ the same contributions as in Eqs. (7.474)–(7.479), except that the expectation values are to be taken in the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$, where only $a_{\mathbf{k},s}|0_{\text{“phys”}}\rangle = 0$ and $\langle 0_{\text{“phys”}} | a_{\mathbf{k},s}^\dagger = 0$. As a consequence, there are contributions from the expectation values of the terms (7.476), yielding a polarization sum

$$\epsilon^{\mu*}(\mathbf{k}, \bar{s}) \epsilon^\nu(\mathbf{k}, s) + \epsilon^{\mu*}(\mathbf{k}, s) \epsilon^\nu(\mathbf{k}, \bar{s}),$$

which, together with the transverse sum (7.480), adds up to

$$\sum_{\sigma=\pm 1} \epsilon^{\mu*}(\mathbf{k}, \sigma) \epsilon^\nu(\mathbf{k}, \sigma) - \epsilon^{\mu*}(\mathbf{k}, s) \epsilon^\nu(\mathbf{k}, \bar{s}) - \epsilon^{\mu*}(\mathbf{k}, \bar{s}) \epsilon^\nu(\mathbf{k}, s) = -g^{\mu\nu}. \quad (7.508)$$

For $x_0 < x'_0$, the same expression is found with spacetime and Lorentz indices interchanged: $x \leftrightarrow x'$, $\mu \leftrightarrow \nu$, so that the propagator becomes

$$\begin{aligned} G^{\mu\nu}(x, x') &= \langle 0_{\text{“phys”}} | T A^\mu(x) A^\nu(x') | 0_{\text{“phys”}} \rangle \\ &= -g^{\mu\nu} \left[\Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{-ik(x-x')} + \Theta(x'_0 - x_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{ik(x-x')} \right]. \end{aligned} \quad (7.509)$$

Up to the prefactor $-g^{\mu\nu}$, this agrees with Eq. (7.47) for the propagator $G(x, x')$ of the Klein-Gordon field for zero mass, which we write as in (7.62) in the form

$$\begin{aligned} G^{\mu\nu}(x, x') &= \langle 0 | T A^\mu(x) A^\nu(x') | 0 \rangle \\ &= -g^{\mu\nu} \left[\Theta(x_0 - x'_0) G^{(+)}(x, x') + \Theta(x'_0 - x_0) G^{(-)}(x, x') \right] \\ &= -g^{\mu\nu} G(x, x'). \end{aligned} \quad (7.510)$$

This photon propagator is much simpler than the previous one in (7.361), making it much easier to perform calculations, which is the main virtue of the Gupta-Bleuler quantization scheme. A second advantage of the propagator (7.510) is that, in contrast to the noncovariant propagator (7.366), it is a proper Green function associated with the wave equation (7.389) in the $\alpha = 0$ -gauge, satisfying the inhomogeneous field equation

$$-\partial^2 G^{\mu\nu}(x - x') = -g^{\mu\nu} i\delta^{(4)}(x - x'). \quad (7.511)$$

A further special feature of the Gupta-Bleuler quantization procedure that is worth pointing out is that the condition $a_{\mathbf{k},s}|\psi_{\text{“phys”}}\rangle = 0$ does not uniquely fix the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$. The vacuum state $|0_{\text{“phys”}}\rangle$ is only one possible choice, but infinitely many other states are equally good candidates, as long as their physical photon number is zero. Focussing attention only on states of a fixed

photon momentum parallel to the z -axis, the zero-norm states (7.408) all satisfy the condition $a_{\mathbf{k},s}|\psi_{\text{phys}}\rangle = 0$. As a consequence, any superposition of such states

$$|\tilde{0}\rangle = |0\rangle + c_{\mathbf{k}}^{(1)}|0\rangle_1 + c_{\mathbf{k}}^{(2)}|0\rangle_2 + \dots \quad (7.512)$$

has a unit norm. It contains no transverse photon and satisfies the condition $a_{\mathbf{k},s}|\tilde{0}\rangle = 0$, and is thus an equally good pseudo-vacuum state of the system.

The expectation value of the vector potential A^μ in this vacuum is nonzero. Its $\mathbf{k}$ th component is equal to the coefficient $c_{\mathbf{k}}^{(1)}$ associated with this momentum, i.e., it is some function $c(\mathbf{k})$. Because of the second of the commutation rules (7.430), its $\mathbf{k}$ th Fourier component $\epsilon^\mu(\mathbf{k}, \nu)a_{\mathbf{k},\nu}$ has an expectation $\epsilon^\mu(\mathbf{k}, s)$, with a coefficient $c_{\mathbf{k}} = c_{\mathbf{k}}^{(1)}$:

$$\langle \tilde{0} | A^\mu | \tilde{0} \rangle = c_{\mathbf{k}} \epsilon^\mu(\mathbf{k}, s), \quad (7.513)$$

i.e., it is proportional to the four-momentum k^μ . In x -space, the expectation value of such a field is equal to a pure gradient $\partial^\mu \Lambda(x)$, so that it carries no electromagnetic field.

The condition (7.502) implies that

$$\langle \tilde{0} | a_{\mathbf{k},0}^\dagger a_{\mathbf{k},0} | \tilde{0} \rangle = \langle \tilde{0} | a_{\mathbf{k},3}^\dagger a_{\mathbf{k},3} | \tilde{0} \rangle. \quad (7.514)$$

The two sides are equal to some function of $\mathbf{k}$, say $k^{02} \chi(\mathbf{k})$. In a covariant way, the vacuum is thus characterized by the expectations

$$\begin{aligned} \langle \tilde{0} | a_{\mathbf{k},\nu}^\dagger a_{\mathbf{k}',\nu'} | \tilde{0} \rangle &= k_\mu \epsilon^{\mu*}(\mathbf{k}, \nu) k_\nu \epsilon^\nu(\mathbf{k}, \nu') \chi(\mathbf{k}) \delta_{\mathbf{k},\mathbf{k}'} \\ \langle \tilde{0} | a_{\mathbf{k},\nu} a_{\mathbf{k}',\nu'}^\dagger | \tilde{0} \rangle &= [-g^{\nu\nu'} + k_\mu \epsilon^{\mu*}(\mathbf{k}, \nu) k_\nu \epsilon^\nu(\mathbf{k}, \nu') \chi(\mathbf{k})] \delta_{\mathbf{k},\mathbf{k}'} \end{aligned} \quad (7.515)$$

If we use any of these vacua and do not impose the condition (7.502), the propagator

$$G_0^{\mu\nu}(x - x') = \langle \tilde{0} | T A^\mu(x) A^\nu(x') | \tilde{0} \rangle \quad (7.516)$$

is a gauge-transformed version of the original one. Let us calculate it explicitly. Using (7.515), we obtain

$$\begin{aligned} G_0^{\mu\nu}(x - x') &= \langle \tilde{0} | T A^\mu(x) A^\nu(x') | \tilde{0} \rangle \\ &= \frac{1}{V} \sum_{\mathbf{k}, \nu, \nu'} \frac{1}{2k^0} e^{-ik(x-x')} [-\Theta(x_0 - x'_0) g^{\nu\nu'} + k_\mu \epsilon^{\mu'*}(\mathbf{k}, \nu) k_\nu \epsilon^{\nu'}(\mathbf{k}, \nu') \chi(\mathbf{k})] \\ &\quad \times \epsilon^{\mu*}(\mathbf{k}, \nu) \epsilon^\nu(\mathbf{k}, \nu') \\ &= \frac{1}{V} \sum_{\mathbf{k}, \nu, \nu'} \frac{1}{2k^0} e^{ik(x-x')} [-\Theta(x'_0 - x_0) g^{\nu\nu'} + k_\mu \epsilon^{\mu'*}(\mathbf{k}, \nu) k_\nu \epsilon^{\nu'}(\mathbf{k}, \nu') \chi(\mathbf{k})] \\ &\quad \times \epsilon^{\mu*}(\mathbf{k}, \nu) \epsilon^\nu(\mathbf{k}, \nu') \\ &= \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{-ik(x-x')} [-\Theta(x_0 - x'_0) g^{\mu\nu} + k^\mu k^\nu \chi(\mathbf{k})] \\ &\quad + \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{ik(x-x')} [-\Theta(x'_0 - x_0) g^{\mu\nu} + k^\mu k^\nu \chi(\mathbf{k})]. \end{aligned} \quad (7.517)$$

The $g^{\mu\nu}$ -terms are again equal to $G^{\mu\nu}$ of Eq. (7.510). The $k^\mu k^\nu$ terms may be placed outside the integrals where they become spacetime derivatives $-\partial^\mu \partial^\nu$ of a function

$$F(x - x') = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} [e^{-ik(x-x')} + e^{ik(x-x')}] \chi(\mathbf{k}). \quad (7.518)$$

Thus we find

$$G_0^{\mu\nu}(x - x') = G_0^{\mu\nu}(x - x') - \partial^\mu \partial^\nu F(x - x'). \quad (7.519)$$

Physical observables must, of course, be independent of $F(x - x')$. This will be proven in Chapter 12 after Eq. (12.101).

Note that in contrast to $G^{\mu\nu}(x - x')$, the Fourier components of $F(x - x')$ are restricted to the light cone. This is seen more explicitly by rewriting the sums in (7.518) as integrals, and introducing the δ -function

$$\delta(k^2) = \frac{1}{2\omega_{\mathbf{k}}} [\delta(k^0 - \omega_{\mathbf{k}}) + \delta(k^0 + \omega_{\mathbf{k}})], \quad (7.520)$$

so that $F(x - x')$ is equal to the four-dimensional integral

$$F(x - x') = \int \frac{d^4 k}{(2\pi)^4} e^{-ik(x-x')} 2\pi \delta(k^2) \chi(\mathbf{k}). \quad (7.521)$$

The function $F(x - x')$ is therefore a solution of the Klein-Gordon equation $\partial^2 F(x - x') = 0$. This is the same type of freedom we are used to from all Green functions that satisfy the same inhomogeneous differential equation

$$-\partial^2 G^{\mu\nu} = -ig^{\mu\nu} \delta^{(4)}(x - x'). \quad (7.522)$$

All solutions of this equation differ from each other by solutions of the homogeneous differential equation, and so do the propagators $G_0^{\mu\nu}(x - x')$ and $G_0^{\mu\nu}(x - x')$ coming from different vacuum states.

Remedy to Wrong Vacuum Energy in Gupta-Bleuler Approach

In the Hamilton operators (7.504) and (7.506) we found an important failure of the Gupta-Bleuler quantization scheme. The energy contains also the vacuum oscillations of the two unphysical degrees of freedom oscillating in the $\mathbf{0}$ - and the $\mathbf{k}$ -direction. Due to the opposite commutation rules of the associated creation and annihilation operators, there is no cancellation of the two contributions. The Gupta-Bleuler approach eliminates the unphysical modes from all multiparticle states except for the vacuum. The elimination of this vacuum energy in the covariant approach was achieved almost two decades later by Faddeev and Popov [?]. Their method was developed for the purpose of quantizing nonabelian gauge theories. In these theories, the elimination of the unphysical gauge degrees of freedom cannot be

achieved with the help of a Gupta-Bleuler type of subsidiary condition (7.502). Essential to their approach is the use of the functional-integral formulation of quantum field theory. In it, all operator calculations are replaced by products of infinitely many integrals over classical fluctuating fields. This formulation will be introduced in Chapter 14. When fixing a covariant gauge in the gauge-invariant quantum partition function of the electromagnetic fields, one must multiply the functional integral by a factor that removes the unphysical modes from the partition function. At zero temperature, this factor subtracts, in the abelian gauge theory of QED, precisely the vacuum energies of the two unphysical modes. The removal requires an equal amount of negative vacuum energy. In Eq. (7.245) we have observed that fermions have negative vacuum energies. The subtraction of the unphysical vacuum energies can therefore be achieved by introducing two fictitious Fermi fields, a ghost field $C(x)$ and an anti-ghost field $\bar{C}(x)$. They are completely unphysical objects with spin zero, so that they do not appear in the physical Hilbert space,²⁰ i.e., the physical state vectors satisfy the conditions

$$C^\dagger(x)|0_{\text{phys}}\rangle = 0, \quad \bar{C}^\dagger(x)|0_{\text{phys}}\rangle = 0. \quad (7.523)$$

These fields are called *Faddeev-Popov ghosts*. In QED with gauge $\partial_\mu A^\mu(x) = 0$, their *only* contribution lies in the negative vacuum energy

$$E_0^{\text{ghosts}} = -2 \sum_{\mathbf{k}} \frac{k^0}{2} \quad (7.524)$$

which cancels the excessive vacuum energy (7.505) in the Gupta-Bleuler approach.

In quantum electrodynamics, the effect of the ghosts is trivial so that their introduction is superfluous for all purposes except for calculating the vacuum energy. This is the reason why their role was recognized only late in the development [13]. In nonabelian gauge theories, the ghost fields have nontrivial interactions with the physical particles, which must be included in all calculations to make the theory consistent.

In the light of this development, the correct way of writing the Lagrangian density of the free-photon field is

$$\mathcal{L}_{\text{tot}} = \mathcal{L} + \mathcal{L}_{\text{GF}} + \mathcal{L}_{\text{ghost}} = -\frac{1}{4}F_{\mu\nu}^2 - D(x)\partial^\mu A_\mu(x) + \alpha D^2(x)/2 - i\partial_\mu \bar{C}\partial^\mu C. \quad (7.525)$$

We shall see that this Lagrangian has an interesting new global symmetry between the Bose fields A^μ, D and the Fermi fields $C, \bar{C}$, called supersymmetry, which will be discussed in Chapter 25. In this context it is called BRS symmetry [?].

The Gupta-Bleuler gauge condition plus the subsidiary ghost conditions (7.523) eliminating the unphysical degrees of freedom are equivalent to requiring that the charges generating all global symmetry transformations annihilate the physical vacuum. Although structurally somewhat complicated, this is the most satisfactory way of formulating the covariant quantization procedure of the photon field.

²⁰For this reason, the failure to display the spin-statistics connection to be derived in Section 7.10 does not produce any causality problems.

The pseudophysical vacuum $|0_{\text{phys}'}\rangle$ of the Gupta-Bleuler approach has a unit norm, which is an important advantage over the physical vacuum $|0_{\text{phys}}\rangle$ of the Dirac approach. In axiomatic quantum field theory it can be proved that for any local operator $\mathcal{O}(x)$, one has

$$\mathcal{O}(x)|0\rangle = 0 \text{ if and only if } \mathcal{O}(x) = 0. \quad (7.526)$$

This is the reason why the Gupta-Bleuler subsidiary condition involves necessarily nonlocal operators. Recall that the operator in (7.502) contains only the positive-frequency part of the local field $D(x)$. The negative frequencies would be needed to make the field local. This will become clear in the proof of the spin-statistic theorem in Section 7.10.

Arbitrary Gauge Parameter α

A quantization of the electromagnetic field is also possible for different values of the gauge parameter α in the Lagrangian density (7.377) which so far has been set equal to unity, for simplicity. For an arbitrary value of α , the field equation (7.381) can be written as

$$L_{\mu\nu}(i\partial)A^\nu(x) = 0, \quad (7.527)$$

with the differential operator

$$L_{\mu\nu}(i\partial) \equiv -\partial^2 g_{\mu\nu} + \left(1 - \frac{1}{\alpha}\right) \partial_\mu \partial_\nu. \quad (7.528)$$

Multiplying Eq. (7.527) by ∂^μ , we find that the vector potential cannot have any four-divergence:

$$\partial_\mu A^\mu(x) = 0. \quad (7.529)$$

In a gauge-invariant formulation, this property can be chosen as the *Lorenz gauge condition*. If the Lagrangian contains a gauge-fixing part like (7.377), the Lorenz condition $\partial_\mu A^\mu(x) = 0$ is a consequence of the equations of motion. For such a field, the equations of motion reduce to four Klein-Gordon equations, just as before in the Feynman case $\alpha = 1$ [see (7.389)]:

$$-\partial^2 A^\mu(x) = 0. \quad (7.530)$$

We shall not go through the entire quantization procedure and the derivation of the propagator in this case. What can be given without much work is the Green function defined by the inhomogeneous field equation

$$L^{\mu\nu}(i\partial)G_{\nu\kappa}(x - x') = -i\delta^\mu_\kappa \delta^{(4)}(x - x'). \quad (7.531)$$

In momentum space, it reads

$$L^{\mu\nu}(k)G_{\nu\kappa}(k) = -i\delta^\mu_\kappa, \quad (7.532)$$

with the 4×4 -matrix

$$L^{\mu\nu}(k) = k^2 \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2} \right) + \frac{k^2}{\alpha} \frac{k^\mu k^\nu}{k^2}. \quad (7.533)$$

This matrix has an eigenvector k^μ with an eigenvalue k^2/α , and three eigenvectors orthogonal to it with eigenvalues k^2 . For a finite α , the matrix has an inverse, which is most easily found by decomposing $L_{\mu\nu}(k)$ as

$$L^{\mu\nu}(k) = k^2 P_T^{\mu\nu}(k) + \frac{k^2}{\alpha} P_L^{\mu\nu}(k), \quad (7.534)$$

with

$$\begin{aligned} P_T^{\mu\nu}(k) &= g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2}, \\ P_L^{\mu\nu}(k) &= \frac{k^\mu k^\nu}{k^2}. \end{aligned} \quad (7.535)$$

These matrices are projections. Indeed, they both satisfy the defining relation

$$P^{\mu\nu} P_\nu{}^\kappa = P^{\mu\kappa}. \quad (7.536)$$

In the decomposition (7.534), the inverse is found by inverting the coefficients in front of the projections $P_T(k)$ and $P_L(k)$:

$$L^{-1\mu\nu}(k) = \frac{1}{k^2} P_T^{\mu\nu}(k) + \frac{\alpha}{k^2} P_L^{\mu\nu}(k) = \frac{1}{k^2} \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2} \right) + \frac{\alpha}{k^2} \frac{k^\mu k^\nu}{k^2}. \quad (7.537)$$

After this, we can solve (7.532) by

$$G^{\mu\nu}(k) = -i L^{-1\mu\nu}(k). \quad (7.538)$$

The propagator has therefore the Fourier representation

$$G^{\mu\nu}(x - x') = \int \frac{d^4 k}{(2\pi)^4} e^{-ik(x-x')} \frac{i}{k^2 + i\eta} \left[-g^{\mu\nu} + (1 - \alpha) \frac{k^\mu k^\nu}{k^2 + i\eta} \right]. \quad (7.539)$$

As usual, we have inserted imaginary parts $i\eta$ to regularize the integral in the same way as in the propagator of the scalar field. For the term $k^\mu k^\nu/(k^2 + i\eta)$ the prescription how to place the additional poles is not immediately obvious. The best way to derive it is by giving the photon a small mass and setting it later equal to zero. The reader is referred to the next section where the massive vector meson is treated. He may be worried about the physical meaning of the double-pole in the integrand of the propagator (7.539). A pole in the propagator is associated with a particle state in Hilbert space. How does a double pole manifest itself in Hilbert space? Heisenberg called the associated state a *dipole ghost* [16]. Instead of satisfying a Schrödinger equation

$$(E - H)|\psi\rangle = 0, \quad (7.540)$$

such a state satisfies the two equations

$$(E - H)|\psi\rangle \neq 0, \quad (E - H)^2|\psi\rangle = 0. \quad (7.541)$$

It is unphysical. In the present context, such states do not cause any harm. They are an artifact of the gauge fixing procedure and do not contribute to any observable quantity, due to gauge invariance. A similar situation will arise from moving charges in Chapter 12.

Since the $D(x)$ -field is now equal to $\partial_\mu A^\mu(x)/\alpha$ [recall (7.379)], the gauge parameter α enters in various commutation relations involving $A^\mu(\mathbf{x}, t)$ and $\dot{A}^\mu(\mathbf{x}, t)$. Proceeding as in Eqs. (7.395)–(7.403), we find that the gauge parameter α enters into the commutation rules among $A^\mu(\mathbf{x}, t)$ and $\dot{A}^\mu(\mathbf{x}, t)$ of Eqs. (7.399)–(7.402) as follows:

$$[\dot{A}^0(\mathbf{x}, t), A^0(\mathbf{x}', t)] = \alpha[D(\mathbf{x}, t), A^0(\mathbf{x}', t)] = i\alpha\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (7.542)$$

$$[\dot{A}^i(\mathbf{x}, t), \dot{A}^j(\mathbf{x}', t)] = 0, \quad (7.543)$$

$$[\dot{A}^0(\mathbf{x}, t), \dot{A}^i(\mathbf{x}', t)] = -(1 - \alpha)i\partial_i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (7.544)$$

$$[\dot{A}^0(\mathbf{x}, t), \dot{A}^0(\mathbf{x}', t)] = 0. \quad (7.545)$$

The other commutators (7.397), (7.400), and (7.401) remain unchanged.

These commutators are needed to verify that the vacuum expectation of the time-ordered product

$$G^{\mu\nu}(x - x') \equiv \langle 0|T A^\mu(x) A^\nu(x')|0\rangle \quad (7.546)$$

satisfies the field equation with a δ -function source (7.656). The proof of this is nontrivial:

$$\begin{aligned} & - \left[\partial^2 g_{\mu\nu} - \left(1 - \frac{1}{\alpha}\right) \partial_\mu \partial_\nu \right] G^{\nu\kappa}(x - x') = \\ & - \langle 0|T \left[\partial^2 g_{\mu\nu} - \left(1 - \frac{1}{\alpha}\right) \partial_\mu \partial_\nu \right] A^\nu(x) A^\kappa(x')|0\rangle - \delta(x^0 - x'^0) g_{\mu\nu} \langle 0|[\dot{A}^\nu(x), A^\kappa(x')]|0\rangle \\ & + \left(1 - \frac{1}{\alpha}\right) g_{0\mu} \delta(x^0 - x'^0) \langle 0|[\partial_\nu A^\nu(x), A^\kappa(x')]|0\rangle = -i\delta_\mu{}^\kappa \delta^{(4)}(x - x'), \end{aligned} \quad (7.547)$$

the right-hand side requiring the commutation relations (7.542)–(7.545).

It is useful to check the consistency of the propagator with the canonical commutation rules. This is done in Appendix 7C.

7.5.4 Behavior under Discrete Symmetries

Under P,C,T, the vector potential has the transformation properties [recall Section 4.6]:

$$A^\mu(x) \xrightarrow{P} A_P'^\mu(x) = \tilde{A}^\mu(\tilde{x}), \quad (7.548)$$

$$A^\mu(x) \xrightarrow{T} A_T'^\mu(x) = \tilde{A}^\mu(x_T), \quad (7.549)$$

$$A^\mu(x) \xrightarrow{C} A_C'^\mu(x) = -A^\mu(x). \quad (7.550)$$

The photon has a negative charge parity which coincides with that of the vector current $V^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x)$ formed from Dirac fields (see Table 4.12.8), to which it will later be coupled (see Chapter 12).

These properties are implemented in the second-quantized Hilbert space by transforming the photon creation operators as follows:

$$\mathcal{P}a_{\mathbf{k},\nu}^\dagger\mathcal{P}^{-1} \equiv a_{-\mathbf{k},-\nu}^\dagger, \quad (7.551)$$

$$\mathcal{T}a_{\mathbf{k},\nu}^\dagger\mathcal{T}^{-1} \equiv a_{-\mathbf{k},\nu}^\dagger, \quad (7.552)$$

$$\mathcal{C}a_{\mathbf{k},\nu}^\dagger\mathcal{C}^{-1} \equiv -a_{\mathbf{k},\nu}^\dagger. \quad (7.553)$$

The annihilation operators transform by the Hermitian-adjoint relations.

7.6 Massive Vector Bosons

Besides the massless photons, there exist also massive vector bosons. The most important examples are the fundamental vector bosons mediating the weak interactions, to be discussed in detail in Chapter 27. They can be electrically neutral or carry an electric charge of either sign: $\pm e$. There also exist strongly interacting vector particles of a composite nature. They are short-lived and only observable as resonances in scattering experiments, the most prominent being a resonance in the two-pion scattering amplitude. These are the famous ρ -mesons which will be discussed in Chapter 24. They also carry charges $0, \pm e$. The actions of a neutral and charged massive vector field $V^\mu(x)$ are:

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left(-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}M^2V_\mu V^\mu \right), \quad (7.554)$$

and

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left(-\frac{1}{2}F_{\mu\nu}^*F^{\mu\nu} + M^2V_\mu^*V^\mu \right), \quad (7.555)$$

with the equations of motion

$$\partial_\mu F^{\mu\nu} + M^2V^\nu = 0, \quad (7.556)$$

or

$$[(-\partial^2 - M^2)g_{\mu\nu} + \partial_\mu\partial_\nu]V^\mu(x) = 0. \quad (7.557)$$

These imply that the vector field $V^\mu(x)$ has no four-divergence:

$$\partial_\mu V^\mu(x) = 0, \quad (7.558)$$

and that each component satisfies the Klein-Gordon equation

$$(-\partial^2 - M^2)V^\mu(x) = 0. \quad (7.559)$$

It will sometimes be convenient to view the photon as an $M \rightarrow 0$ -limit of a massive vector meson. For this purpose we have to add a gauge fixing term to the Lagrangian to allow for a proper limit. The extended action reads

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} M^2 V_\mu V^\mu - \frac{1}{2\alpha} (\partial_\mu V^\mu)^2 \right], \quad (7.560)$$

resulting in the field equation

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu + \frac{1}{\alpha} \partial^\nu \partial_\mu V^\mu = 0, \quad (7.561)$$

which reads more explicitly

$$\left[(-\partial^2 - M^2) g_{\mu\nu} + \left(1 - \frac{1}{\alpha} \right) \partial_\mu \partial_\nu \right] V^\mu(x) = 0. \quad (7.562)$$

Multiplying (7.561) with ∂_ν from the left gives, for the divergence $\partial_\nu V^\nu$, the Klein-Gordon equation

$$(\partial^2 + \alpha M^2) \partial_\nu V^\nu(x) = 0, \quad (7.563)$$

from which the constraint (7.558) follows in the limit of large α .

7.6.1 Field Quantization

The canonical field momenta are

$$\pi_\mu = \frac{\partial \mathcal{L}}{\partial [\partial_0 V^\mu]} = -F_{0\mu}^*, \quad (7.564)$$

where the complex conjugation is, of course, irrelevant for a real field. As for electromagnetic fields, the zeroth component $V^0(x)$ has no canonical field momentum. The vanishing of π_0 is a primary constraint. It expresses the fact that the Euler-Lagrange equation (4.811) for $V^0(x)$ is not a dynamical field equation.

For the spatial components $V^i(x)$, there are nonvanishing canonical equal-time commutation rules:

$$\begin{aligned} [\pi_i(\mathbf{x}, t), V^j(\mathbf{x}', t)] &= -i \delta_i^j \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\pi_i^\dagger(\mathbf{x}, t), V^{j\dagger}(\mathbf{x}', t)] &= -i \delta_i^j \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (7.565)$$

From these we can calculate commutators involving $V^0(\mathbf{x}, t)$ by using relation (4.811). The results are

$$[V^{0\dagger}(\mathbf{x}, t), V^i(\mathbf{x}', t)] = \frac{i}{M^2} \partial_i \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (7.566)$$

and

$$[V^0(\mathbf{x}, t), V^i(\mathbf{x}', t)] = 0. \quad (7.567)$$

To exhibit the particle content in the second-quantized fields, we now expand $V^\mu(x)$ into the complete set of classical solutions of Eqs. (7.556) and (7.558) in a large but finite volume V :

$$V^\mu(x) = \sum_{\mathbf{k}, s_3=0, \pm 1} \frac{1}{\sqrt{2V k^0}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, s_3) a_{\mathbf{k}, s_3} + e^{ikx} \epsilon^{\mu*}(\mathbf{k}, s_3) b_{\mathbf{k}, s_3}^\dagger \right]. \quad (7.568)$$

If the vector fields are real, the same expansion holds with particles and antiparticles being identified. Dealing with massive vector particles, we may label the polarization states by the third components s_3 of angular momentum in the particle's rest frame. The polarization vectors were given explicitly in Eq. (4.815).

As for scalar and Dirac fields, we have associated the expansion coefficients of the plane waves of negative energy e^{ikx} with a creation operator $b_{\mathbf{k}, s_3}^\dagger$ rather than a second type of annihilation operator $d_{\mathbf{k}, s_3}$. In principle, the polarization vector associated with the antiparticles could have been some charge-conjugate polarization vector $\epsilon_c^\mu(\mathbf{k}, s_3)$, by analogy with the spinors $v(\mathbf{p}, s_3) = u^c(\mathbf{p}, s_3)$ [recall (4.678)]. In the present case of a vector field, that is multiplied with a Lorentz transformation by a real 4×4 -Lorentz matrix $\Lambda^\mu{}_\nu$. Charge conjugation exchanges the polarization vector (or tensor) by its complex conjugate. This is a direct consequence of the charge conjugation property (7.309) of the four-vector currents to which the standard massive vector fields are coupled in the action. For the vector potential $V^\mu(x) \equiv A^\mu(x)$ of electromagnetism this will be seen most explicitly in Eq. (12.54).

Alternatively we may expand the field $V^\mu(x)$ in terms of helicity polarization states as

$$V^\mu(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V k^0}} \sum_{\lambda=\pm 1, 0} \left[e^{-ipx} \epsilon_H^\mu(\mathbf{k}, \lambda) a_{\mathbf{k}, \lambda} + e^{ipx} \epsilon_H^{\mu*}(\mathbf{k}, \lambda) b_{\mathbf{k}, \lambda}^\dagger \right], \quad (7.569)$$

where $\epsilon_H^\mu(\mathbf{k}, \lambda)$ are the polarization vectors (4.822).

The quantization of the massive vector field with the action (7.560) proceeds most conveniently by introducing a transverse field

$$V_\mu^T(x) \equiv V_\mu + \frac{1}{\alpha M^2} \partial_\mu \partial_\nu V^\nu(x), \quad (7.570)$$

which is divergenceless, as a consequence of (7.563):

$$\partial^\mu V_\mu^T(x) = 0. \quad (7.571)$$

The full vector field is then a sum of a purely transverse field and the gradient of a scalar field $\partial_\nu V^\nu(x)$:

$$V_\mu(x) = V_\mu^T(x) - \frac{1}{\alpha M^2} \partial_\mu \partial_\nu V^\nu(x). \quad (7.572)$$

It can be expanded in terms of three creation and annihilation operators $a_{\mathbf{k}, \lambda}^\dagger$, $a_{\mathbf{k}, \lambda}$ for the three physical polarization states with helicities $\lambda = 0, \pm 1$, and an extra pair of operators $a_{\mathbf{k}, s}^\dagger$, $a_{\mathbf{k}, s}$ for the scalar degree of freedom. The commutation rules are

$$\begin{aligned} [a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}] &= [a_{\mathbf{k}, \lambda}^\dagger, a_{\mathbf{k}', \lambda'}^\dagger] = 0, \\ [a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}^\dagger] &= -\delta_{\mathbf{k}, \mathbf{k}'} g_{\lambda \lambda'}, \end{aligned} \quad (7.573)$$

where λ runs through the helicities $0, \pm 1$, and s . The metric $g_{\lambda\lambda'}$ has a negative sign for $\lambda = 0, \pm 1$, and a positive one for $\nu = s$. These commutation rules have the same form as those in (7.404), except for the different meaning of the labels ν . The properly quantized field is then

$$V^\mu(x) = \sum_{\mathbf{k}} \left\{ \sum_{\lambda=0,\pm 1} \frac{1}{\sqrt{2Vk^0}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, \lambda) a_{\mathbf{k},\lambda} + \epsilon^{\mu*}(\mathbf{k}, \lambda) a_{\mathbf{k},\lambda}^\dagger \right] + \frac{1}{\sqrt{2Vk^0}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, s) a_{\mathbf{k},s} + \epsilon^{\mu*}(\mathbf{k}, s) a_{\mathbf{k},s}^\dagger \right] \right\}. \quad (7.574)$$

7.6.2 Energy of Massive Vector Particles

The energy can be calculated by close analogy with that of photons. We shall consider a real field, and admit an additional coupling to an external current density $j^\mu(x)$, with an interaction

$$\mathcal{L}_{\text{int}} = -j^\mu(x) V_\mu(x). \quad (7.575)$$

This causes only minor additional labor but will be useful to understand a special feature of the massive propagator to be calculated in the next section. The current term changes the equations of motion (7.556) to

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu - j^\nu = 0, \quad (7.576)$$

implying, for the non-dynamical zeroth component of $V^\mu(x)$, the relation

$$V^0(x) = \frac{1}{M^2} \left[\nabla \cdot \dot{\mathbf{V}}(x) + \nabla^2 V^0(x) - j^0(x) \right], \quad (7.577)$$

rather than (4.811). As in electromagnetism, we define the negative vector of the canonical field momenta (7.564) as the “electric” field strength of the massive vector field:

$$\mathbf{E}(x) \equiv -\boldsymbol{\pi}(x) = -\dot{\mathbf{V}}(x) - \nabla V^0(x). \quad (7.578)$$

Combining this with (7.577), we obtain

$$\dot{\mathbf{V}}(x) = -\mathbf{E}(x) - \nabla V^0(x) = -\mathbf{E}(x) + \frac{1}{M^2} \nabla [\nabla \cdot \mathbf{E}(x) - j^0(x)]. \quad (7.579)$$

We now form the Hamiltonian density (7.340) as the Legendre transform

$$\mathcal{H} = \boldsymbol{\pi} \dot{\mathbf{V}} - \mathcal{L}_0 - \mathcal{L}_{\text{int}}. \quad (7.580)$$

Inserting (7.579), we obtain

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}, \quad (7.581)$$

with a free Hamiltonian density

$$\mathcal{H}_0 = \frac{1}{2} \left[\mathbf{E}^2 + \mathbf{B}^2 + \frac{V_0}{M^2} (\nabla \cdot \mathbf{E}) + M^2 \mathbf{V}^2 \right], \quad (7.582)$$

and an interaction energy density

$$\mathcal{H}_{\text{int}} = \mathbf{j} \cdot \mathbf{V} - \frac{1}{M^2} j^0 \nabla \cdot \mathbf{E} + \frac{1}{M^2} j^{02}. \quad (7.583)$$

Here we have introduced the field

$$\mathbf{B}(x) = \nabla \times \mathbf{V}(x) \quad (7.584)$$

by analogy with the magnetic field of electromagnetism [compare (7.340)].

Discarding again the external current, we form the free Hamiltonian $H_0 = \int d^3x \mathcal{H}_0$, express $\mathbf{E}(x)$ as $-\dot{\mathbf{V}} - \nabla V^0$, and $\nabla \cdot \mathbf{E}$ as $-M^2 V^0$, and find the Hamiltonian

$$H_0 = \int d^3x \left\{ \frac{1}{2} \left[-\dot{V}^\mu \dot{V}_\mu - \nabla V^\mu \cdot \nabla V_\mu - M^2 V^\mu V_\mu \right] - \nabla \cdot (\mathbf{E} V^0) \right\}. \quad (7.585)$$

The last term is a surface term that can be omitted in an infinite volume. Inserting the expansion (7.569) for the field operator, and proceeding as in the case of the photon energy (7.356), we obtain the energy

$$H_0 = \sum_{\mathbf{k}, \lambda=0, \pm 1} k^0 \left(a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda} + \frac{1}{2} \right). \quad (7.586)$$

This contains a vacuum energy

$$E_0 \equiv \langle 0 | H_0 | 0 \rangle = \frac{1}{2} \sum_{\mathbf{k}, \lambda=0, \pm 1} k^0 = \frac{3}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}}, \quad (7.587)$$

due to the zero-point oscillations. The factor 3 accounts for the different polarization states.

7.6.3 Propagator of Massive Vector Particles

Let us now calculate the propagator of a massive vector particle from the vacuum expectation value of the time-ordered product of two vector fields. As in (7.360) we find

$$\begin{aligned} G^{\mu\nu}(x, x') &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{k^0} e^{-ik(x-x')} \sum_{\lambda} \epsilon^\mu(\mathbf{k}, \lambda) \epsilon^{\nu*}(\mathbf{k}, \lambda) \\ &+ \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{k^0} e^{ik(x-x')} \sum_{\lambda} \epsilon^\nu(\mathbf{k}, \lambda) \epsilon^{\mu*}(\mathbf{k}, \lambda), \end{aligned} \quad (7.588)$$

and insert the completeness relation (4.820) to write

$$\begin{aligned} G^{\mu\nu}(x, x') &= \Theta(x_0 - x'_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{k^0} e^{-ik(x-x')} \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{M^2} \right) \\ &+ \Theta(x'_0 - x_0) \frac{1}{2V} \sum_{\mathbf{k}} \frac{1}{k^0} e^{ik(x-x')} \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{M^2} \right). \end{aligned} \quad (7.589)$$

This expression has precisely the general form (7.283), with the polarization sums of particles and antiparticles being equal to one another. The common polarization sum can be pulled in front of the Heaviside functions, yielding

$$\begin{aligned} G^{\mu\nu}(x, x') &= \left(-g^{\mu\nu} - \frac{\partial^\mu \partial^\nu}{M^2} \right) \left[\Theta(x_0 - x'_0) G^{(+)}(x - x') + \Theta(x'_0 - x_0) G^{(-)}(x - x') \right] \\ &+ \frac{1}{M^2} \{ [\partial^\mu \partial^\nu, \Theta(x^0 - x'^0)] G^{(+)}(x - x') + [\partial^\mu \partial^\nu, \Theta(x'^0 - x^0)] G^{(-)}(x - x') \}. \end{aligned} \quad (7.590)$$

The bracket in the first expression is equal to the Feynman propagator of the scalar field. The second term only contributes if both μ and ν are 0. For $\mu = i$ and $\nu = j$, it vanishes trivially. For $\mu = 0$ and $\nu = i$, it gives

$$\frac{1}{M^2} [\partial^i \delta(x^0 - x'^0) G^{(+)}(x - x') + \partial^i \delta(x'^0 - x^0) G^{(-)}(x - x')].$$

Since

$$\delta(x^0 - x'^0) G^{(+)}(x - x') = \delta(x'^0 - x^0) G^{(-)}(x - x'),$$

these components vanish. If both components μ and ν are zero, we use the trivial identities

$$\begin{aligned} [\partial_0 \partial_0, \Theta(x^0 - x'^0)] &= \partial_0 \delta'(x^0 - x'^0) + 2\delta(x^0 - x'^0) \partial_0, \\ [\partial_0 \partial_0, \Theta(x'^0 - x^0)] &= -\partial_0 \delta(x'^0 - x^0) - 2\delta(x^0 - x'^0) \partial_0, \end{aligned}$$

and the relation

$$\partial_0 G^{(\pm)}(x - x') \Big|_{x_0=x'_0=0} = \mp \frac{i}{2} \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (7.591)$$

to obtain $-2i\delta^{(4)}(x - x')$ from the last two terms in (7.590). By a calculation like (7.44), we see that the first terms remove a factor 2 from this, so that we find for the Feynman propagator of the massive vector field the expression

$$\begin{aligned} G^{\mu\nu}(x, x') &= - \int \frac{d^4 k}{(2\pi)^4} e^{-ik(x-x')} \frac{i}{k^2 - M^2 + i\eta} \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2} \right) \\ &- \frac{i}{M^2} \delta_{\mu 0} \delta_{\nu 0} \delta^{(4)}(x - x'). \end{aligned} \quad (7.592)$$

Only the first term is a Lorentz tensor. The second term destroys the covariance. It is known as a *Schwinger term*.

Let us trace its origin in momentum space. If we replace the Heaviside functions in (7.588) by their Fourier integral representations (7.63), we find a representation of the type (7.290) for the propagator:

$$G^{\mu\nu}(x - x') = \int \frac{d^4 k}{(2\pi)^4} \frac{i}{2\omega_{\mathbf{k}}} \left[\frac{P^{\mu\nu}(\omega_{\mathbf{k}}, \mathbf{k})}{k^0 - \omega_{\mathbf{k}} + i\eta} - \frac{P^{\mu\nu}(-\omega_{\mathbf{k}}, \mathbf{k})}{k^0 + \omega_{\mathbf{k}} - i\eta} \right] e^{-ip(x-x')}, \quad (7.593)$$

with the on-shell projection matrices

$$P^{\mu\nu}(\omega_{\mathbf{k}}, k) \equiv P^{\mu\nu}(k^0, \mathbf{k}) \Big|_{k^0=\omega_{\mathbf{k}}} \equiv - \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2} \right) \Big|_{k^0=\omega_{\mathbf{k}}}. \quad (7.594)$$

Expression (7.593) is a tensor only if the on-shell energy $k^0 = \omega_{\mathbf{k}}$ in the argument of $P^{\mu\nu}(k^0, \mathbf{k})$ is replaced by the off-shell integration variable k^0 . The difference between (7.594) and such a covariant version has two contributions: one from the linear term in k^0 , and one from the quadratic term. The first vanishes by the same mechanism as in the Dirac discussion of (7.290). The quadratic term contributes only for $(\mu, \nu) = (0, 0)$, where

$$P^{00}(\omega_{\mathbf{k}}, \mathbf{k}) - P^{00}(k^0, k) = \frac{\omega_{\mathbf{k}}^2 - k^{02}}{M^2}. \quad (7.595)$$

The combination $\omega_{\mathbf{k}}^2 - k^{02} = M^2 - k^2$ cancels the denominators in (7.593), thus producing precisely Schwinger's δ -function term (7.592).

The covariant part of the propagator coincides with the Green function of the field equation (7.557). Indeed, the differential operator on the left-hand side can be written by analogy with (7.534) as

$$L_{\mu\nu}(i\partial)G^{\nu\kappa}(x - x') = -i\delta_\mu^\kappa \delta^{(4)}(x - x'), \quad (7.596)$$

so that the calculation of the Green function requires inverting the matrix in momentum space [the analog of (7.534)]

$$L_{\mu\nu}(k) = (k^2 - M^2)P_{T\mu\nu}(k) - M^2 P_{L\mu\nu}(k). \quad (7.597)$$

This has the inverse

$$L^{-1\mu\nu}(k) = \frac{1}{k^2 - M^2} P_T^{\mu\nu}(k) - \frac{1}{M^2} P_L^{\mu\nu}(k) = \frac{1}{k^2 - M^2} \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2} \right), \quad (7.598)$$

yielding the solution of (7.596) in momentum space:

$$G^{\mu\nu}(k) = -iL^{-1\mu\nu}(k). \quad (7.599)$$

This is precisely the Fourier content in the first term of (7.592). The mass contains an infinitesimal $-i\eta$ to ensure that particles and antiparticles decay both at positive infinite times.

For a massive vector meson whose action contains a gauge fixing term as in (7.560), the matrix (7.597) reads

$$L_{\mu\nu}(k) = (k^2 - M^2)P_{T\mu\nu}(k) + \left(\frac{k^2}{\alpha} - M^2 \right) P_{L\mu\nu}(k). \quad (7.600)$$

It has an inverse (7.598):

$$\begin{aligned} L^{-1\mu\nu}(k) &= \frac{1}{k^2 - M^2} P_T^{\mu\nu}(k) + \frac{\alpha}{k^2 - \alpha M^2} P_L^{\mu\nu}(k) \\ &= \frac{1}{k^2 - M^2} \left[g^{\mu\nu} - (1 - \alpha) \frac{k^\mu k^\nu}{k^2 - \alpha M^2} \right]. \end{aligned} \quad (7.601)$$

Due to the Schwinger term, the propagator is different from the Green function associated with the field equation (7.557). In Chapters 9, 10, and 14, we shall see that in the presence of interactions there are two ways of evaluating the physical consequences. One of them is based on the interaction picture of quantum mechanics and the Schwinger-Dyson perturbation expansion for scattering amplitudes derived in Section 1.6. The other makes use of functional integrals and eventually leads to similar results. The first is based on a Hamiltonian approach in which time-ordered propagators play a central role, and interactions are described with the help of an interaction Hamiltonian. The second is centered on a spacetime formulation of the action, where covariant Green functions are relevant, rather than time-ordered propagators. Eventually, the results will be the same in both cases, as we shall see. The cancellation of all Schwinger terms will be caused by the last term in the Hamiltonian density (7.583).

The commutator of two vector fields is

$$[V^{\mu\dagger}(x), V^\nu(x')] = C^{\mu\nu}(x - x'), \quad (7.602)$$

with

$$\begin{aligned} C^{\mu\nu}(x - x') &= \int \frac{d^4 k}{(2\pi)^4} e^{-ik(x-x')} 2\pi\epsilon(k^0) \delta(k^2 - M^2) \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{M^2} \right) \\ &= \left(-g^{\mu\nu} - \frac{\partial^\mu \partial^\nu}{M^2} \right) C(x - x'). \end{aligned} \quad (7.603)$$

At equal times, we rewrite in the integrand

$$\delta(k^2 - M^2) = \frac{1}{2\omega_{\mathbf{k}}} [\delta(k^0 - \omega_{\mathbf{k}}) + \delta(k^0 + \omega_{\mathbf{k}})],$$

with $\omega_{\mathbf{k}} \equiv \sqrt{\mathbf{k}^2 + M^2}$, and see that the oddness of $\epsilon(k^0)$ makes the commutator vanish, except for $(\mu, \nu) = (0, i)$, where $k^0 \epsilon(k^0) = |k^0|$ produces at equal times an even integral

$$\int d^4 k e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \epsilon(k^0) \delta(k^2 - M^2) k^0 k^i = \int d^3 k k^i e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} = -i \partial^i \delta^{(3)}(\mathbf{x} - \mathbf{x}') = i \partial_i \delta^{(3)}(\mathbf{x} - \mathbf{x}'),$$

thus verifying the canonical commutation relation (7.566).

Let us end this section by justifying the earlier-used $i\eta$ -prescription in the propagator (7.539) of the photon field. For this we add a mass term to the electromagnetic

Lagrangian (7.376) with the gauge-fixing Lagrangian, which leads to a massive vector photon Lagrangian

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}M^2 A_\mu A^\mu - D(x)\partial^\mu A_\mu(x) + \frac{\alpha}{2}D^2(x), \quad \alpha \geq 0. \quad (7.604)$$

The Euler-Lagrange equations are now [compare (7.381)]

$$\left[(-\partial^2 - M^2)g_{\mu\nu} + \left(1 - \frac{1}{\alpha}\right)\partial_\mu\partial_\nu\right]A^\nu(x) = 0, \quad (7.605)$$

so that the propagator in momentum space obeys the equation

$$\left[(k^2 - M^2)g_{\mu\nu} - \left(1 - \frac{1}{\alpha}\right)k_\mu k_\nu\right]G^{\nu\kappa}(k) = -i\delta^\mu_\kappa. \quad (7.606)$$

The matrix on the left-hand side is decomposed into transverse and longitudinal parts as

$$L_{\mu\nu}(k) = (k^2 - M^2)P_{T\mu\nu}(k) + \frac{1}{\alpha}(k^2 - \alpha M^2)P_{L\mu\nu}(k), \quad (7.607)$$

from which we obtain the inverse

$$\begin{aligned} L^{-1\mu\nu}(k) &= \frac{1}{k^2 - M^2}P_T^{\mu\nu}(k) + \frac{\alpha}{k^2 - \alpha M^2}P_L^{\mu\nu}(k), \\ &= \frac{1}{k^2 - M^2}\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2}\right) + \frac{\alpha}{k^2 - \alpha M^2}\frac{k^\mu k^\nu}{k^2}, \end{aligned} \quad (7.608)$$

which can be rearranged to

$$L^{-1\mu\nu}(k) = \frac{g^{\mu\nu}}{k^2 - M^2} + (\alpha - 1)\frac{k^\mu k^\nu}{(k^2 - \alpha M^2)(k^2 - M^2)}, \quad (7.609)$$

so that (7.547) is solved by the matrix

$$G^{\mu\nu}(k) = -iL^{-1\mu\nu}(k). \quad (7.610)$$

The condition $\alpha > 0$ in the Lagrangian (7.604) ensures that both poles in the second denominator lie at a physical mass square.

Adding to the mass an infinitesimal imaginary part $-i\eta$ with $\alpha > 0$, and letting $M \rightarrow 0$, we obtain precisely the $i\eta$ -prescription of Eq. (7.539).

7.7 Wigner Rotation of Spin-1 Polarization Vectors

Let us verify that the polarization vectors $\epsilon^\mu(\mathbf{k}, s_3)$ and their complex-conjugates $\epsilon^{\mu*}(\mathbf{k}, s_3)$ lead to the correct Wigner rotations for the annihilation and creation operators $a_{\mathbf{k}, s_3}$ and $b_{\mathbf{k}, s_3}^\dagger$. These have to be the spin-1 generalizations of (4.736) and (4.742), or (4.737) and (4.738). The simplest check are the analogs of Eqs. (4.743).

For this we form the 4×3 -matrices corresponding to $u(\mathbf{0})$ and $v(\mathbf{0})$ in (4.743) [recall (4.669) and (4.670)]

$$\epsilon^\mu(\mathbf{k}) \equiv \mp \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ i & 0 & -i \\ 0 & 0 & 0 \end{pmatrix}, \quad \epsilon^{\mu*}(\mathbf{k}) \equiv \mp \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ -i & 0 & i \\ 0 & 0 & 0 \end{pmatrix}. \quad (7.611)$$

Multiplying these by the 4×4 -generators [recall (4.54)–(4.56)]

$$L_3 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad L_1 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad L_2 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (7.612)$$

from the left, we find the same result as by applying the 3×3 spin-1 representation matrices [recall (4.848)–(4.849)]:

$$D^j(L_3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad D^j(L_1) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad D^j(L_2) = \frac{-i}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad (7.613)$$

from the right.

For finite Lorentz transformation, the polarization vectors undergo the Wigner rotations

$$\epsilon^\mu(\mathbf{k}, s_3) \xrightarrow{\Lambda} \epsilon'^\mu(\mathbf{k}, s_3) = \Lambda^\mu{}_\nu \epsilon^\nu(\mathbf{k}, s_3) = \sum_{s'_3=-1}^1 \epsilon^\mu(\mathbf{p}, s'_3) W_{s'_3, s_3}^{(1)}(p', \Lambda, p), \quad (7.614)$$

$$\epsilon^{\mu*}(\mathbf{k}, s_3) \xrightarrow{\Lambda} \epsilon'^{\mu*}(\mathbf{k}, s_3) = \Lambda^\mu{}_\nu \epsilon^{\nu*}(\mathbf{k}, s_3) = \sum_{s'_3=-1}^1 \epsilon^{\mu*}(\mathbf{p}, s'_3) W_{s'_3, s_3}^{(1)*}(p', \Lambda, p), \quad (7.615)$$

where $W_{s'_3, s_3}^{(1)}$ is the spin-1 representation of the 2×2 Wigner rotations (4.736). The second transformation law follows from the first as a consequence of the reality of the Lorentz transformations $\Lambda^\mu{}_\nu$.

In closer analogy with (4.678), we can obtain the charge-conjugate polarization vectors by forming

$$\epsilon_c^\mu(\mathbf{k}, s_3) \equiv -\epsilon^\mu(\mathbf{k}, s'_3) c_{s'_3, s_3}^{(1)}, \quad (7.616)$$

where $c_{s'_3, s_3}^{(s)}$ denotes the spin- s representation of the rotation matrix $c = e^{-i\pi\sigma_2/2}$ introduced in Eq. (4.900). It is easy to verify that $\epsilon_c^\mu(\mathbf{k}, s_3)$ coincides with $\epsilon^{\mu*}(\mathbf{k}, s_3)$. The matrix $c_{s'_3, s_3}^{(s)}$ turns the spin into the opposite direction:

$$c_{s_3, s'_3}^{(s)} = \langle s, s_3 | e^{-i\hat{L}_2\pi/2} | s, s'_3 \rangle = d_{s_3, s'_3}^s(\pi) = (-)^{s+s_3} \delta_{s_3, -s'_3}, \quad (7.617)$$

and has the property [recall (4.901)]:

$$D^j(R)c^{(j)} = c^{(j)}D^{j*}(R), \quad (7.618)$$

which confirms that $\epsilon_c^\mu(\mathbf{k}, s_3)$ transforms with the complex-conjugate of the Wigner rotation of $\epsilon^\mu(\mathbf{k}, s_3)$.

In principle, there exists also a fourth vector which may be called *scalar polarization vector* to be denoted by

$$\epsilon^\mu(\mathbf{k}, s) \equiv k^\mu. \quad (7.619)$$

This polarization vector will be of use later in Subsecs. 4.9.6 and 7.5.2. It corresponds to a pure gauge degree of freedom since in x -space it has the form $\partial^\mu \Lambda$. As such, it transforms under an extra independent and irreducible representation of the Lorentz group describing a scalar particle degree of freedom and no longer forms part of the vector particle. It certainly does not contribute to the gauge-invariant electromagnetic action.

Observe that for a very small mass where $\omega_{\mathbf{k}} \rightarrow |\mathbf{k}|$, the scalar polarization vector has the limit

$$M\epsilon^\mu(\mathbf{k}, s) \xrightarrow{M \rightarrow 0} |\mathbf{k}| \begin{pmatrix} 1 \\ \hat{\mathbf{k}} \end{pmatrix} = k^\mu, \quad (7.620)$$

i.e., it goes over into the unphysical scalar degree of freedom. This is why the longitudinal polarization does not contribute to the action of a massless vector particle.

7.7.1 Behavior under Discrete Symmetry Transformations

Under the discrete transformations P, T , and C , a massive vector field transforms in the same way as the vector potential of electromagnetism in Eqs. (7.548)–(7.552), except for different possible phases η_P, η_T, η_C .

In the second-quantized Hilbert space, these amount to the following transformation laws for the creation and annihilation operators of particles of helicity λ . Under parity we have:

$$\mathcal{P}a_{\mathbf{k},\lambda}^\dagger \mathcal{P}^{-1} \equiv a_{\mathbf{k},\lambda}'^\dagger = \eta_P a_{-\mathbf{k},-\lambda}^\dagger, \quad (7.621)$$

with $\eta_P = \pm 1$. Under time reversal:

$$\mathcal{T}a_{\mathbf{k},\lambda}^\dagger \mathcal{T}^{-1} \equiv a_{\mathbf{k},\lambda}'^\dagger = \eta_T a_{-\mathbf{k},\lambda}^\dagger, \quad (7.622)$$

with an arbitrary phase factor η_T , and under charge conjugation

$$\mathcal{C}a_{\mathbf{k},\lambda}^\dagger \mathcal{C}^{-1} \equiv a_{\mathbf{k},\lambda}'^\dagger = \eta_C a_{\mathbf{k},\lambda}^\dagger, \quad (7.623)$$

with $\eta_C = \pm 1$.

Vector mesons such as the ρ -meson of mass $m_\rho \approx 759$ MeV and the ω -meson of mass $m_\omega \approx 782$ MeV transform with the three phase factors η_P, η_T, η_C being equal

to those of a photon. This is a prerequisite for the theory of *vector meson dominance* of electromagnetic interactions which approximate all electromagnetic interactions of strongly interacting particles by assuming the photon to become a mixture of a neutral ρ -meson and an ω -meson, which then participate in strong interactions.

We omit the calculation of the Hamilton operator since the result is an obvious generalization of the previous expression (7.586) for neutral vector bosons:

$$H = \sum_{\mathbf{p}} p^0 \sum_{\lambda=\pm 1,0} \left(a_{\mathbf{p},\lambda}^\dagger a_{\mathbf{p},\lambda} - b_{\mathbf{p},\lambda} b_{\mathbf{p},\lambda}^\dagger \right) = \sum_{\mathbf{p}} p^0 \sum_{s_3=\pm 1,0} \left(a_{\mathbf{p},s_3}^\dagger a_{\mathbf{p},s_3} - b_{\mathbf{p},s_3} b_{\mathbf{p},s_3}^\dagger \right). \quad (7.624)$$

7.8 Spin-3/2 Fields

The Rarita-Schwinger field of massive spin-3/2 particles is expanded just like (7.224) as follows:

$$\psi_\mu(x) = \sum_{\mathbf{p}, S_3} \frac{1}{\sqrt{V p^0 / M}} \left[e^{-ipx} u_\mu(\mathbf{p}, S_3) a_{\mathbf{p}, S_3} + e^{ipx} v_\mu(\mathbf{p}, S_3) b^\dagger(\mathbf{p}, S_3) \right], \quad (7.625)$$

where the spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(\mathbf{p}, S_3)$ are solutions of equations analogous to (4.663):

$$L^{\mu\nu}(p) u_\nu(\mathbf{p}, S_3) = 0, \quad L^{\mu\nu}(-p) v_\nu(\mathbf{p}, S_3) = 0. \quad (7.626)$$

By analogy with the Dirac matrices $(\not{p} - M)$ and $(-\not{p} - M)$ in those equations, the matrices $L^{\mu\nu}(p)$ and $L^{\mu\nu}(-p)$ are the Fourier-transformed differential operators (4.955) with positive mass shell energy $p^0 = \sqrt{\mathbf{p}^2 + M^2}$. The Rarita-Schwinger spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(\mathbf{p}, S_3)$ can be constructed explicitly from those of spin 1/2 and the polarization vectors (7.616) of spin 1 with the help of the Clebsch-Gordan coefficients in Table 4.2:

$$u_\mu(\mathbf{p}, S_3) = \sum_{s_3, s'_3} \langle \tfrac{3}{2}, S_3 | 1, s_3; \tfrac{1}{2}, s'_3 \rangle \epsilon_\mu(\mathbf{p}, s_3) u(\mathbf{p}, s'_3), \quad (7.627)$$

$$v_\mu(\mathbf{p}, S_3) = \sum_{s_3, s'_3} \langle \tfrac{3}{2}, S_3 | 1, s_3; \tfrac{1}{2}, s'_3 \rangle \epsilon_\mu(\mathbf{p}, s_3) v(\mathbf{p}, s'_3). \quad (7.628)$$

The calculation of the propagator

$$S_{\mu\nu}(x, x') = \langle 0 | T \psi_\mu(x) \bar{\psi}_\nu(x') | 0 \rangle \quad (7.629)$$

is now somewhat involved. As in the case of spin-zero, spin-1/2, and massive spin-1 fields, the result can be derived most directly by inverting the matrix $L_{\mu\nu}(p)$. For this we make use of the fact that, for reasons of covariance, $L^{-1}_{\mu\nu}$ may be expanded into the tensors $g_{\mu\nu}, \gamma_\mu \gamma_\nu, \gamma_\mu p_\nu, \gamma_\nu p_\mu, p_\mu p_\nu$ with coefficients of the form $A + B \not{p}$. When

multiplying this expansion by $L^{\nu\lambda}(p)$ and requiring the result to be equal to δ_μ^λ , we find $L^{-1}_{\mu\nu}$ to be equal to the 4×4 spinor matrix

$$L^{-1}_{\mu\nu} = \left\{ \frac{\not{p} + M}{p^2 - M^2} \left[-g_{\mu\nu} + \frac{1}{3}\gamma_\mu\gamma_\nu + \frac{1}{3M}(\gamma_\mu p_\nu - \gamma_\nu p_\mu) + \frac{2}{3} \frac{p_\mu p_\nu}{M} \right] - \frac{1}{6M^2} \frac{w+1}{(2w+1)^2} [(4w+2)\gamma_\mu p_\nu + (w+1)\not{p}\gamma_\mu\gamma_\nu + 2wp_\mu\gamma_\nu - 2wM\gamma_\mu\gamma_\nu] \right\}. \quad (7.630)$$

For simplicity, we have stated this matrix only for the case of a real w . By analogy with (7.289), the propagator is equal to the Fourier transform of $L^{-1}_{\mu\nu}(p)$:

$$S_{\mu\nu}(x, x') = \int \frac{d^4p}{(2\pi)^4} L^{-1}_{\mu\nu}(p) e^{-ip(x-x')}. \quad (7.631)$$

The wave equation has a nontrivial solution where $L^{-1}(p)$ has a singularity. From (7.630) we see that this happens only on the positive- and negative-energy mass shells at

$$p^0 = \pm \sqrt{\mathbf{p}^2 + M^2}. \quad (7.632)$$

By writing the prefactor in (7.630) as

$$\frac{\not{p} + M}{p^2 - M^2} = \frac{1}{\not{p} - M}, \quad (7.633)$$

we see that only solutions of

$$(\not{p} - M)_\alpha^{\alpha'} \psi_{\mu\alpha'}(p) = 0, \quad p^0 = \pm \sqrt{\mathbf{p}^2 + M^2} \quad (7.634)$$

can cause this singularity. These are the spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(-\mathbf{p}, S_3)$, respectively. The residue matrix accompanying the singularity is independent of the parameter c . It must have the property of projecting precisely into the subspace of $\psi_{\mu\alpha}(p)$ in which the wave equation $L^{\mu\nu}(p)\psi_\nu(p) = 0$ is satisfied. Let

$$L^{-1\mu\nu}(p) = \frac{2M}{p^2 - M^2} P^{\mu\nu}(p) + \text{regular piece}. \quad (7.635)$$

After a little algebra, we find

$$P^{\mu\nu}(p) = \frac{\not{p} + M}{2M} \left[-g_{\mu\nu} + \frac{1}{3}\gamma_\mu\gamma_\nu + \frac{1}{3M}(p_\mu\gamma_\nu - p_\nu\gamma_\mu) + \frac{2}{3} \frac{p_\mu p_\nu}{M^2} \right]. \quad (7.636)$$

The residue matrix $P^{\mu\nu}(p)$ is uniquely fixed only for p_0 on the upper and lower mass shells $p_0 = \pm \sqrt{\mathbf{p}^2 + M^2}$. There it has the form $P_\pm^{\mu\nu}(\mathbf{p})$, respectively. The expression (7.636) is a common covariant off-shell extension of these two matrices.

These matrices and their extension $P^{\mu\nu}(p)$ are independent of the parameter c . They are projection matrices, satisfying

$$P^{\mu\nu}g_{\nu\kappa}P^{\kappa\lambda} = P^{\mu\lambda}. \quad (7.637)$$

It is easy to verify that for $p^2 = M^2$, the matrix $P_{\mu\nu}(\mathbf{p})$ satisfies the same equations as the Rarita-Schwinger spinors $u_\mu(\mathbf{p}, S_3)$:

$$(\not{p} - M)P_{\mu\nu}(p) = 0, \quad (7.638)$$

$$P_{\mu\nu}(p)p^\nu = 0, \quad (7.639)$$

$$P_{\mu\nu}(p)\gamma^\nu = 0. \quad (7.640)$$

For this reason, $P_{\mu\nu}(\pm p)$ with $p^0 = \omega_{\mathbf{p}}$ can be expanded as

$$P_{\mu\nu}(p) = \sum_{s_3} u_\mu(\mathbf{p}, S_3) \bar{u}_\nu(\mathbf{p}, S_3), \quad (7.641)$$

$$P_{\mu\nu}(-p) = - \sum_{s_3} v_\mu(\mathbf{p}, S_3) \bar{v}_\nu(\mathbf{p}, S_3). \quad (7.642)$$

The projection matrix is equal to the polarization sums of the spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(\mathbf{p}, S_3)$, except for a minus sign accounting for the fact that $\bar{v}(\mathbf{p}, S_3)v(\mathbf{p}, S_3) = -\bar{u}(\mathbf{p}, S_3)u(\mathbf{p}, S_3)$, just as in the Dirac case [recall the discussion after Eq. (4.705)].

The behavior under discrete symmetry transformations of the creation and annihilation operators of a Rarita-Schwinger field is the same as that of a product of a Dirac operator and a massive vector meson operator, i.e., it is given by a combination of the transformation laws (7.301), (7.322), (7.306) and (7.621), (7.622), (7.623).

7.9 Gravitons

In order to quantize the gravitational field we first have to rewrite the action as squares of first derivative terms. After a partial integration, it reads

$$\mathcal{A} = \frac{1}{8\kappa} \int d^4x \left[\partial_\lambda h^{\mu\nu} \partial^\lambda h_{\mu\nu} - 2\partial^\nu h^{\mu\lambda} \partial_\lambda h_{\mu\nu} + 2\partial_\mu h \partial_\nu h^{\mu\nu} - \partial_\mu h \partial_\nu h \right], \quad (7.643)$$

where $h \equiv h^\mu{}_\mu$. A few further partial integrations bring this to the alternative form

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \frac{1}{2} \int d^4x \pi_{\lambda\mu\nu} \partial_\lambda h_{\mu\nu}, \quad (7.644)$$

where

$$\pi_{\lambda\mu\nu} \equiv \frac{1}{8\kappa} [\partial_\lambda h_{\mu\nu} - \partial_\mu h_{\lambda\nu} + g_{\lambda\nu} \partial_\mu h - g_{\mu\nu} \partial_\lambda h + g_{\mu\nu} \partial^\kappa h_{\kappa\lambda} - g_{\lambda\nu} \partial^\kappa h_{\kappa\mu}] + (\mu \leftrightarrow \nu) \quad (7.645)$$

is defined by

$$\pi_{\lambda\mu\nu}(x) \equiv \frac{\partial \mathcal{L}(x)}{\partial [\partial_\lambda h_{\mu\nu}(x)]}. \quad (7.646)$$

It is antisymmetric in $\lambda\mu$ and symmetric in $\mu\nu$. The components $\pi_{0\mu\nu}$ play the role of the canonical field momenta. Similar to the electromagnetic case, four of the six independent components π_{0ij} vanish, as a consequence of the invariance of the action under gauge transformations (4.380):

$$h_{\mu\nu}(x) \rightarrow h_{\mu\nu}(x) + \partial_\mu \Lambda_\nu(x) + \partial_\nu \Lambda_\mu(x). \quad (7.647)$$

Going over to the field $\phi_{\mu\nu}(x)$ of Eq. (4.403) and the Hilbert gauge (4.403), we expand the field into plane waves e^{-ikx} with $k^0 = |\mathbf{k}|$ and two transverse polarization tensors (4.403):

$$\phi^{\mu\nu}(x) = \frac{1}{\sqrt{2Vp^0}} \sum_{\mathbf{k}} \sum_{\lambda=\pm 2} \left[a_{\mathbf{k},\lambda} \epsilon^{\mu\nu}(\mathbf{k}, \lambda) e^{-ikx} + a_{\mathbf{k},\lambda}^\dagger \epsilon^{\mu\nu*}(\mathbf{k}, \lambda) e^{ikx} \right]. \quad (7.648)$$

The behavior under discrete symmetry transformations of the creation and annihilation operators of a free graviton field is the same as that of a product of two photon operators in Eqs. (7.548)–(7.550).

7.10 Spin-Statistics Theorem

When quantizing Klein-Gordon and Dirac fields we directly used commutation rules for spin 0 and anticommutation rules for spin 1/2. In nonrelativistic quantum field theory this procedure was dictated by experimental facts. It is one of the important successes of relativistic quantum field theory that this connection between spin and statistics is a necessity if one wants to quantize free fields canonically. Let us first look at the real scalar field theory, and consider the field commutator expanded as in (7.11):

$$\begin{aligned} i[\partial^0 \phi(\mathbf{x}, t), \phi(\mathbf{x}', t)] \\ = \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{\sqrt{2Vp^0 2Vp'^0}} \left(e^{i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} p^0 [a_{\mathbf{p}}, a_{\mathbf{p}'}^\dagger] + e^{-i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} (-p^0) [a_{\mathbf{p}}^\dagger, a_{\mathbf{p}'}] \right). \end{aligned} \quad (7.649)$$

Here we have left out terms with vanishing commutators $[a_{\mathbf{p}}, a_{\mathbf{p}'}]$ and $[a_{\mathbf{p}}^\dagger, a_{\mathbf{p}'}^\dagger]$. Inserting the commutators (7.15), we see that both contributions just add up correctly to give a δ -function, as they should, in order to satisfy the canonical field commutation rules (7.2)–(7.4). Suppose now for a moment that the particles obeyed Fermi statistics. Then the symbol $[\partial^0 \phi(\mathbf{x}, t), \phi(\mathbf{x}', t)]$ would stand for anticommutators, and the two contributions would have to be subtracted from each other, giving zero. Thus a real relativistic scalar field cannot be quantized according to the (wrong) Fermi statistics. The situation is similar for a complex scalar field, where we obtain

$$\begin{aligned} i[\partial^0 \phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t)] \\ = \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{\sqrt{2Vp^0 2Vp'^0}} \left(e^{i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} p^0 [a_{\mathbf{p}}, a_{\mathbf{p}'}^\dagger] + e^{-i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} (-p^0) [b_{\mathbf{p}}^\dagger, b_{\mathbf{p}'}] \right). \end{aligned} \quad (7.650)$$

Here all vanishing commutators have been omitted. Again, the two terms add up correctly to give a $\delta^{(3)}$ -function, while the use of anticommutators would have led to a vanishing of the right-hand side.

These observations are related to another remark made earlier when we expanded the free complex field into the solutions of the wave equation, and where we wrote down immediately creation operators $b_{\mathbf{p}}^\dagger$ for the negative energy solutions e^{ipx} as a generalization of $a_{\mathbf{p}}^\dagger$ for the real field. At that place we could, in principle, have had the option of using $b_{\mathbf{p}}$. But looking at (7.650), we realize that this would not have led to canonical commutation rules in either statistics.

Consider now the case of spin-1/2 fields. Here we calculate the anticommutator expanded via (7.223):

$$\begin{aligned} \{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)\} &= \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{\sqrt{Vp^0/M} \sqrt{Vp'^0/M}} \sum_{s_3, s'_3 = \pm 1/2} \\ &\times \left[e^{i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} \{a_{\mathbf{p}, s_3}, a_{\mathbf{p}', s'_3}^\dagger\} u(\mathbf{p}, s_3) u^\dagger(\mathbf{p}', s'_3) \right. \\ &\left. + e^{-i(\mathbf{p}\mathbf{x} - \mathbf{p}'\mathbf{x}')} \{b_{\mathbf{p}, s_3}^\dagger, b_{\mathbf{p}', s'_3}\} v(\mathbf{p}, s_3) v^\dagger(\mathbf{p}', s'_3) \right]. \end{aligned} \quad (7.651)$$

Inserting here the anticommutation rules (7.228) and (7.229),

$$\begin{aligned} \{a_{\mathbf{p}, s_3}, a_{\mathbf{p}', s'_3}^\dagger\} &= \delta_{\mathbf{p}, \mathbf{p}'} \delta_{s_3, s'_3}, \\ \{b_{\mathbf{p}, s_3}^\dagger, b_{\mathbf{p}', s'_3}\} &= \delta_{\mathbf{p}, \mathbf{p}'} \delta_{s_3, s'_3}, \end{aligned} \quad (7.652)$$

and the polarization sums (4.702) and (4.703),

$$\begin{aligned} \sum_{s_3} u(\mathbf{p}, s_3) u^\dagger(\mathbf{p}, s_3) &= \frac{\not{p} + M}{2M} \gamma_0, \\ \sum_{s_3} v(\mathbf{p}, s_3) v^\dagger(\mathbf{p}, s_3) &= \frac{\not{p} - M}{2M} \gamma_0, \end{aligned} \quad (7.653)$$

we find

$$\begin{aligned} \{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)\} &= \sum_{\mathbf{p}} \frac{1}{Vp^0/M} \left(e^{-ip(x-x')} \frac{\not{p} + M}{2M} \gamma_0 + e^{ip(x-x')} \frac{\not{p} - M}{2M} \gamma_0 \right) \\ &= \sum_{\mathbf{p}} \frac{1}{V} e^{i\mathbf{p}(\mathbf{x} - \mathbf{x}')} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (7.654)$$

The function $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$ arises from the $p^0\gamma^0$ -terms after a cancellation of the terms with M and $\mathbf{p}\boldsymbol{\gamma}$ in the numerator.

Let us see what would happen if we use commutators for quantization and thus the wrong particle statistics. Then the $[b_{\mathbf{p}, s_3}^\dagger, b_{\mathbf{p}, s_3}]$ -term would change its sign and fail to produce the desired $\delta^{(3)}$ -function. At first sight, one might want to correct this by using, in the expansion of $\psi(\mathbf{x}, t)$, annihilation operators $d_{\mathbf{p}, s_3}$ rather than creators $b_{\mathbf{p}, s_3}^\dagger$. Then the commutator $[b_{\mathbf{p}, s_3}^\dagger, b_{\mathbf{p}, s_3}]$ would be replaced by $[d_{\mathbf{p}, s_3}, d_{\mathbf{p}, s_3}^\dagger]$, and give indeed a correct sign after all!

However, the problem would then appear at a different place. When calculating the energy in (7.624), we found

$$H = \sum_{\mathbf{p}, s_3} p^0 \left(a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s_3} - b_{\mathbf{p}, s_3} b_{\mathbf{p}, s_3}^\dagger \right), \quad (7.655)$$

independent of statistics. Changing $b_{\mathbf{p}, s_3}$ to $d_{\mathbf{p}, s_3}^\dagger$ in the field expansion, would give instead

$$H = \sum_{\mathbf{p}, s_3} p^0 \left(a_{\mathbf{p}, s_3}^\dagger a_{\mathbf{p}, s_3} - d_{\mathbf{p}, s_3}^\dagger d_{\mathbf{p}, s_3} \right). \quad (7.656)$$

But this is an operator whose eigenvalues can take arbitrarily large negative values on states containing a large number of creation operators $d_{\mathbf{p}, s_3}^\dagger$ applied to the vacuum state $|0\rangle$. Such an energy is unphysical since it would imply the existence of a perpetuum mobile.

The spin-statistics relation can be extended in a straightforward way to vector and tensor fields, and further to fields of any spin s . For each of these fields, quantization with the wrong statistics would imply either a failure of locality or of the positivity of the energy.

We shall sketch the general proof only for the spinor field $\xi(x)$ introduced in Section 4.19. This is expanded into plane waves (4.19) as before, assigning creation operators of antiparticles to the Fourier components of the negative-energy solutions:

$$\xi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}} \left[e^{-ipx} w(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ipx} w^c(\mathbf{p}, s_3) b_{\mathbf{p}, s_3}^\dagger \right]. \quad (7.657)$$

Here

$$w^c(\mathbf{p}, s_3) = c^{\{2s\}} w^*(\mathbf{p}, s_3) = w(\mathbf{p}, s'_3) c_{s'_3, s_3}^{(s)} = w(\mathbf{p}, -s_3) (-1)^{s-s_3} \quad (7.658)$$

are the charge-conjugate spinors. The matrices $c^{\{2s\}}$ have the labels $c_{n_1, n_2; n'_1, n'_2}^{\{2s\}}$. They are the spin-2s equivalent of the matrices $c_{s_3, s'_3}^{(s)}$ reversing the spin direction by a rotation around the y -axis by an angle π [recall the defining equation (4.900)]. The relation between their indices n_1, n_2 and s_3 is the same as in the rest spinors (4.938). These matrices have the property

$$c^{\{2s\}} c^{\{2s\}^\dagger} = 1, \quad \left(c^{\{2s\}} \right)^2 = (-1)^{2s}. \quad (7.659)$$

The commutation or anticommutation relation between two such spinor fields has the form

$$\begin{aligned} i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_{\mp} &= \sum_{\mathbf{p}} \frac{1}{2Vp^0} \left[e^{-ip(x-x')} \sum_{s_3} w(\mathbf{p}, s_3) w^*(\mathbf{p}, s_3) \right. \\ &\quad \left. \pm e^{ip(x-x')} \sum_{s_3} w^c(\mathbf{p}, s_3) w^{c*}(\mathbf{p}, s_3) \right]. \quad (7.660) \end{aligned}$$

Recalling the polarization sum (4.940)

$$P(p) \equiv \sum_{s_3} w^{\{2s\}}(\mathbf{p}, s_3) w^{\{2s\}*}(\mathbf{p}, s_3) = \left(\frac{p\sigma}{M}\right)^{\{2s\}}, \quad (7.661)$$

and noting that the charge-conjugate spinors have the same sum, this becomes

$$i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_{\mp} = \sum_{\mathbf{p}} \frac{1}{2Vp^0} P(p) \left[e^{-ip(x-x')} \mp e^{ip(x-x')} \right]. \quad (7.662)$$

The polarization sum $P(p)$ is a homogenous polynomial in p^0 and $\mathbf{p}$ of degree $2s$. It has therefore the symmetry property $P(-p) = (-1)^{2s} P(p)$. The energy p^0 lies on the mass shell $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$. Replacing all even powers $\omega_{\mathbf{p}}^{2n}$ by $(\mathbf{p}^2 + M^2)^n$, and all odd powers $\omega_{\mathbf{p}}^{2n+1}$ by $\omega_{\mathbf{p}}(\mathbf{p}^2 + M^2)^n$, we obtain for $P(p)$ the following generic dependence on the spatial momenta

$$P(p) = P_0(\mathbf{p}) + \omega_{\mathbf{p}} P_1(\mathbf{p}), \quad (7.663)$$

where $P_0(\mathbf{p})$ and $P_1(\mathbf{p})$ are polynomials of $\mathbf{p}$ with the reflection properties

$$P_0(-\mathbf{p}) = (-1)^{2s} P_0(\mathbf{p}), \quad P_1(-\mathbf{p}) = -(-1)^{2s} P_1(\mathbf{p}). \quad (7.664)$$

Thus we can write

$$\begin{aligned} i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_{\mp} &= \sum_{\mathbf{p}} \frac{1}{2Vp^0} \left\{ [P_0(\mathbf{p}) + p^0 P_1(\mathbf{p})] e^{-ip(x-x')} \mp (-1)^{2s} [P_0(-\mathbf{p}) - p^0 P_1(-\mathbf{p})] e^{ip(x-x')} \right\}. \end{aligned} \quad (7.665)$$

After replacing $\pm \mathbf{p}$ by spatial derivatives $-i\nabla$, the momentum-dependent factors can be taken outside the momentum sums, and we obtain

$$\begin{aligned} i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_{\mp} &= P_0(-i\nabla) \sum_{\mathbf{p}} \frac{1}{2Vp^0} \left[e^{-ip(x-x')} \mp (-1)^{2s} e^{ip(x-x')} \right] \\ &+ P_1(-i\nabla) \sum_{\mathbf{p}} \frac{1}{2V} \left[e^{-ip(x-x')} \pm (-1)^{2s} e^{ip(x-x')} \right]. \end{aligned} \quad (7.666)$$

In the limit of infinite volume, the right-hand side becomes [recall (7.47)]

$$\begin{aligned} &P_0(-i\nabla) \left[G^{(+)}(x-x') \mp (-1)^{2s} G^{(+)}(x-x') \right] \\ &+ P_1(-i\nabla) \left[G^{(+)}(x-x') \pm (-1)^{2s} G^{(+)}(x-x') \right]. \end{aligned} \quad (7.667)$$

At equal times, this reduces to

$$\begin{aligned} &P_0(-i\nabla) [1 \mp (-1)^{2s}] G^{(+)}(\mathbf{x} - \mathbf{x}', 0) \\ &+ P_1(-i\nabla) [1 \pm (-1)^{2s}] \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \quad (7.668)$$

Locality requires that the commutator at spacelike distances vanishes. Since $G^{(+)}(\mathbf{x} - \mathbf{x}', 0) \neq 0$, the prefactor of the first term must be zero, and hence

$$(-1)^{2s} = \begin{cases} 1 & \text{for bosonic commutators,} \\ -1 & \text{for fermionic anticommutators.} \end{cases} \quad (7.669)$$

This proves the spin-statistics relation for spin- s spinor fields $\xi(x)$.

Note that the locality of the free fields always forces particles and antiparticles to have the same mass and spin.

7.11 CPT-Theorem

All of the above local free-field theories have a universal property under the discrete symmetry operations C , P , and T . When being subjected to a product CPT of the three operations, the Lagrangian is invariant. We shall see later in Chapter 27 that this remains true also in the presence of interactions that violate CP - or P -invariance, as long as these are local and Lorentz-invariant.

When introducing local interactions between local fields they will always have the property of being invariant under the operation CPT . This is the content of the so-called CPT-theorem. This property guarantees that the equality of masses and spins of particles and antiparticles remains true also in the presence of interactions. If there is a mass difference in nature, it must be extremely small. Direct measurements of masses of electrons and protons and their antiparticles are too insensitive to detect a difference with present experiments.

7.12 Physical Consequences of Vacuum Fluctuations — Casimir Effect

For each of the above relativistic quantum fields we have found an infinite vacuum energy due to the vacuum fluctuations of the field. For a real scalar field, this energy is [see (7.32)]

$$E_0 = \frac{1}{2} \sum_{\mathbf{k}} k^0 = \frac{1}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}} = \frac{\hbar c}{2} \sum_{\mathbf{k}} \sqrt{\mathbf{k}^2 + c^2 M^2 / \hbar^2}, \quad (7.670)$$

where $\mathbf{k} = \mathbf{p}/\hbar$ are the wave vectors. In many calculations, this energy is irrelevant and can be discarded. There are, however, some important physical phenomena where this energy matters. One of them is the cosmological constant as discussed on p. 479. The other appears in electromagnetism and is observable in the form of van der Waals forces between different dielectric media.

In the present context of free fields in a vacuum, the most relevant phenomenon is the *Casimir effect*. Vacuum fluctuations of electromagnetic fields cause an attraction between two parallel closely spaced silver plates in an otherwise empty space. The basic electromagnetic property of a silver plate is to enforce the vanishing of the

parallel electric field at its surface, due to the high conductivity. Let us study a specific situation and suppose the silver plates to be parallel to the xy -plane, one at $z = 0$ and the other at $z = d$. To have discrete momenta the whole system is imagined to be enclosed in a very large conducting box

$$x \in (-L_x/2, L_x/2), \quad y \in (-L_y/2, L_y/2), \quad z \in (-L_z/2, L_z/2). \quad (7.671)$$

The plates divide the box into a thin slice of volume $L_x L_y d$, and two large pieces of volumes $L_y L_z/2$ below, and $L_x L_y (L_z/2 - d)$ above the slice (see Fig. 7.5). These are three typical resonant cavities of classical electrodynamics. For waves of frequency ω , the Maxwell equations $\partial_\mu F^{\mu\nu} = 0$ read, in natural units with $c = 1$ [recall (4.247)],

$$\nabla \times \mathbf{B} = \dot{\mathbf{E}} = -i\omega \mathbf{E}, \quad \nabla \cdot \mathbf{E} = 0. \quad (7.672)$$

Since the field components parallel to the conducting surface vanish, the first equation implies that the same is true for the magnetic field components normal to the surface. Combining the Maxwell equations (7.672) with the equations

$$\nabla \times \mathbf{E} = i\omega \mathbf{B}, \quad \nabla \cdot \mathbf{B} = 0. \quad (7.673)$$

which follow from the Bianchi identity $\partial_\mu \tilde{F}^{\mu\nu} = 0$ [recall (4.246)], the fields $\mathbf{E}$ and $\mathbf{B}$ are seen to satisfy the *Helmholtz equations*

$$(\nabla^2 + \omega^2) \begin{Bmatrix} \mathbf{E}(\mathbf{x}) \\ \mathbf{B}(\mathbf{x}) \end{Bmatrix} = 0. \quad (7.674)$$

They are solved by the plane-wave ansatz

$$\begin{Bmatrix} \mathbf{E}(\mathbf{x}) \\ \mathbf{B}(\mathbf{x}) \end{Bmatrix} = \begin{Bmatrix} \mathbf{E}_0(\mathbf{x}_\perp) \\ \mathbf{B}_0(\mathbf{x}_\perp) \end{Bmatrix} e^{ik_z z}, \quad (7.675)$$

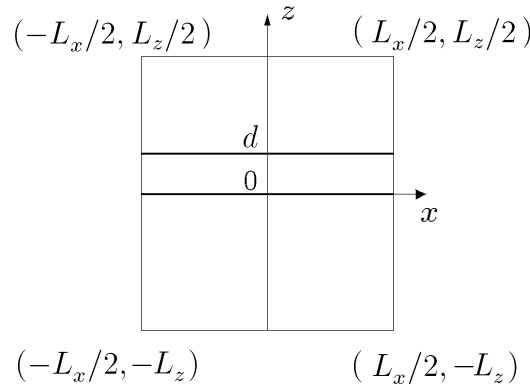


FIGURE 7.5 Geometry of the plates for the calculation of the Casimir effect.

where $\mathbf{x}_\perp \equiv (x, y)$ are the components of $\mathbf{x}$ parallel to the plates. The fields $\mathbf{E}_0(\mathbf{x}_\perp)$, $\mathbf{B}_0(\mathbf{x}_\perp)$ satisfy the differential equation

$$\left(\nabla_\perp^2 + \omega^2 - k_z^2 \right) \begin{Bmatrix} \mathbf{E}_0(\mathbf{x}_\perp) \\ \mathbf{B}_0(\mathbf{x}_\perp) \end{Bmatrix} = 0, \quad (7.676)$$

where $\nabla_\perp$ is the transverse derivative

$$\nabla_\perp \equiv (\nabla_x, \nabla_y, 0). \quad (7.677)$$

We now split the original fields $\mathbf{E}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$ into a component parallel and orthogonal to the unit vector $\hat{z}$ along the z -axis:

$$\begin{aligned} \mathbf{E} &= E_z \hat{z} + \mathbf{E}_\perp \\ \mathbf{B} &= B_z \hat{z} + \mathbf{B}_\perp. \end{aligned} \quad (7.678)$$

Now we observe that the Maxwell equations (7.672) can be solved for $\mathbf{E}_\perp, \mathbf{B}_\perp$ in terms of E_z, B_z :

$$\begin{aligned} \mathbf{B}_\perp &= \frac{1}{\omega^2 + \nabla_\perp^2} [\nabla_\perp \partial_z B_z + i\omega \hat{z} \times \nabla_\perp E_z], \\ \mathbf{E}_\perp &= \frac{1}{\omega^2 + \nabla_\perp^2} [\nabla_\perp \partial_z E_z - i\omega \hat{z} \times \nabla_\perp B_z]. \end{aligned} \quad (7.679)$$

Therefore we only have to find E_z, B_z . Let us see what boundary conditions the field components satisfy at the conducting surfaces, where we certainly have

$$\mathbf{E}_\perp = 0, \quad B_z = 0. \quad (7.680)$$

Due to (7.679), this implies $\nabla_\perp \partial_z E_z|_{\text{surface}} = 0$. The Maxwell equations admit two types of standing-wave solutions with these conditions:

1) Transverse magnetic waves

$$\begin{aligned} B_z &\equiv 0, \\ E_z &= \varphi_E(\mathbf{x}_\perp) \cos \frac{\pi z}{d} n \quad n = 0, 1, 2, \dots \end{aligned} \quad (7.681)$$

2) Transverse electric waves

$$\begin{aligned} E_z &\equiv 0, \\ B_z &= \varphi_B(\mathbf{x}_\perp) \sin \frac{\pi z}{d} n \quad n = 1, 2, 3, \dots, \end{aligned} \quad (7.682)$$

where $\varphi_{E,B}(\mathbf{x}_\perp)$ solve the transverse Helmholtz equation

$$\left(\nabla_\perp^2 + \omega^2 - k_z^2 \right) \varphi_{E,B}(\mathbf{x}_\perp) = 0. \quad (7.683)$$

If the dimensions of the box along x - and y -axes are much larger than d , the quantization of the transverse momenta becomes irrelevant. Any boundary condition

will yield a nearly continuous set of states with the transverse density of states $L_x L_y / (2\pi)^2$. Thus we may record that there are two standing waves for each momentum

$$\mathbf{k} = \left(k_x, k_y, k_z^n = \frac{\pi}{d} n \right), \quad (7.684)$$

except for the case $n = 0$ when there is only one wave, namely the transverse magnetic wave. Using the discrete momenta in the sum (7.670), the energy between the plates may therefore be written as

$$E_d = \frac{\hbar c}{2} L_x L_y \int \frac{dk_x dk_y}{(2\pi)^2} 2 \sum'_{k_z^n} \sqrt{k_x^2 + k_y^2 + k_z^2}. \quad (7.685)$$

We have reinserted the proper fundamental constants $\hbar$ and c . The sum carries a prime which is supposed to record the presence of an extra factor $\frac{1}{2}$ for $n = 0$. In the two semi-infinite regions outside the two plates, also the momentum k_z may be taken as a continuous variable so that there are the additional vacuum energies

$$\begin{aligned} E_{\text{outside}} &= \frac{\hbar c}{2} L_x L_y \frac{L_z}{2} \int \frac{dk_x dk_y dk_z}{(2\pi)^3} 2 \sqrt{k_x^2 + k_y^2 + k_z^2} \\ &+ \frac{\hbar c}{2} L_x L_y \left(\frac{L_z}{2} - d \right) \int \frac{dk_x dk_y dk_z}{(2\pi)^3} 2 \sqrt{k_x^2 + k_y^2 + k_z^2}. \end{aligned} \quad (7.686)$$

Let us now compare this energy with the corresponding expression in the absence of the plates

$$E_0 = \frac{\hbar c}{2} L_x L_y L_z \int \frac{dk_x dk_y dk_z}{(2\pi)^3} 2 \sqrt{k_x^2 + k_y^2 + k_z^2}. \quad (7.687)$$

By subtracting this from $E_d + E_{\text{outside}}$, we find the change of the energy due to the presence of the plates

$$\Delta E = \hbar c L_x L_y \int \frac{dk_x dk_y}{(2\pi)^2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) \sqrt{k_x^2 + k_y^2 + k_z^2}. \quad (7.688)$$

It is caused by the difference in the particle spectra, once with discrete k_z^n between the plates and once with continuous k_z without plates. The evaluation of (7.688) proceeds in two steps. First we integrate over the $k_\perp = (k_x, k_y)$ variables, but enforce the convergence by inserting a *cutoff function* $f(k_\perp^2 + k_z^2)$. It is identical to unity up to some large $\mathbf{k}^2 = k_\perp^2 + k_z^2$, say $\mathbf{k}^2 \leq \Lambda^2$. For $\mathbf{k}^2 \gg \Lambda^2$, the cutoff function decreases rapidly to zero. Later we shall take the limit $\Lambda^2 \rightarrow \infty$. The cutoff function is necessary to perform the mathematical operations. In the physical system a function of this type is provided by the finite thickness and conductivity of the plates. This will have the effect that, for wavelengths much smaller than the thickness, the plates become transparent to the electromagnetic waves. Thus they are no longer able to enforce the boundary conditions which are essential for the discreteness of the spectrum. Since the energy difference comes mainly from long wavelengths, the precise way in which the short wavelengths are cut off is irrelevant.

We then proceed by considering the remaining function of k_z

$$g(k_z) \equiv \int dk_{\perp}^2 \sqrt{k_{\perp}^2 + k_z^2} f(k_{\perp}^2 + k_z^2), \quad (7.689)$$

in terms of which the energy difference is given by

$$\Delta E = \hbar c L_x L_y \frac{1}{4\pi^2} \left(\sum'_{k_z=k_z^n} - \int_0^{\infty} \frac{dk_z d}{\pi} \right) g(k_z). \quad (7.690)$$

To evaluate this expression it is convenient to change the variables from k_z^n to $n = k_z d/\pi$ and from $k_{\perp}^2$ to $\nu^2 = k_{\perp}^2 d^2/\pi^2$, and to introduce the auxiliary function

$$\begin{aligned} G(n) &\equiv \frac{d^3}{\pi^4} g(\pi n/d) = \frac{d^3}{\pi^3} \int_{\pi^2 n^2/d^2}^{\infty} dk^2 k f(k^2) \\ &= \int_{n^2}^{\infty} d\nu^2 \nu f(\pi^2 \nu^2/d^2). \end{aligned} \quad (7.691)$$

Then ΔE can be written as

$$\Delta E = \hbar c L_x L_y \frac{\pi^2}{4d^3} \left[\sum'_{n=0} G(n) - \int_0^{\infty} dn G(n) \right]. \quad (7.692)$$

The difference between a sum and an integral over the function $G(n)$ is given by the well-known *Euler-Maclaurin formula* which reads [see Eq. (7A.20) in Appendix 7A]

$$\begin{aligned} \frac{1}{2}G(0) + G(1) + G(2) + \dots + G(n-1) + \frac{1}{2}G(n) - \int_0^n dn G(n) \\ = \sum_{p=1}^{\infty} \frac{B_{2p}}{(2p)!} [G^{(2p-1)}(n) - G^{(2p-1)}(0)]. \end{aligned} \quad (7.693)$$

Here B_p are the Bernoulli numbers, defined by the Taylor expansion [see (7A.15)]

$$\frac{t}{e^t - 1} = \sum_{p=0}^{\infty} B_p \frac{t^p}{p!}, \quad (7.694)$$

whose lowest values are [see (7A.6)]

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = 0, \quad B_4 = -\frac{1}{30}, \quad B_5 = 0, \quad B_6 = \frac{1}{42}, \quad \dots \quad (7.695)$$

The primed sum in (7.685) is therefore obtained from the expansion

$$\begin{aligned} \sum'_{n=0} G(n) - \int_0^{\infty} dn G(n) &= -\frac{B_2}{2!} [G'(0) - G'(\infty)] \\ &\quad - \frac{B_4}{4!} [G'''(0) - G'''(\infty)] \\ &\quad - \frac{B_6}{6!} [G^{(5)}(0) - G^{(5)}(\infty)] \\ &\quad \vdots \end{aligned} \quad (7.696)$$

Since the cutoff function $f(\mathbf{k}^2)$ vanishes exponentially fast at infinity, the function $G(n)$ and all its derivatives vanish in the limit $n \rightarrow \infty$ (so that the factor $1/2$ at the upper end of the primed sum is irrelevant). For $n = 0$, only one expansion coefficient turns out to be nonzero. To see this, we denote $f(\pi^2 n^2/d^2)$ by $\tilde{f}(n^2)$ and calculate

$$\begin{aligned} G'(0) &= -[2n^2 \tilde{f}(n^2)]_{n=0} = 0, \\ G''(0) &= -[4n \tilde{f}(n^2) + 4n^3 \tilde{f}'(n^2)]_{n=0} = 0, \\ G'''(0) &= -[4 \tilde{f}(n^2) + 18n^2 \tilde{f}'(n^2) + 8n^4 \tilde{f}''(n^2)]_{n=0} = -4, \\ G^{(l)}(0) &= 0, \quad l > 3. \end{aligned} \quad (7.697)$$

The higher derivatives contain an increasing number of derivatives of $\tilde{f}(\nu^2)$. Since $\tilde{f}(\nu^2)$ starts out being unity up to large arguments, all derivatives vanish at $\nu = 0$. Thus we arrive at

$$\sum_{n=0}^{\infty} {}' G(n) - \int_0^{\infty} dn G(n) = 4 \frac{B_4}{4!} = -\frac{1}{180}. \quad (7.698)$$

This yields the energy difference

$$\Delta E = -L_x L_y \hbar c \frac{\pi^2}{720 d^3}. \quad (7.699)$$

There is an *attractive* force between silver plates decreasing with the inverse forth power of the distance:

$$F = -L_x L_y \hbar c \frac{\pi^2}{240 d^4}. \quad (7.700)$$

Between steel plates of an area 1 cm^2 at a distance of $0.5 \text{ } \mu\text{m}$, the force is 0.2 dyne/cm^2 . The existence of this force was verified experimentally [17].

Experiments are often done by bringing a conducting sphere close to a plate. Then the force (7.701) is modified by a factor $2\pi R d/3$ to

$$F = -\frac{2\pi R d}{3} \hbar c \frac{\pi^2}{240 d^4}. \quad (7.701)$$

In dielectric media, a similar calculation renders the important van der Waals forces between two plates of different dielectric constants.²¹

It is also interesting to study the force between an electrically conducting plate and a magnetically conducting plate. The transverse electric modes have the form (7.681), but with n running through the half-integer values $n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$. These values ensure that the electric field is maximal at the second plate so that the transverse magnetic field vanishes. The transverse magnetic modes have the form (7.681)

²¹See H. Kleinert, Phys. Lett. A 136, 253 (1989), and references therein.

with n running through the same half-integer values. The relevant modification of the Euler-MacLaurin formula is

$$\begin{aligned} G(\tfrac{1}{2}) + G(\tfrac{3}{2}) + \dots G(\tfrac{n}{2}) - \int_0^n dx G(x) \\ = \sum_{p=1}^{\infty} \frac{1}{p!} B_p(\omega) \left[G^{(2p-1)}(n) - G^{(2p-1)}(0) \right]. \end{aligned} \quad (7.702)$$

It is a special case of the general formula [see Eq. (7A.25) in Appendix 7A]

$$\begin{aligned} \sum_{n=0}^{m-1} G(a + nh + \omega h) - \int_a^b dx G(x) \\ = \sum_{p=1}^{\infty} \frac{h^{p-1}}{p!} B_p(\omega) \left[G^{(2p-1)}(b) - G^{(2p-1)}(a) \right], \end{aligned} \quad (7.703)$$

where $b = a + mh$. Here $B_p(\omega)$ are the Bernoulli functions defined by the generalization of formula (7.694):

$$\frac{te^{\omega t}}{e^t - 1} = \sum_{p=0}^{\infty} B_p(\omega) \frac{t^p}{p!}. \quad (7.704)$$

They are related to the Bernoulli numbers B_p by

$$B_n(\omega) = \sum_{p=1}^n \binom{n}{p} B_p \omega^{n-p}. \quad (7.705)$$

For instance

$$B_n(\tfrac{1}{2}) = -(1 - 2^{1-n}) B_n, \quad (7.706)$$

so that

$$B_0(\tfrac{1}{2}) = 1, \quad B_1(\tfrac{1}{2}) = 0, \quad B_2(\tfrac{1}{2}) = -\tfrac{1}{12}, \quad B_3(\tfrac{1}{2}) = 0, \quad B_4(\tfrac{1}{2}) = \tfrac{7}{240}, \quad B_5(\tfrac{1}{2}) = 0, \dots \quad (7.707)$$

For $h = 1$ and $\omega = \tfrac{1}{2}$ this is reduced to (7.702).

The right-hand side is a modified version of (7.696):

$$\begin{aligned} \sum_{n=1}^{\infty} ' G(\tfrac{n}{2}) - \int_0^{\infty} dx G(x) &= -\frac{B_2(\tfrac{1}{2})}{2!} [G'(0) - G'(\infty)] \\ &\quad - \frac{B_4(\tfrac{1}{2})}{4!} [G'''(0) - G'''(\infty)] \\ &\quad - \frac{B_6(\tfrac{1}{2})}{6!} [G^{(5)}(0) - G^{(5)}(\infty)] \\ &\quad \vdots \end{aligned} \quad (7.708)$$

and the previous result (7.698) is replaced by

$$\sum_{n=1}^{\infty} ' G(\tfrac{n}{2}) - \int_0^{\infty} dx G(x) = 4 \frac{B_4(\tfrac{1}{2})}{4!}. \quad (7.709)$$

Since $B_4(\frac{1}{2}) = \frac{7}{240} = -\frac{7}{8}B_4$, the energy difference (7.699) is modified by a factor $-7/8$:

$$\Delta E = L_x L_y \hbar c \frac{7}{8} \frac{\pi^2}{720d^3}. \quad (7.710)$$

The force is now *repulsive* and a little weaker than the previous attraction [17].

7.13 Zeta Function Regularization

There exists a more elegant method of evaluating the energy difference (7.688) without using a cutoff function $f(\mathbf{k}^2)$. This method has become popular in recent years in the context of the field theories of critical phenomena near second-order phase transitions. The method will be discussed in detail when calculating the properties of interacting particles in Chapter 11. The Casimir effect presents a good opportunity for a short introduction. We observe that we can rewrite an arbitrary negative power of a positive quantity a as an integral

$$a^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty \frac{d\tau}{\tau} \tau^z e^{-\tau a}. \quad (7.711)$$

This follows by a simple rescaling from the integral representation for the Gamma function²²

$$\Gamma(z) = \int_0^\infty \frac{d\tau}{\tau} \tau^z e^{-\tau}, \quad (7.712)$$

which converges for $\text{Re } z > 0$. Then we rewrite the energy difference (7.688) as

$$\Delta E = \hbar c L_x L_y \int \frac{dk_x dk_y}{(2\pi)^2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) (k_x^2 + k_y^2 + k_z^2)^{-z}, \quad (7.713)$$

and evaluate this exactly for sufficiently large z , where sum and integrals converge. At the end we continue the result analytically to $z = -1/2$.

If we do not worry about the convergence at each intermediate step, this procedure is equivalent to using formula (7.714) for $z = -1/2$

$$\sqrt{a} = \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} e^{-\tau a}, \quad (7.714)$$

and by rewriting the energy difference (7.688) as

$$\Delta E = \hbar c L_x L_y \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} \int \frac{dk_x dk_y}{(2\pi)^2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau(k_x^2 + k_y^2 + k_z^2)}. \quad (7.715)$$

²²I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.310.1.

Being Gaussian, the integrals over k_x, k_y can immediately be done, yielding

$$\Delta E = \hbar c L_x L_y \frac{1}{4\pi\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2}. \quad (7.716)$$

The remaining sum-minus-integral over k_z is evaluated as follows. First we write

$$\left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2} = \frac{1}{2} \left(\sum_{n=-\infty}^\infty - \int_{-\infty}^\infty dn \right) e^{-\tau \pi^2 n^2 / d^2}. \quad (7.717)$$

Then we make use of the Poisson summation formula (1.205):

$$\sum_{m=-\infty}^\infty e^{2\pi i \mu m} = \sum_{n=-\infty}^\infty \delta(\mu - n). \quad (7.718)$$

This allows us to express the sum over n as an integral over n , which is restricted to the original sum with the help of an extra sum over integers m :

$$\frac{1}{2} \sum_{n=-\infty}^\infty e^{-\alpha n^2} = \frac{1}{2} \sum_{m=-\infty}^\infty \int_{-\infty}^\infty dn e^{-\alpha n^2 + 2\pi i n m}. \quad (7.719)$$

The Gaussian integral over n can then be performed after a quadratic completion. It gives

$$\frac{1}{2} \sum_{n=-\infty}^\infty e^{-\alpha n^2} = \frac{1}{2} \sum_{m=-\infty}^\infty \sqrt{\frac{\pi}{\alpha}} e^{-4\pi^2 m^2 / \alpha}. \quad (7.720)$$

The two sides are said to be the *dual transforms* of each other. The left-hand side converges fast for large α , the right-hand side does so for small α . This duality transformation is fundamental to the theoretical description of many phase transitions where the partition functions over fundamental excitations can be brought to different forms by such transformations, one converging fast for low temperatures, the other for high temperatures.²³

Now, subtracting from the sum (7.720) over n the integral over dn removes precisely the $m = 0$ term from the auxiliary sum over m on the right-hand side, so that we find the difference between sum and integral:

$$\frac{1}{2} \left(\sum_{n=-\infty}^\infty - \int_{-\infty}^\infty dn \right) e^{-\alpha n^2} = \sum_{m=1}^\infty \sqrt{\frac{\pi}{\alpha}} e^{-4\pi^2 m^2 / \alpha}. \quad (7.721)$$

The left-hand side appears directly in (7.717), which therefore becomes

$$\left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2} = \frac{d}{\sqrt{\pi\tau}} \sum_{m=1}^\infty e^{-d^2 m^2 / \tau}. \quad (7.722)$$

²³For a comprehensive discussion see the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I, *Superflow and Vortex Lines*, pp. 1–744, World Scientific, Singapore 1989 (<http://www.physik.fu-berlin.de/~kleinert/b1>). See also Vol. II, *Stresses and Defects*, pp. 744–1443, World Scientific, Singapore 1989 (<http://www.physik.fu-berlin.de/~kleinert/b2>).

To obtain the energy difference (7.716), this has to be multiplied by $\tau^{-3/2}$ and integrated over $d\tau/\tau$. In the dually transformed integral, convergence at small τ is automatic. The τ -integral can be done yielding

$$\int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \frac{d}{\sqrt{\pi\tau}} \sum_{m=1}^\infty e^{-d^2 m^2/\tau} = \frac{d}{\sqrt{\pi}} \frac{\Gamma(2)}{d^4} \sum_{m=1}^\infty \frac{1}{m^4}. \quad (7.723)$$

The sum over m involves Riemann's zeta function

$$\zeta(z) \equiv \sum_{m=1}^\infty \frac{1}{m^z}, \quad (7.724)$$

encountered before in calculations of statistical mechanics [see (2.277)]. Here it is equal to [recall (2.317)]

$$\zeta(4) = \frac{8\pi^4}{4!} |B_4| = \frac{8\pi^4}{4!} \frac{1}{30}. \quad (7.725)$$

With this number, the energy difference (7.716) becomes, recalling the values of the Gamma function $\Gamma(2) = 1$ and $\Gamma(-1/2) = -2\sqrt{\pi}$,

$$\begin{aligned} \Delta E &= \hbar c L_x L_y \frac{1}{4\pi\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2} \\ &= \hbar c L_x L_y \frac{\Gamma(2)}{4\pi^{3/2}\Gamma(-\frac{1}{2})d^3} = -L_x L_y \hbar c \frac{\pi^2}{720d^3}. \end{aligned} \quad (7.726)$$

This is the same result as in Eq. (7.699). To be satisfactory, these calculations should all be done for the general expression (7.713), followed by an analytic continuation of the power z to $-1/2$ at the end.

While being formal, with the above justification via analytic continuation, we may be mathematically even more sloppy, and process the τ -integral in the energy difference (7.716) as a shortcut via (7.717) and write

$$\begin{aligned} \int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2} &= \frac{1}{2} \left(\sum_{n=-\infty}^\infty - \int_{-\infty}^\infty dn \right) \int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} e^{-\tau \pi^2 n^2/d^2} \\ &= \Gamma(-\tfrac{3}{2}) \left(\sum'_{n=-\infty}^\infty - \int_0^\infty dn \right) n^3. \end{aligned} \quad (7.727)$$

The divergent sum-minus-integral over n^3 can formally be identified with the zeta function $\sum_{n=1}^\infty n^{-z}$ at the negative argument $z = -3$. With the help of formula (2.314), we find

$$\zeta(-3) = -\frac{B_4}{4} = \frac{1}{120}. \quad (7.728)$$

Inserting this together with $\Gamma(-\frac{3}{2}) = -\frac{2}{3}\Gamma(-\frac{1}{2})$ into (7.727), and this further into (31.15), we obtain

$$\Delta E = -L_x L_y \hbar c \frac{\pi^2}{720d^3}. \quad (7.729)$$

The correctness of this formal approach is ensured by the explicit duality transformation done before.

The formal procedure of evaluating apparently meaningless sum-minus-integrals over powers n^ν with $\nu > -1$, using zeta functions of negative arguments defined by analytic continuation, is known as the *zeta function regularization* method. We shall see later in Eq. (11.127), that by a similar analytic continuation the integral $\int_0^\infty dk k^\alpha$ vanishes for all α . For this reason, the zeta-function regularization applies even to the pure sum, allowing us to replace $\sum_{n=1}^\infty n^\nu$ by $\zeta(\nu)$.

Let us rederive also the repulsive result (7.710) with the help of this regularization method. The energy difference has again the form (7.716), but with the discrete values of k_z^n running through all $\pi n/d$ with half-integer values of $n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$. Thus we must calculate (7.717) with the sum over all half-integer n . This can be done with a slight modification of the Poisson summation formula (1.205):

$$\sum_{m=-\infty}^{\infty} e^{2\pi i \mu m} (-1)^m = \sum_{m=-\infty}^{\infty} e^{2\pi i (\mu - \frac{1}{2})m} = \sum_{n=-\infty}^{\infty} \delta(\mu - n - \frac{1}{2}). \quad (7.730)$$

As a result we obtain a modified version of (7.723):

$$\int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \frac{d}{\sqrt{\pi\tau}} \sum_{m=1}^{\infty} e^{-d^2 m^2/\tau} (-1)^m = \frac{d}{\sqrt{\pi}} \frac{\Gamma(2)}{d^4} \sum_{m=1}^{\infty} \frac{(-1)^m}{m^4}. \quad (7.731)$$

It contains the modified zeta function

$$\bar{\zeta}(x) \equiv \sum_{m=1}^{\infty} \frac{(-1)^m}{m^x}. \quad (7.732)$$

It is now easy to derive the identity

$$\bar{\zeta}(x) \equiv \sum_{m=1}^{\infty} \left[-\frac{1}{m^x} + 2 \frac{1}{(2m)^x} \right] = -(1 - 2^{1-x}) \zeta(x), \quad (7.733)$$

so that

$$\bar{\zeta}(4) \equiv -\left(1 - \frac{1}{8}\right) \zeta(4) = -\frac{7}{8} \zeta(4). \quad (7.734)$$

As in the previous result (7.710), there is again a sign change and a factor 7/8 with respect to the attractive result (7.726) that was obtained there from the Euler-MacLaurin summation formula.

7.14 Dimensional Regularization

The above results can also be obtained without the duality transformation (7.720) by a calculation in an arbitrary dimension D , and continuing everything to the physical dimension $D = 3$ at the end. In D spatial dimensions, the energy difference (7.713) becomes

$$\Delta E = \hbar c V_{D-1} \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) (k_x^2 + k_y^2 + k_z^2)^{-z}, \quad (7.735)$$

where V_{D-1} is the $D - 1$ -dimensional volume of the plates, the dimensional extension of the area $L_x L_y$. After using the integral formula (7.714), we obtain the D -dimensional generalization of (7.715):

$$\Delta E = \hbar c V_{D-1} \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau(k_x^2 + k_y^2 + k_z^2)}. \quad (7.736)$$

Performing now the $D - 1$ Gaussian momentum integrals yields

$$\Delta E = \hbar c V_{D-1} \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} \left(\frac{1}{4\pi\tau} \right)^{\frac{D-1}{2}} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2}. \quad (7.737)$$

After integrating over all τ , this becomes

$$\Delta E = \hbar c V_{D-1} \frac{\Gamma(-\frac{D}{2})}{\Gamma(-\frac{1}{2})} \left(\frac{1}{4\pi} \right)^{\frac{D-1}{2}} \left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) k_z^D. \quad (7.738)$$

Inserting $k_z = k_z^n = \pi n/d$, the last factor is seen to be equal to

$$\left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) k_z^D = \left(\frac{\pi}{d} \right)^D \left(\sum'_n - \int_0^\infty dn \right) n^D. \quad (7.739)$$

We now make use of the heuristic *Veltman integral rule*. This states that in any renormalizable quantum field theory (which a free-field theory trivially is), we may always set the following integrals equal to zero:

$$\int_0^\infty dk k^\alpha = 0. \quad (7.740)$$

The proof of this can be found in the textbook [7] around Eq. (8.33). With this rule we shall rewrite the sum-minus-integral expression in the energy difference (7.738), using a zeta function (7.724) as

$$\left(\sum'_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) k_z^D = \left(\frac{\pi}{d} \right)^D \zeta(-D), \quad (7.741)$$

and the energy difference (7.738) becomes

$$\Delta E = \hbar c V_{D-1} \frac{\Gamma(-\frac{D}{2})}{\Gamma(-\frac{1}{2})} \left(\frac{1}{4\pi} \right)^{\frac{D-1}{2}} \left(\frac{\pi}{d} \right)^D \zeta(-D). \quad (7.742)$$

For $D = 3$ dimensions, this is equal to

$$\Delta E = \hbar c V_2 \frac{\Gamma(-\frac{3}{2})}{\Gamma(-\frac{1}{2})} \left(\frac{1}{4\pi} \right) \left(\frac{\pi}{d} \right)^3 \zeta(-3). \quad (7.743)$$

Inserting $\Gamma(-\frac{3}{2}) = 4\sqrt{\pi}/3$, $\Gamma(-1/2) = -2\sqrt{\pi}$, this becomes

$$\Delta E = -\hbar c V_2 \frac{\pi^2}{6d^3} \zeta(-3). \quad (7.744)$$

The value of $\zeta(-3)$ cannot be calculated from the definition (7.724) since the sum diverges. There exists, however, an integral representation for $\zeta(z)$ which agrees with (7.724) for $z > 1$ where the sum converges, but which can also be evaluated for $z \leq 1$. From this, one can derive the *reflection formula*

$$\Gamma(z/2)\pi^{-z/2}\zeta(z) = \Gamma((1-z)/2)\pi^{-(1-z)/2}\zeta(1-z). \quad (7.745)$$

This allows us to calculate

$$\zeta(-3) = \frac{3}{4\pi^4}\zeta(4) = \frac{1}{120}, \quad (7.746)$$

so that

$$\Delta E = -\hbar c V_2 \frac{\pi^2}{6d^3} \frac{3}{4\pi^4} \zeta(4) = -V_2 \hbar c \frac{\pi^2}{720d^3}, \quad (7.747)$$

in agreement with Eq. (7.729).

Note that this result via dimensional regularization agrees with what was obtained before with the help of the sloppy treatment in Eq. (7.716). The reason for this is the fact that the reflection formula (7.745) is a direct consequence of the duality transformation in Eq. (7.720), which was the basis for the previous treatment.

The derivation of the factor $-7/8$ for the energy between the mixed electric and magnetic conductor plates is more direct in the present approach than before. Here the expression (7.748) becomes

$$\left(\sum_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) k_z^D = \left(\frac{\pi}{d} \right)^D \left(\sum_{n=1/2, 3/2, \dots}^\infty - \int_0^\infty dn \right) n^D, \quad (7.748)$$

and we may express the right-hand side in terms of the *Hurwitz zeta function* defined by²⁴

$$\zeta(x, q) \equiv \sum_{n=0}^\infty \frac{1}{(q+n)^x} \quad (7.749)$$

as

$$\left(\sum_{k_z=k_z^n} - \int_0^\infty \frac{dk_z d}{\pi} \right) k_z^D = \left(\frac{\pi}{d} \right)^D \zeta(-D, 1/2). \quad (7.750)$$

Now we use the property²⁵

$$\zeta(x, q) = (2^x - 1)\zeta(x), \quad (7.751)$$

²⁴I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 9.521

²⁵ibid., Formula 9.535.1

to calculate the right-hand side of (7.750) as

$$\zeta(-3, 1/2) = -\frac{7}{8}\zeta(-3). \quad (7.752)$$

This exhibits immediately the desired factor $-7/8$ with respect to (7.747).

At a finite temperature, the sum over the vacuum energies $2\hbar \sum_{\mathbf{k}} \omega_{\mathbf{k}}/2$ is modified by the Bose occupation factor n_{ω} of Eq. (2.264),

$$n_{\omega_{\mathbf{k}}} = \frac{1}{2} + \frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_B T} - 1} = \frac{1}{2} \coth \frac{\hbar\omega_{\mathbf{k}}}{2k_B T}. \quad (7.753)$$

It becomes $2\hbar \sum_{\mathbf{k}} \omega_{\mathbf{k}} n_{\omega_{\mathbf{k}}}$.

How does this modify the vacuum energy, which in Eq. (7.744) was shown to be equal to

$$\Delta E = -\hbar c V_2 \frac{\pi^2}{6d^3} \zeta(-3)? \quad (7.754)$$

For small T , the sum over n^3 in $\zeta(-3)$ is replaced by a sum over $2n^D k_B T/n$. The subject is discussed in detail in Ref. [17], and the resulting force between a plate and a sphere of radius R is

$$F = \frac{\zeta(3)}{4} \frac{R k_B T}{d^2}. \quad (7.755)$$

This has apparently been observed recently.

7.15 Accelerated Frame and Unruh Temperature

The vacuum oscillations of a field show unusual properties when they are observed from an accelerated frame. Such a frame is obtained by applying to a rest frame an infinitesimal boost $e^{-id\zeta \cdot \mathbf{M}}$, successively after each proper time interval $d\tau$. The rapidity ζ increases as a function of the invariant time τ like $\zeta(\tau) = a\tau/c$, where a is the invariant acceleration. Hence the velocity $v = c \operatorname{arctanh} \zeta$ increases as a function of τ like

$$v(\tau) = c \operatorname{arctan}(a\tau/c) \quad (7.756)$$

If the acceleration points into the z -direction, the space and time coordinates evolve like

$$z(\tau) = (c/a) \cosh(a\tau/c), \quad t(\tau) = (c/a) \sinh(a\tau/c). \quad (7.757)$$

The velocity seen from the initial Minkowski frame increases therefore like

$$dv(t)/dt = a(1 - v^2/c^2)^{3/2}. \quad (7.758)$$

The energy of a particle transforms into

$$p_0(\tau) = \cosh \zeta(\tau) p_0 + \sinh \zeta(\tau) p_3. \quad (7.759)$$

A massless particle has $p_3 = p_0$, where this becomes simply

$$p_0(\tau) = e^{\zeta(\tau)} p_0 = e^{a\tau/c} p_0. \quad (7.760)$$

The temporal oscillations of the wave function of the particle $e^{i\omega\tau}$ with $\omega = cp_0/\hbar$ is observed in an accelerated frame to have a frequency $e^{-\omega(\tau)\tau} = e^{-\omega e^{a\tau/c}\tau}$. As a consequence, a wave of a single momentum p_3 in the rest frame is seen to have an entire spectrum of frequencies. Their distribution can be calculated by a simple Fourier transformation [18]:

$$f(\omega, \Omega) = \int_{-\infty}^{\infty} dt e^{-i\Omega t} e^{-i\omega e^{at/c}t} = \left(i \frac{\omega c}{a}\right)^{-i\Omega c/a} \Gamma\left(i \frac{\Omega c}{a}\right), \quad (7.761)$$

or

$$f(\omega, \Omega) = e^{\pi\Omega c/2a} \Gamma\left(i \frac{\Omega c}{a}\right) e^{-i\Omega c/a \log(\omega c/a)} \frac{c}{a}, \quad (7.762)$$

$$f(\omega, -\Omega) = e^{-\pi\Omega c/2a} \Gamma\left(-i \frac{\Omega c}{a}\right) e^{i\Omega c/a \log(\omega c/a)} \frac{c}{a}. \quad (7.763)$$

We see that the probability to find the frequency Ω in $f(\omega, \Omega)$ is $|f(\omega, \Omega)|^2 = |e^{-\pi\Omega c/2a} \Gamma(-i\Omega c/a) c/a|^2$. Since

$$\Gamma(-ix)\Gamma(ix) = \pi/x \sinh(\pi x), \quad (7.764)$$

we obtain

$$|f(\omega, \Omega)|^2 = \frac{2\pi c}{\Omega a} \frac{1}{e^{2\pi\Omega c/a} - 1} = \frac{2\pi c}{\Omega a} n_{\Omega}. \quad (7.765)$$

The factor n_{Ω} is the thermal Bose-Einstein distribution of the frequencies Ω [recall Eq. (14.199)] at a temperature $T_U = \hbar a/2\pi c k_B$, the so-called *Unruh temperature* [19]. The particles in this heat bath can be detected by suitable particle reactions (for details see Ref. [20]).

Let us describe the situation in terms of the quantum field. For simplicity, we focus attention upon the relevant dimensions z and t and study the field only at the origin $z = 0$, where it has the expansion [compare (7.16)]

$$\phi(0, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\sqrt{c\hbar}}{2\omega_k} \left(e^{-i\omega_k t} a_k + e^{i\omega_k t} a_k^{\dagger} \right), \quad \omega_k \equiv c|k|. \quad (7.766)$$

The creation and annihilation operators satisfy the commutation rules

$$\begin{aligned} [a_k, a_{k'}] &= [a_k^{\dagger}, a_{k'}^{\dagger}] = 0, \\ [a_k, a_{k'}^{\dagger}] &= 2k^0 2\pi \delta(k - k'). \end{aligned} \quad (7.767)$$

They can be recovered from the fields by the Fourier transform [compare (7.16)] :

$$\begin{Bmatrix} a_k \\ a_k^{\dagger} \end{Bmatrix} = 2c\omega_k \int_{-\infty}^{\infty} dt e^{\pm i\omega_k t} \phi(0, t). \quad (7.768)$$

The accelerated field has the form

$$\phi_a(z, t) = \int \frac{dk}{2\pi} \frac{1}{2\omega_k} \left(e^{-ie^{at/c}\omega_k t} a_k + e^{i\omega_k t} a_k^\dagger \right). \quad (7.769)$$

Inverting the Fourier transformation (7.761), we can expand

$$\phi_a(z, t) = c \int \frac{dK}{2\pi} \left(e^{-iK(ct-z)} A_K + e^{iK(ct-z)} A_K^\dagger \right), \quad (7.770)$$

where

$$A_K = \int \frac{dk}{2\pi}. \quad (7.771)$$

In the following sections we shall study the quantum-statistical properties of this field in a thermal environment of temperature T .

7.16 Photon Propagator in Dirac Quantization Scheme

Let us calculate the propagator of the A_μ -field in the Dirac quantization scheme. We expand the vector field A^μ as in (7.419) and calculate

$$G^{\mu\nu}(x, x') = \langle 0_{\text{phys}} | T A^\mu(x) A^\nu(x') | 0_{\text{phys}} \rangle, \quad (7.772)$$

obtaining for the time-ordered operators between the vacuum states the same terms as in (7.478)–(7.479). The transverse polarization terms contribute, as before, a sum

$$\epsilon^\mu(\mathbf{k}, 1)^* \epsilon^\nu(\mathbf{k}, 1) + \epsilon^\mu(\mathbf{k}, 2)^* \epsilon^\nu(\mathbf{k}, 2). \quad (7.773)$$

However, in contrast to the Gupta-Bleuler case, the creation operators $a_{\mathbf{k},s}^\dagger$ annihilate the physical vacuum to their right, and $a_{\mathbf{k},s}$ do the same thing to their left. Hence there are no contributions proportional to $\epsilon^\mu(\mathbf{k}, \bar{s})^* \epsilon^\nu(\mathbf{k}, s)$ and $\epsilon^\mu(\mathbf{k}, s)^* \epsilon^\nu(\mathbf{k}, \bar{s})$. For the same reason, there are no contributions from (7.479). Thus we obtain, instead of (7.509),

$$\begin{aligned} G^{\mu\nu}(x, x') &= \langle 0_{\text{phys}} | T A^\mu(x) A^\nu(x') | 0_{\text{phys}} \rangle \\ &= \Theta(x_0 - x'_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{-ik(x-x')} \sum_{\lambda=1}^2 \epsilon^\mu(\mathbf{k}, \lambda)^* \epsilon^\nu(\mathbf{k}, \lambda) \\ &+ \Theta(x'_0 - x_0) \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2k^0} e^{ik(x-x')} \sum_{\lambda=1}^2 \epsilon^\mu(\mathbf{k}, \lambda)^* \epsilon^\nu(\mathbf{k}, \lambda). \end{aligned} \quad (7.774)$$

This is the same propagator as the one in Eq. (7.361), which was obtained in the noncovariant quantization scheme where only the physical degrees of freedom of the vector potential became operators. Thus, although the field operators have been quantized with covariant commutation relations (7.386), the selection procedure of the physical states has made the propagator noncovariant.

7.17 Free Green Functions of n Fields

For free fields of spin 0 and $1/2$ quantized in the preceding sections we have shown that the vacuum expectation value of the time-ordered product of two field operators, i.e., the field propagator is equal to the Green function associated with the differential equation obeyed by the field. In the case of the real Klein-Gordon field we had, for example,

$$G(x_1, x_2) = G(x_1 - x_2) \equiv \langle 0 | \hat{T} \phi(x_1) \phi(x_2) | 0 \rangle, \quad (7.775)$$

satisfying

$$(-\partial^2 - M^2)G(x, x_2) = i\delta^{(4)}(x - x_2). \quad (7.776)$$

It is useful to define a generalization of the vacuum expectation values (7.775) to any number n of free fields:

$$G^{(n)}(x_1, x_2, x_3, \dots, x_n) \equiv \langle 0 | \hat{T} \phi(x_1) \dots \phi(x_n) | 0 \rangle. \quad (7.777)$$

This object will be referred to as the free n -point *propagator*, or n -point function. For massive vector fields and other massive fields with spin larger than $1/2$, one must watch out for the discrepancy between propagator and Green function by Schwinger terms. For scalar fields, there is no problem of this kind. For complex scalar fields, the appropriate definition is

$$G^{(n,m)}(x_1, \dots, x_n; x'_1, \dots, x'_m) \equiv \langle 0 | \hat{T} \phi(x_1) \dots \phi(x_n) \phi^\dagger(x'_1) \dots \phi^\dagger(x'_m) | 0 \rangle. \quad (7.778)$$

For free fields, the latter is nonzero only for $n = m$. Corresponding expressions are used for fields of any spin. We shall see later that the set of all free n -point functions plays a crucial role in extracting the information contained in an arbitrary interacting field theory.

The n -point functions (7.778) may be considered as the relativistic generalizations of the set of all nonrelativistic many-particle Schrödinger wave functions. In the local $\mathbf{x}$ -basis, these would consist of all scalar products

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \psi(t) \rangle = \langle 0 | \psi(\mathbf{x}_1, 0) \dots \psi(\mathbf{x}_n, 0) | \psi(t) \rangle. \quad (7.779)$$

Choosing for the wave vectors $|\psi(t)\rangle$ any state in the local n -particle basis

$$|\mathbf{x}'_1, \dots, \mathbf{x}'_n; t\rangle = \psi^\dagger(\mathbf{x}'_1, t) \dots \psi^\dagger(\mathbf{x}'_n, t) | 0 \rangle, \quad (7.780)$$

we arrive at the scalar products

$$\langle 0 | \psi(\mathbf{x}, 0) \dots \psi(\mathbf{x}_n, 0) \psi^\dagger(\mathbf{x}'_1, t) \dots \psi^\dagger(\mathbf{x}'_n, t) | 0 \rangle. \quad (7.781)$$

These, in turn, are a special class of propagators:

$$G^{(n,m)}(\mathbf{x}_1, 0, \mathbf{x}_2, 0, \dots, \mathbf{x}_n, 0; \mathbf{x}'_1, t, \dots, \mathbf{x}'_m, t), \quad (7.782)$$

where only two time arguments appear. When going to relativistic theories, the set of such equal-time objects is no longer invariant under Lorentz transformations. Two events which happen simultaneously in one frame do not do so in another frame. This is why the propagators $G^{(n,m)}(x, \dots, x_n; x'_1, \dots, x'_m)$ require arbitrary spacetime arguments to represent the relativistic generalization of the local wave functions. This argument does not yet justify the time ordering in the relativistic propagators in contrast to the relevance of the causal propagator in the nonrelativistic case. Its advantage will become apparent only later in the development of perturbation theory.

At the present level where we are dealing only with free quantum fields, the n -point functions have a special property. They can all be expanded into a sum of products of the simple propagators. Before we develop the main expansion formula it is useful to recall that normal products were introduced in Subsecs. 7.1.5 and 7.4.2 for Bose and Fermi fields, respectively. They were contrived as a simple trick to eliminate a bothersome infinite energy of the vacuum to the zero-point oscillations of free fields, that helped us to avoid a proper physical discussion. This product is useful in a purely mathematical discussion to evaluate vacuum expectation values of products of any number of field operators.

Given an arbitrary set of n free field operators $\phi_1(x_1) \cdots \phi_n(x_n)$, each of them consists of a creation and an annihilation part:

$$\phi_i(x_i) = \phi_i^c(x_i) + \phi_i^a(x_i). \quad (7.783)$$

Some ϕ_i may be commuting Bose fields, some anticommuting Fermi fields. The normally ordered product or *normal product* of n of these fields was introduced in (7.34) as $:\phi_1(x)\phi(x_2)\dots\phi(x_n):$. From now on we shall prefer a notation that is more parallel to that of the time-ordered product: $\hat{N}(\phi_1(x)\phi(x_2)\dots\phi(x_n))$. For the subsequent discussion, the function symbol $\hat{N}(\dots)$ will be more convenient than the earlier double-dot notation. The normal product is a function of a product of field operators which has the following two properties:

- i) **Linearity:** The normal product is a linear function of all its n arguments, i.e., it satisfies

$$\hat{N}((\alpha\phi_1 + \beta\phi'_1)\phi_2\phi_3\cdots\phi_n) = \alpha\hat{N}(\phi_1\phi_2\phi_3\cdots\phi_n) + \beta\hat{N}(\phi'_1\phi_2\phi_3\cdots\phi_n). \quad (7.784)$$

If every ϕ_i is replaced by $\phi_i^c + \phi_i^a$, it can be expanded into a linear combination of terms which are all pure products of creation and annihilation operators.

- ii) **Normal Reordering:** The normal product reorders all products arising from a complete linear expansion of all fields according to i) in such a way that all annihilators stand to the right of all creators. If the operators ϕ_i describe fermions, the definition requires a factor -1 to be inserted for every transmutation of the order of two operators.

For example, let ϕ_1, ϕ_2, ϕ_3 be scalar fields, then normal ordering produces for two field operators

$$\begin{aligned}\hat{N}(\phi_1^c \phi_2^c) &= \phi_1^c \phi_2^c = \phi_2^c \phi_1^c, \\ \hat{N}(\phi_1^c \phi_2^a) &= \phi_1^c \phi_2^a, \\ \hat{N}(\phi_1^a \phi_2^c) &= \phi_2^c \phi_1^a, \\ \hat{N}(\phi_1^a \phi_2^a) &= \phi_1^a \phi_2^a = \phi_2^a \phi_1^a,\end{aligned}\tag{7.785}$$

and for three field operators

$$\begin{aligned}\hat{N}(\phi_1^c \phi_2^c \phi_3^a) &= \phi_1^c \phi_2^c \phi_3^a = \phi_2^c \phi_1^c \phi_3^a, \\ \hat{N}(\phi_1^c \phi_2^a \phi_3^c) &= \phi_1^c \phi_3^c \phi_2^a = \phi_3^c \phi_1^c \phi_2^a, \\ \hat{N}(\phi_1^a \phi_2^c \phi_3^c) &= \phi_2^c \phi_3^c \phi_1^a = \phi_3^c \phi_2^c \phi_1^a.\end{aligned}\tag{7.786}$$

If the operators ϕ_i are fermions, the effect is

$$\begin{aligned}\hat{N}(\phi_1^c \phi_2^c) &= \phi_1^c \phi_2^c = -\phi_2^c \phi_1^c, \\ \hat{N}(\phi_1^c \phi_2^a) &\equiv \phi_1^c \phi_2^a, \\ \hat{N}(\phi_1^a \phi_2^c) &= -\phi_2^c \phi_1^a, \\ \hat{N}(\phi_1^a \phi_2^a) &= \phi_1^a \phi_2^a = -\phi_2^a \phi_1^a,\end{aligned}\tag{7.787}$$

and

$$\begin{aligned}\hat{N}(\phi_1^c \phi_2^c \phi_3^a) &= \phi_1^c \phi_2^c \phi_3^a = -\phi_2^c \phi_1^c \phi_3^a, \\ \hat{N}(\phi_1^c \phi_2^a \phi_3^c) &= -\phi_1^c \phi_3^c \phi_2^a = \phi_3^c \phi_1^c \phi_2^a, \\ \hat{N}(\phi_1^a \phi_2^c \phi_3^c) &= \phi_2^c \phi_3^c \phi_1^a = -\phi_3^c \phi_2^c \phi_1^a.\end{aligned}\tag{7.788}$$

The normal product is uniquely defined. The remaining order of creation or annihilation parts among themselves is irrelevant, since these commute or anticommute with each other by virtue of the canonical free-field commutation rules. In the following, the fields ϕ may be Bose or Fermi fields and the sign of the Fermi case will be recorded underneath the Bose sign.

The advantage of normal products is that their vacuum expectation values are zero. There is always an annihilator on the right-hand side or a creator on the left-hand side which produces 0 when matched between vacuum states. The method of calculating all n -point functions will consist in expanding all time-ordered products of n field operators completely into normal products. Then only the terms with no operators will survive between vacuum states. This will be the desired value of the n -point function.

Let us see how this works for the simplest case of a time-ordered product of two identical field operators

$$\hat{T}(\phi(x_1)\phi(x_2)) \equiv \Theta(x_1^0 - x_2^0)\phi(x_1)\phi(x_2) \pm \Theta(x_2^0 - x_1^0)\phi(x_2)\phi(x_1).\tag{7.789}$$

The basic expansion formula is

$$\hat{T}(\phi(x_1)\phi(x_2)) = \hat{N}(\phi(x_1)\phi(x_2)) + \langle 0|\hat{T}(\phi(x_1)\phi(x_2))|0\rangle. \quad (7.790)$$

For brevity, we shall denote the propagator of two fields as follows:

$$\langle 0|\hat{T}(\phi(x_1)\phi(x_2))|0\rangle = \overline{\phi(x_1)\phi(x_2)} = G(x_1 - x_2). \quad (7.791)$$

The hook which connects the two fields is referred to as a *contraction* of the fields.

We shall prove the basic expansion formula (7.790) by considering it separately for the creation and annihilation parts ϕ^c and ϕ^a . This will be sufficient since the time-ordered product is linear in each field just as the normal product. Now, in both cases $x_1^0 \gtrless x_2^0$ we have

$$\begin{aligned} \hat{T}(\phi^c(x_1)\phi^c(x_2)) &= \left\{ \begin{array}{c} \phi^c(x_1)\phi^c(x_2) \\ \pm \phi^c(x_2)\phi^c(x_1) \end{array} \right\} \\ &= \phi^c(x_1)\phi^c(x_2) + \langle 0|\left\{ \begin{array}{c} \phi^c(x_1)\phi^c(x_2) \\ \pm \phi^c(x_2)\phi^c(x_1) \end{array} \right\}|0\rangle, \end{aligned} \quad (7.792)$$

which is true since $\phi^c(x_1)\phi^c(x_2)$ commute or anticommute with each other, and annihilate the vacuum state $|0\rangle$. The same equation holds for $\phi^a(x_1)\phi^a(x_2)$. The only nontrivial cases are those with a time-ordered product of $\phi^c(x_1)\phi^a(x_2)$ and $\phi^a(x_1)\phi^c(x_2)$. The first becomes for $x_1^0 \gtrless x_2^0$:

$$\begin{aligned} \hat{T}(\phi^c(x_1)\phi^a(x_2)) &= \left\{ \begin{array}{c} \phi^c(x_1)\phi^a(x_2) \\ \pm \phi^a(x_2)\phi^c(x_1) \end{array} \right\} \\ &= \phi^c(x_1)\phi^a(x_2) + \langle 0|\left\{ \begin{array}{c} \phi^c(x_1)\phi^a(x_2) \\ \pm \phi^a(x_2)\phi^c(x_1) \end{array} \right\}|0\rangle. \end{aligned} \quad (7.793)$$

For $x_1^0 > x_2^0$, this equation is obviously true. For $x_1^0 < x_2^0$, the normal ordering produces an additional term

$$\pm(\phi^a(x_2)\phi^c(x_1) \mp \phi^c(x_1)\phi^a(x_2)) = \pm[\phi^a(x_2), \phi^c(x_1)]_{\mp}. \quad (7.794)$$

As the commutator or anticommutator of free fields is a c -number, they may equally well be evaluated between vacuum states, so that we may replace (7.794) by

$$\pm\langle 0|[\phi^a(x_2), \phi^c(x_1)]_{\mp}|0\rangle. \quad (7.795)$$

Moreover, since ϕ^a annihilates the vacuum, this reduces to

$$\pm\langle 0|\phi^a(x_2), \phi^c(x_1)|0\rangle. \quad (7.796)$$

The oppositely ordered operators $\phi^a(x_1)\phi^c(x_2)$ can be processed by complete analogy.

We shall now generalize this basic result to an arbitrary number of field operators. In order to abbreviate the expressions let us define the concept of a contraction inside a normal product

$$\begin{aligned} \hat{N} \left(\phi_1 \cdots \phi_{i-1} \overbrace{\phi_i \phi_{i+1} \cdots \phi_{j-1} \phi_j \phi_{j+1} \cdots \phi_n} \right) \\ \equiv \eta \overbrace{\phi_i \phi_j} \hat{N} (\phi_1 \cdots \phi_{i-1} \phi_{i+1} \cdots \phi_{j-1} \phi_{j+1} \cdots \phi_n). \end{aligned} \quad (7.797)$$

The phase factor η is equal to 1 for bosons and $(-1)^{j-i-1}$ for fermions accounting for the number of fermion transmutations necessary to reach the final order. A normal product with several contractions is defined by the successive execution of each of them. If only one field is left inside the normal ordering symbol, it is automatically normally ordered so that

$$\hat{N}(\phi) = \phi. \quad (7.798)$$

Similarly, if all fields inside a normal product are contracted, the result is no longer an operator and the symbol $\hat{N}$ may be dropped using linearity and the trivial property

$$\hat{N}(1) \equiv 1. \quad (7.799)$$

The fully contracted normal product will be the relevant one in determining the n -particle propagator. With these preliminaries we are now ready to prove Wick's theorem for the expansion of a time-ordered product in terms of normally ordered products.²⁶

7.17.1 Wick's Theorem

The theorem may be stated as follows. An arbitrary time ordered product of free fields can be expanded into a sum of normal products, one for each different contraction between pairs of operators:

$$\begin{aligned} \hat{T}(\phi_1 \cdots \phi_n) &= \hat{N}(\phi_1 \cdots \phi_n) \quad (\text{no contraction}) \\ &+ \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4} \cdots \phi_n) + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4} \cdots \phi_n) + \dots + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4} \cdots \phi_n) \\ &+ \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4} \cdots \phi_n) + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_4} \cdots \phi_n) + \dots \quad (\text{one contraction}) \\ &+ \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4} \overbrace{\phi_5} \cdots \phi_n) + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4 \phi_5} \cdots \phi_n) + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4 \phi_5} \cdots \phi_n) \\ &+ \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4 \phi_5} \cdots \phi_n) + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_4 \phi_3 \phi_5} \cdots \phi_n) \\ &\quad + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_4 \phi_5 \phi_3} \cdots \phi_n) + \dots \quad (\text{two contractions}) \\ &+ \dots + \hat{N}(\overbrace{\phi_1 \phi_2 \phi_3 \phi_4 \phi_5 \phi_6} \cdots \phi_n) \cdots \phi_{n-1} \phi_n). \quad (\text{remaining contractions}) \end{aligned} \quad (7.800)$$

²⁶G.C. Wick, Phys. Rev. 80, 268 (1950); F. Dyson, Phys. Rev. 82, 428 (1951).

In this particular expression we have assumed n to be even so that it is possible to contract all operators. Otherwise each term in the last row would have contained one uncontracted field. In either case the expansion on the right-hand side will be abbreviated as

$$\sum_{\text{all pair contractions}} \hat{N}(\phi_1 \cdots \phi_n), \quad (7.801)$$

i.e., we shall state Wick's theorem in the form

$$\hat{T}(\phi_1 \cdots \phi_n) = \sum_{\text{all pair contractions}} \hat{N}(\phi_1 \cdots \phi_n). \quad (7.802)$$

Using Wick's theorem, it is a trivial matter to calculate an arbitrary n -point function of free fields. Since the vacuum expectation values of all normal products are zero except for the fully contracted ones, we may immediately write for an even number of real fields:

$$\begin{aligned} G^{(n)}(x_1 \cdots x_n) &= \langle 0 | \hat{T}(\phi(x_1) \cdots \phi(x_n)) | 0 \rangle \\ &= \sum_{\text{all full pair contractions}} \hat{N}(\phi(x_1) \cdots \phi(x_n)). \end{aligned} \quad (7.803)$$

A simple combinatorical analysis shows that the right-hand side consists of

$$n!/(n/2)!2^{n/2} = 1 \cdot 3 \cdot 5 \cdots (n-1) \equiv (n-1)!!$$

pair terms.

In the case of complex fields, $G^{(n,m)}$ can only be nonzero for $n = m$ and all contractions $\dot{\phi}\dot{\phi}$ and $\dot{\phi}^\dagger\dot{\phi}^\dagger$ vanish. Thus there are altogether $n!$ different contractions.

The proof of (7.802) goes by induction: For $n = 2$ the theorem was proved in Eq. (7.790). Let it be true for a product of n fields $\phi_1 \cdots \phi_n$, and allow for an additional field ϕ . We may assume that it is earlier in time than the other fields $\phi_1, \dots, \phi_n$. For if it were not, we could always choose the earliest of the n fields, move it completely to the right in the time ordered product, with a well-defined phase factor due to Fermi permutations, and proceed. Once the rightmost field is the earliest, it may be removed trivially from the time ordered product. The resulting product can be expanded according to the Wick's theorem for a product of n field operators as

$$\hat{T}(\phi_1 \cdots \phi_n \phi) = \hat{T}(\phi_1 \cdots \phi_n) \phi = \sum_{\text{all pair contractions}} \hat{N}(\phi_1 \cdots \phi_n) \phi. \quad (7.804)$$

We now incorporate the extra field ϕ on the right-hand side into each of the normal products in the expansion. When doing so we obtain, from each term, precisely the contractions required by Wick's theorem for $n+1$ field operators. The crucial formula which yields these is

$$\begin{aligned} \hat{N}(\phi_1 \cdots \phi_n) \phi &= \hat{N}(\phi_1 \cdots \phi_n \phi) + \hat{N}(\overbrace{\phi_1 \phi_2 \cdots \phi_n} \phi) + \hat{N}(\phi_1 \overbrace{\phi_2 \cdots \phi_n} \phi) \\ &+ \hat{N}(\phi_1 \cdots \overbrace{\phi_{n-1} \phi_n} \phi) + \hat{N}(\phi_1 \cdots \overbrace{\phi_n} \phi), \end{aligned} \quad (7.805)$$

which is valid as long as ϕ is earlier than the others. This formula is proved by splitting ϕ into creation and annihilation parts and considering each part separately, which is allowed because of the linearity of the normal products. For $\phi = \phi^a$, the formula is trivially true since all contractions vanish. Indeed, for a field ϕ^a with an earlier time argument than that of all others, we find:

$$\overline{\phi_i \phi^a} \equiv \langle 0 | \hat{T}(\phi(x_i) \phi^a(x)) | 0 \rangle = \langle 0 | \phi(x_i) \phi^a(x) | 0 \rangle \equiv 0. \quad (7.806)$$

For $\phi = \phi^c$, let us for a moment assume that all other ϕ_i 's are annihilating parts ϕ_i^a . If one or more creation parts ϕ_i^c are present, they will appear as left-hand factors in each normally ordered term of (7.805), and participate only as spectators in all further operations. Thus we shall prove that

$$\hat{N}(\phi_1^a \cdots \phi_n^a) \phi^c = \hat{N}(\phi_1^a \cdots \phi_n^a \phi^c) + \hat{N}(\overline{\phi_1^a \cdots \phi_n^a} \phi^c) + \dots + \hat{N}(\phi_1^a \cdots \overline{\phi_n^a} \phi^c), \quad (7.807)$$

for any creation part of a field ϕ^c that lies earlier than the annihilation parts ϕ_i^a 's. The proof proceeds by induction.

To start, we show that (7.807) is true for $n = 2$:

$$\hat{N}(\phi^a) \phi^c = \hat{N}(\phi^a \phi^c) + \hat{N}(\overline{\phi^a} \phi^c). \quad (7.808)$$

Using (7.798), the left-hand side is equal to $\phi^a \phi^c$, which can be rewritten as

$$\phi^a \phi^c = \pm \phi^c \phi^a [\phi^a, \phi^c]_{\mp}. \quad (7.809)$$

Since the commutator or anticommutator is a c -number, it can be replaced as in (7.795) by its vacuum expectation value, and thus by a contraction (7.806):

$$[\phi^a, \phi^c]_{\mp} = \langle 0 | [\phi^a, \phi^c]_{\mp} | 0 \rangle = \overline{\phi^a} \phi^c. \quad (7.810)$$

Rewriting $\pm \phi^c \phi^a$ as $\hat{N}(\phi^a \phi^c)$ and trivially as $\dot{\phi}^a \dot{\phi}^c$, we see that (7.808) is true.

Now suppose (7.807) to be true for n factors and consider one more annihilation field ϕ_0^a inside a normal product. This field can immediately be taken outside:

$$\hat{N}(\phi_0^a \phi_1^a \cdots \phi_n^a) \phi^c = \phi_0^a \hat{N}(\phi_1^a \cdots \phi_n^a) \phi^c. \quad (7.811)$$

The remainder can be expanded via (7.807):

$$\begin{aligned} \hat{N}(\phi_0^a \phi_1^a \phi_2^a \cdots \phi_n^a) \phi^c &= \phi_0^a [N(\phi_1^a \phi_2^a \cdots \phi_n^a \phi^c) + \hat{N}(\overline{\phi_1^a \phi_2^a \cdots \phi_n^a} \phi^c) \\ &+ \hat{N}(\overline{\phi_1^a \phi_2^a \cdots \phi_n^a} \phi^c) + \dots + \hat{N}(\phi_1^a \phi_2^a \cdots \overline{\phi_n^a} \phi^c)]. \end{aligned} \quad (7.812)$$

The additional ϕ_0^a can now be taken *into* all terms where the creation operator ϕ^c appears in a contraction:

$$\begin{aligned} \hat{N}(\phi_0^a \phi_1^a \phi_2^a \cdots \phi_n^a) \phi^c &= \phi_0^a + N(\phi_0^a \phi_1^a \phi_2^a \cdots \phi_n^a \phi^c) + \hat{N}(\phi_0^a \overline{\phi_1^a \phi_2^a \cdots \phi_n^a} \phi^c) \\ &+ \hat{N}(\phi_0^a \phi_1^a \overline{\phi_2^a \cdots \phi_n^a} \phi^c) + \dots + \hat{N}(\phi_1^a \phi_2^a \cdots \overline{\phi_n^a} \phi^c). \end{aligned} \quad (7.813)$$

Only in the first term work is needed to reorder the uncontracted creation operator. Writing out the normal product explicitly, this term reads

$$\eta \phi_0^a \phi_1^c \phi_1^a \cdots \phi_n^a, \quad (7.814)$$

where η denotes the number of fermion transmutations necessary to bring ϕ^c from the right-hand side to its normal position. This product can now be rewritten in normal form by using one additional commutator or anticommutator:

$$\pm \eta \phi^c \phi_0^a \phi_1^a \cdots \phi_n^a + \eta [\phi_0^a, \phi^c]_{\mp} \phi_1^a \cdots \phi_n^a. \quad (7.815)$$

But the commutator or anticommutator is again a c -number, and since ϕ^c is earlier than ϕ_0^a , it is equal to the contraction $\overline{\phi_0^a \phi^c}$. The two terms in (7.815) can therefore be rewritten as normal products

$$\hat{N}(\phi_0^a \cdots \phi_n^a \phi^c) + \hat{N}(\overline{\phi_0^a \phi^c} \phi_1^a \cdots \phi_n^a). \quad (7.816)$$

In both terms we have brought the field ϕ^c back to its original position, thereby canceling the sign factors η and $\pm \eta$ in (7.815). These two are just the missing terms in (7.812) to verify the expansion (7.807) for $n+1$ operators, and thus Wick's theorem (7.802).

Examples are

$$T(\phi_1 \phi_2 \phi_3) = \hat{N}(\phi_1 \phi_2 \phi_3) + \overline{\phi_1 \phi_2} N(\phi_3) \pm \overline{\phi_1 \phi_3} N(\phi_2) + \overline{\phi_2 \phi_3} N(\phi_1), \quad (7.817)$$

and

$$\begin{aligned} \hat{T}(\phi_1 \phi_2 \phi_3 \phi_4) &= \hat{N}(\phi_1 \phi_2 \phi_3 \phi_4) \\ &+ \overline{\phi_1 \phi_2} N(\phi_3 \phi_4) \pm \overline{\phi_1 \phi_3} N(\phi_2 \phi_4) + \overline{\phi_1 \phi_4} N(\phi_2 \phi_3) \\ &+ \overline{\phi_2 \phi_3} N(\phi_1 \phi_4) \pm \overline{\phi_2 \phi_4} N(\phi_1 \phi_3) + \overline{\phi_3 \phi_4} N(\phi_1 \phi_2) \\ &= \overline{\phi_1 \phi_2} \overline{\phi_3 \phi_4} \pm \overline{\phi_1 \phi_3} \overline{\phi_2 \phi_4} + \overline{\phi_1 \phi_4} \overline{\phi_2 \phi_3}. \end{aligned} \quad (7.818)$$

Each expansion contains $(n-1)!!$ fully contracted terms.

There is a useful lemma to Wick's theorem which helps in evaluating vacuum expectation values of ordinary products of field operators rather than time-ordered ones. An ordinary product can be expanded in a sum of normal products with all possible pair contractions just as in (7.801), except that contractions stand for commutators of the creation and annihilation parts of the fields, which are c -numbers:

$$\overline{\phi(x_1) \phi(x_2)} \equiv [\phi^a(x_1), \phi^c(x_2)]. \quad (7.819)$$

The proof proceeds by induction in the same way as before, except that one does not have to make the assumption of the additional field ϕ in the induction being the earliest of all field operators. For the calculation of scattering amplitudes we shall need both expansions.

7.18 Functional Form of Wick's Theorem

Although Wick's rule for expanding the time ordered product of n fields in terms of normal products is quite transparent, it is somewhat cumbersome to state them explicitly for any n , as we can see in formula (7.801). It would be useful to find an algorithm which specifies the expansion compactly in mathematical terms. This would greatly simplify further manipulations of operator products. Such an algorithm can easily be found. Let $\delta/\delta\phi(x)$ denote the functional differentiations for functions of space and time, i.e.,

$$\frac{\delta\phi(x)}{\delta\phi(x')} = \delta^{(4)}(x - x'). \quad (7.820)$$

Then we see immediately that the basic formula (7.790) can be rewritten as

$$\hat{T}(\phi(x_1)\phi(x_2)) = \left(1 \pm \frac{1}{2} \int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta\phi(y_2)}\right) \hat{N}(\phi(x_1)\phi(x_2)), \quad (7.821)$$

where functional differentiation treats field variables as c -numbers. The differentiation produces the single possible contraction which by (7.791) is equal to the free propagator $G(x_1, x_2)$. For three operators, the Wick expansion

$$\begin{aligned} \hat{T}(\phi(x_1)\phi(x_2)\phi(x_3)) &= \hat{N}(\phi(x_1)\phi(x_2)\phi(x_3)) + \hat{N}(\dot{\phi}(x_1)\dot{\phi}(x_2)\phi(x_3)) \\ &+ \hat{N}(\dot{\phi}(x_1)\phi(x_2)\dot{\phi}(x_3)) + \hat{N}(\phi(x_1)\dot{\phi}(x_2)\dot{\phi}(x_3)) \end{aligned} \quad (7.822)$$

can once more be obtained via the same operation

$$\left(1 \pm \frac{1}{2} \int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta\phi(y_2)}\right) \hat{N}(\phi(x_1)\phi(x_2)\phi(x_3)). \quad (7.823)$$

If we want to recover the correct signs for fermions, we have to imagine the field variables $\phi(x)$ to be anticommuting objects satisfying $\phi(x)\phi(y) = -\phi(y)\phi(x)$, which results in the antisymmetry $G(x_1, x_2) = -G(x_2, x_1)$.

A time-ordered product of four field operators has a Wick expansion

$$\begin{aligned} T(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) &= \hat{N}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \\ &+ \sum_{\text{onepaircontractions}} \hat{N}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \\ &+ \sum_{\text{twopaircontractions}} \hat{N}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)). \end{aligned} \quad (7.824)$$

Here we can obtain the same result by applying the functional differentiation

$$\left\{1 \pm \frac{1}{2} \int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta\phi(y_2)} + \frac{1}{8} \left(\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta\phi(y_2)} \right)^2 \right\}. \quad (7.825)$$

This looks like the first three pieces of a Taylor expansion of the exponential

$$\exp \left\{ \pm \frac{1}{2} \int d^4 y_1 d^4 y_2 \frac{\delta}{\delta \phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta \phi(y_2)} \right\}.$$

Indeed, we shall now prove that the general Wick expansion is given by the functional formula

$$\hat{T}(\phi(x_1) \cdots \phi(x_n)) = e^{\pm \frac{1}{2} \int d^4 y_1 \int d^4 y_2 \frac{\delta}{\delta \phi(y_1)} G(y_1, y_2) \frac{\delta}{\delta \phi(y_2)}} \hat{N}(\phi(x_1) \cdots \phi(x_n)). \quad (7.826)$$

To prepare the tools for deriving this result we introduce the following generating functionals of ordinary, time-ordered, and normal-ordered operator products, respectively:

$$\begin{aligned} O[j] &\equiv e^{i \int d^4 x j(x) \phi(x)}, \\ T[j] &\equiv \hat{T} e^{i \int d^4 x j(x) \phi(x)}, \\ N[j] &\equiv \hat{N} e^{i \int d^4 x j(x) \phi(x)}. \end{aligned} \quad (7.827)$$

Here $j(x)$ is an arbitrary c -number local source term, usually referred to as an *external current*. For Fermi fields $\phi(x)$, the currents have to be anticommuting Grassmann variables which also anticommute with the fields. Under complex conjugation, products of Grassmann variables interchange their order. The product $j(x)\phi(x)$ has therefore the complex-conjugation property

$$[j(x)\phi(x)]^* = -\phi(x)j(x). \quad (7.828)$$

The expressions (7.827) are operators. They have the obvious property that their n th functional derivatives with respect to $j(x)$, evaluated at $j(x) \equiv 0$, give the corresponding operator products of n fields:

$$\phi(x_1) \cdots \phi(x_n) = (-i)^n \frac{\delta}{\delta j(x_1)} \cdots \frac{\delta}{\delta j(x_n)} O[j] \Big|_{j(x) \equiv 0}, \quad (7.829)$$

$$\hat{T}(\phi(x_1) \cdots \phi(x_n)) = (-i)^n \frac{\delta}{\delta j(x_1)} \cdots \frac{\delta}{\delta j(x_n)} T[j] \Big|_{j(x) \equiv 0}, \quad (7.830)$$

$$\hat{N}(\phi(x_1) \cdots \phi(x_n)) = (-i)^n \frac{\delta}{\delta j(x_1)} \cdots \frac{\delta}{\delta j(x_n)} N[j] \Big|_{j(x) \equiv 0}. \quad (7.831)$$

We can now easily prove Wick's lemma for ordinary products of field operators. We simply separate the field in the generating functional $O[j]$ into creation and annihilation parts:

$$O[j] \equiv e^{i \int d^4 x j(x) [\phi^a(x) + \phi^c(x)]}, \quad (7.832)$$

and apply the Baker-Hausdorff formula (4.74) to this expression, with $A \equiv i \int d^4x j(x) \phi^a(x)$ and $B \equiv i \int d^4x j(x) \phi(x)^c$. Because of the anticommutativity of $\phi(x)$ and $j(x)$ for fermions, the commutator $[A, B]$ is

$$[A, B] = - \int d^4x_1 \int d^4x_2 [\phi^a(x_1), \phi^c(x_2)]_{\mp} j(x_1) j(x_2), \quad (7.833)$$

which is a c -number. Thus the expansion on the right-hand side of (4.74) terminates, and we can use the formula as

$$e^{A+B} = e^{-\frac{1}{2}[A,B]} e^A e^B. \quad (7.834)$$

This yields the simple result

$$\begin{aligned} O[j] = \exp \left\{ \frac{1}{2} \int d^4x_1 \int d^4x_2 [\phi^a(x_1), \phi^c(x_2)]_{\mp} j(x_1) j(x_2) \right\} \\ \times e^{i \int d^4x j(x) \phi^c(x)} e^{i \int d^4x j(x) \phi^a(x)}. \end{aligned} \quad (7.835)$$

The operator on the right-hand side of the curly bracket is recognized to be precisely the generating functional of the normal products:

$$N[j] = e^{i \int d^4x j(x) \phi^c(x)} e^{i \int d^4x j(x) \phi^a(x)}. \quad (7.836)$$

Now we observe that the currents $j(x)$ in front of this operator are equivalent to a functional differentiation with respect to the fields, $j(x) \hat{=} -i\delta/\delta\phi(x)$. Wick's lemma can therefore be rewritten in the following concise functional form

$$O[j] = \exp \left\{ \mp \frac{1}{2} \int d^4x_1 \int d^4x_2 [\phi^a(x_1), \phi^c(x_2)]_{\mp} \frac{\delta}{\delta\phi(x_1)} \frac{\delta}{\delta\phi(x_2)} \right\} N[j].$$

The $\pm$ -sign appears when commuting or anticommuting $\delta/\delta\phi(x)$ with $j(x)$.

A Taylor expansion of the exponential prefactor renders, via the functional derivatives, precisely all pair contractions required by Wick's lemma, where a contraction represents a commutator or anticommutator of the fields.

From the earlier proof in Section (7.17.1) it is now clear that exactly the same set of pair contractions appears in the Wick expansion of the time-ordered products of field operators, except that the pair contractions become free-field propagators

$$G(x_1, x_2) \equiv \langle 0 | T(\phi(x_1) \phi(x_2)) | 0 \rangle. \quad (7.837)$$

Thus we may immediately conclude that Wick's theorem has the functional form

$$T[j] = \exp \left\{ \pm \frac{1}{2} \int d^4x_1 \int d^4x_2 G(x_1, x_2) \frac{\delta}{\delta\phi(x_1)} \frac{\delta}{\delta\phi(x_2)} \right\} N[j], \quad (7.838)$$

which becomes, after reexpressing the functional derivatives in terms of the currents,

$$T[j] = e^{-\frac{1}{2} \int d^4y_1 d^4y_2 j(y_1) G(y_1, y_2) j(y_2)} \hat{N}[j]. \quad (7.839)$$

Expanding both sides in powers of $j(x)$, a comparison of the coefficients yields Wick's expansion for products of any number of time-ordered operators.

The functional $T[j]$ has the important property that its vacuum expectation value

$$Z[j] \equiv \langle 0|T[j]|0\rangle \quad (7.840)$$

collects all informations on n -point functions. Indeed, forming the n th functional derivative as in (7.830) we see that

$$G^{(n)}(x_1, \dots, x_n) = (-i)^n \frac{\delta}{\delta j(x_1)} \cdots \frac{\delta}{\delta j(x_n)} Z[j]. \quad (7.841)$$

For this reason, the vacuum expectation value $Z[j]$ is called the *generating functional* of all n -point functions. We can take advantage of Wick's expansion formula and write down a compact formula for all n -point functions of free fields. We only have to observe that the generating functional of normal products $\hat{N}[j]$ has a trivial vacuum expectation value

$$\langle 0|\hat{N}[j]|0\rangle \equiv 1. \quad (7.842)$$

Then (7.839) leads directly to the simple expression

$$Z[j] = e^{-\frac{1}{2} \int d^4 y_1 d^4 y_2 j(y_1) G(y_1, y_2) j(y_2)}. \quad (7.843)$$

Expanding the right-hand side in powers of $j(x)$, each term consists of a sum of combinations of propagators $G(x_i, x_{i+1})$. These are precisely the fully pair contracted terms appearing in the Wick expansions (7.803) for the n -point functions.

There exists another way of proving Eq. (7.843), by making use of the equation of motion for the field $\phi(x)$. For simplicity, we shall consider a Klein-Gordon field satisfying the equation of motion

$$(-\partial^2 - M^2)\phi(x) = 0. \quad (7.844)$$

This equation can be applied to the first functional derivative of $Z[j]$:

$$\frac{\delta Z[j]}{\delta j(x)} = \langle 0|T\phi(x)e^{i \int d^4 y j(y)\phi(y)}|0\rangle, \quad (7.845)$$

to find the differential equation

$$(-\partial^2 - M^2)\frac{\delta Z[j]}{\delta j(x)} = -ij(x)Z[j]. \quad (7.846)$$

The correctness of this equation is verified by integrating it functionally with the initial condition

$$Z[0] = 1, \quad (7.847)$$

and by recovering the known equation (7.843) with $G(x, y) = i/(-\partial^2 - M^2)$. A direct proof of the differential equation (7.846) proceeds by expanding both sides in

a Taylor series in $j(x)$ and processing every expansion term as in (7.43)–(7.45). If we were able to pass $(-\partial^2 - m^2)$ through the time-ordering operation, we would obtain zero. During the passage, however, ∂_0^2 encounters the Heaviside function $\Theta(x_0 - x'_0)$ of the time ordering which generates additional terms. These are collected by the right-hand side of (7.846). The n th power expansion term of $Z[j]$ contributes on the left-hand side a term $nT\phi(x)[\int dz j(z)\phi(z)]^{n-1}/n!$. Applying $(-\partial^2 - m^2)$ and using the steps (7.43)–(7.45), we obtain n times a canonical commutator between $\dot{\phi}(x)$ and $\phi(z)$ which can be written as $-j(x)T[\int dz j(z)\phi(z)]^{n-2}/(n-2)!$. Summing these up gives $-jZ[j]$. These properties will find extensive use in Chapter 13.

The formulas can be generalized to complex fields by using the generating functionals

$$\begin{aligned} O[j, j^\dagger] &= e^{i \int d^4x [j^\dagger(x)\phi(x) + j(x)\phi^\dagger(x)]}, \\ T[j, j^\dagger] &= \hat{T} e^{i \int d^4x [j^\dagger(x)\phi(x) + j(x)\phi^\dagger(x)]}, \\ N[j, j^\dagger] &= \hat{N} e^{i \int d^4x [j^\dagger(x)\phi(x) + j(x)\phi^\dagger(x)]}. \end{aligned} \quad (7.848)$$

Note that for fermions, the interaction $j^\dagger(x)\phi(x)$ is odd under complex conjugation, just as for real anticommuting fields in (7.827).

Now the propagators of n fields ϕ and m fields $\phi^\dagger$ are obtained from the expectation value

$$Z[j, j^\dagger] = \langle 0 | \hat{T}[j, j^\dagger] | 0 \rangle \quad (7.849)$$

as the functional derivatives

$$\begin{aligned} G^{(n,m)}(x_1, \dots, x_n; y_1 \dots y_m) = \\ (-i)^{m+n} \frac{\delta}{\delta j^\dagger(x_1)} \dots \frac{\delta}{\delta j^\dagger(x_n)} \frac{\delta}{\delta j(y_1)} \dots \frac{\delta}{\delta j(y_m)} Z[j, j^\dagger] \Big|_{j(x) \equiv 0}. \end{aligned} \quad (7.850)$$

The explicit form of the generating functional $Z[j, j^\dagger]$ is

$$Z[j, j^\dagger] = e^{-\int d^4x d^4y j^\dagger(x) G(x, y) j(y)}. \quad (7.851)$$

The latter form is valid for fermions if one uses anticommuting currents $j(x)$, $j^\dagger(x)$.

7.18.1 Thermodynamic Version of Wick's Theorem

By analogy with the generalization of the one-particle Green function (7.775) to the thermodynamic n -point functions $G^{(n)}$ of (7.777) it is useful to generalize also the thermal propagator (2.391). We shall treat here explicitly only the nonrelativistic case. The generalization to relativistic fields is straight-forward.

For this we introduce the thermal average of an imaginary-time-ordered product of $n + n'$ fields:

$$\begin{aligned} G^{(n,n')}(x_1, \tau_1, \dots, x_n, \tau_n; x'_1, \tau'_1, \dots, x'_n, \tau'_n) \\ = \frac{\text{Tr} \left[e^{-H_G/k_B T} T_\tau \left(\psi(x_1, \tau_1) \dots \psi(x_n, \tau_n) \psi^\dagger(x'_1, \tau'_1) \dots \psi^\dagger(x'_n, \tau'_n) \right) \right]}{\text{Tr} [e^{-H_G/k_B T}]}, \end{aligned} \quad (7.852)$$

where the free fields are expanded as in (2.405):

$$\psi(\mathbf{x}, \tau) = \int \tilde{d}^3 p f_{\mathbf{p}}(\mathbf{x}, \tau) a_{\mathbf{p}}, \quad (7.853)$$

$$\psi^\dagger(\mathbf{x}, \tau) = \int \tilde{d}^3 p f_{\mathbf{p}}^*(\mathbf{x}, \tau) a_{\mathbf{p}}^\dagger, \quad (7.854)$$

with the wave functions

$$f_{\mathbf{p}}(\mathbf{x}, \tau) \equiv e^{i[\mathbf{p}\mathbf{x} - \xi(\mathbf{p})\tau]/\hbar} \equiv f_{\mathbf{p}}^*(\mathbf{x}, -\tau), \quad \xi(\mathbf{p}) = \varepsilon(\mathbf{p}) - \mu, \quad (7.855)$$

where μ is the chemical potential. We shall write all subsequent equations with an explicit $\hbar$. An explicit evaluation of the thermal propagators (7.852) is much more involved than it was for vacuum expectation values. It proceeds using Wick's theorem, expanding the thermal expectation values in $G^{(n, n')}$ into a sum of products of two-particle thermal propagators, the sum running over all possible pair contractions, just as in Eq. (7.803) for the n -point function in the vacuum. All thermal information is therefore contained in the one-particle propagators which have the Fourier decomposition (2.420) with (2.419). The detailed form is here irrelevant.

To prove now Wick's expansion, we first observe that the free Hamiltonian conserves particle number, so that $G^{(n, n')}$ vanishes unless $n = n'$. As a next step we order the product of field operators according to their imaginary time arguments τ_n , thereby picking up some sign factor ± 1 depending on the number of transpositions of Fermi fields. On the right-hand side of Wick's expansion the corresponding permutations lead to the same sign. Thus we may assume all field operators to be time-ordered. The ordering in τ yields a product in which the fields ψ and $\psi^\dagger$ appear in a mixed fashion. We expand each field as $\int \tilde{d}^3 p f_{\mathbf{p}} \alpha_{\mathbf{p}}$, using the same notation for $\alpha_{\mathbf{p}} = a_{\mathbf{p}}$ and $\alpha_{\mathbf{p}} = a_{\mathbf{p}}^\dagger$, with the tacit understanding that, in the latter case, the wave function is taken as $f_{\mathbf{p}}^*$ rather than $f_{\mathbf{p}}$. Expanding the product of field operators in this way, we have

$$\begin{aligned} G^{(n, n)} &= \int \tilde{d}^3 p_1 \cdots \tilde{d}^3 p_{2n} f_1 \cdots f_{2n} \\ &= \text{Tr} \left(e^{-H_G/k_B T} \alpha_1 \cdots \alpha_{2n} \right) / \text{Tr} \left(e^{-H_G/k_B T} \right), \end{aligned} \quad (7.856)$$

where we have omitted the momentum labels on the operators α , using only their numeric subscripts. There are always equally many creators as annihilators among the α_i 's. In order to reduce the traces to a pure number, let us commute or anti-commute α_1 successively to the right via

$$\begin{aligned} \alpha_1 \alpha_2 \alpha_3 \cdots \alpha_{2n} &= [\alpha_1, \alpha_2]_{\mp} \alpha_3 \cdots \alpha_{2n} \\ &\quad \pm \alpha_2 [\alpha_1, \alpha_3]_{\mp} \alpha_4 \cdots \alpha_{2n} \\ &\quad + \cdots \\ &\quad + \alpha_2 \alpha_3 \cdots [\alpha_1, \alpha_{2n}]_{\mp} \\ &\quad \pm \alpha_2 \alpha_3 \cdots \alpha_{2n} \alpha_1. \end{aligned} \quad (7.857)$$

The commutators or anticommutators among α_1 and α_i will give 0 if both are creators or annihilators, 1 if α_1 is an annihilator and α_i a creator, and ∓ 1 in the opposite case. At any rate, they are c -numbers, so that they may be taken out of the trace leading to

$$\begin{aligned} & \text{Tr} \left(e^{-H_G/k_B T} \alpha_1 \alpha_2 \cdots \alpha_{2n} \right) \mp \text{Tr} \left(e^{-H_G/k_B T} \alpha_2 \cdots \alpha_{2n} \alpha_1 \right) \\ &= [\alpha_1, \alpha_2]_{\mp} \text{Tr} \left(e^{-H_G/k_B T} \alpha_3 \alpha_4 \cdots \alpha_{2n} \right) \pm [\alpha_1, \alpha_3]_{\mp} \text{Tr} \left(e^{-H_G/k_B T} \alpha_2 \alpha_4 \cdots \alpha_{2n} \right) \\ &+ \cdots + [\alpha_1, \alpha_{2n}]_{\mp} \text{Tr} \left(e^{H_G/k_B T} \alpha_2 \alpha_3 \cdots \alpha_{2n-1} \right). \end{aligned} \quad (7.858)$$

Now we make use of the cyclic property of the trace and observe that

$$\alpha_1 e^{-H_G/k_B T} = e^{-H_G/k_B T} \alpha_1 e^{\eta \xi(\mathbf{p})/k_B T}, \quad (7.859)$$

where the sign factor $\eta = \pm 1$ depends on whether α_1 is a creator or an annihilator, respectively. Then we can rewrite the left-hand side in (7.858) as

$$\left(1 \mp e^{\eta \xi(\mathbf{p})/k_B T} \right) \text{Tr} \left(e^{-H_G/k_B T} \alpha_2 \cdots \alpha_{2n} \alpha_1 \right). \quad (7.860)$$

Dividing the prefactor out, we obtain

$$\begin{aligned} \text{Tr} \left(e^{-H_G/k_B T} \alpha_1 \cdots \alpha_{2n} \right) &= \text{Tr} \left(e^{-H_G/k_B T} \dot{\alpha}_1 \dot{\alpha}_2 \alpha_3 \cdots \alpha_{2n} \right) \\ &+ \text{Tr} \left(e^{H_G/k_B T} \dot{\alpha}_1 \alpha_2 \dot{\alpha}_3 \cdots \alpha_{2n} \right) \\ &+ \cdots \\ &+ \text{Tr} \left(e^{-H_G/k_B T} \dot{\alpha}_1 \alpha_2 \alpha_3 \cdots \dot{\alpha}_{2n} \right), \end{aligned} \quad (7.861)$$

where a *thermal contraction* is defined as

$$\dot{\alpha}_1 \dot{\alpha}_i = \frac{[\alpha_1, \alpha_i]_{\mp}}{1 \mp e^{\eta \xi(\mathbf{p})/k_B T}}, \quad (7.862)$$

with the same rules of taking these c -numbers outside the trace as in the ordinary Wick contractions in Subsec. 7.17.1.

These contractions are just the Fourier transforms of the one-particle thermal propagators as given in (2.409) and (2.410). For if α_1 and α_i are both creators or annihilators, this is trivially true: both expressions vanish identically. If α_1 is an annihilator and α_i a creator, we see that [recalling (2.408) and (2.411)]

$$\dot{\alpha}_1 \dot{\alpha}_i = \frac{[a_{\mathbf{p}}, a_{\mathbf{p}'}^{\dagger}]_{\mp}}{1 \mp e^{-\xi(\mathbf{p})/k_B T}} = \delta^{(3)}(\mathbf{p} - \mathbf{p}') (1 \pm n_{\xi(\mathbf{p})}). \quad (7.863)$$

In the opposite case

$$\dot{\alpha}_1 \dot{\alpha}_i = \frac{[a_{\mathbf{p}}^{\dagger}, a_{\mathbf{p}'}]_{\mp}}{1 \mp e^{\xi(\mathbf{p})/k_B T}} = \delta^{(3)}(\mathbf{p} - \mathbf{p}') n_{\xi(\mathbf{p})}. \quad (7.864)$$

Multiplying either of these expressions by the product of wave functions $f_{\mathbf{p}}(\mathbf{x})f_{\mathbf{p}'}^*(\mathbf{x})$, and integrating everything over the entire momentum space, we find that these contractions are precisely the propagators $G(\mathbf{x}, \tau; \mathbf{x}', \tau') = G(\mathbf{x} - \mathbf{x}', \tau - \tau')$:

$$\dot{\psi}(\mathbf{x}, \tau)\dot{\psi}^\dagger(\mathbf{x}', \tau') = \pm \dot{\psi}^\dagger(\mathbf{x}', \tau')\dot{\psi}(\mathbf{x}, \tau) = G(\mathbf{x} - \mathbf{x}', \tau - \tau'). \quad (7.865)$$

In (7.861), the n -particle thermal Green function $G^{(n,n)}$ has been reduced to a sum of $(n-1)$ -particle propagators, each multiplied by an ordinary propagator. Continuing this procedure iteratively, we arrive at Wick's expansion for thermal Green functions.

As before, this result can be expressed most concisely in a functional form. For this we introduce

$$Z[j, j^\dagger] = \text{Tr} \left(e^{-H_G/k_B T} T_\tau e^{i \int d^3x d\tau [j(\mathbf{x}, \tau)\psi^\dagger(\mathbf{x}, \tau) + \psi(\mathbf{x}, \tau)j^\dagger(\mathbf{x}, \tau)]} \right) / \text{Tr} \left(e^{-H_G/k_B T} \right) \quad (7.866)$$

as the generating functional of thermal Green functions. Then Wick's expansion amounts to the statement

$$Z[i, j^\dagger] = e^{-\int d^3x d\tau d^3x' d\tau' j^\dagger(\mathbf{x}, \tau) G(\mathbf{x} - \mathbf{x}', \tau - \tau') j(\mathbf{x}, \tau)}. \quad (7.867)$$

As before, this can be derived from the equation of motion [compare (2.399) and (2.400)]

$$\begin{aligned} \left(-\partial_\tau + \frac{\nabla^2}{2M} + \mu \right) \frac{\delta}{\delta j^\dagger(\mathbf{x}, \tau)} Z[j, j^\dagger] &= -Z[j, j^\dagger] j(\mathbf{x}, \tau), \\ Z[j, j^\dagger] \frac{\overleftarrow{\delta}}{\delta j(\mathbf{x}, \tau)} \left(-\overleftarrow{\partial}_\tau + \frac{\overleftarrow{\nabla}^2}{2M} + \mu \right) &= -j^\dagger(\mathbf{x}, \tau) Z[j, j^\dagger], \end{aligned} \quad (7.868)$$

following the procedure to prove Eq. (7.846). Here the proof is simpler since only one time derivative needs to be passed through the time-ordering operation T_τ producing a canonical equal-time commutator for every pair of fields, as in (2.237). As a check we integrate again (7.868) with the initial condition $Z[0, 0] = 1$, and recover (7.867).

It is worth deriving also a related theorem concerning the thermal expectations of normally ordered field operators. According to Wick's theorem in the operator form (7.802), any product of time ordered operators can be expanded into normal products, so that

$$\begin{aligned} Z[j, j^\dagger] &= e^{-\int d^4x d^4x' j^\dagger(x) G(x-x') j(x)} \\ &\quad \times \frac{\text{Tr} \left(e^{-H_G/k_B T} N e^{i \int d^4x [j^\dagger(x)\psi(x) + \psi^\dagger(x)j(x)]} \right)}{\text{Tr} (e^{-H_G/k_B T})}, \end{aligned} \quad (7.869)$$

where we have used the four-vector notation $x = (\mathbf{x}, \tau)$ and $d^4x = d^3x d\tau$, for brevity. We can show that the expectation of the normal product can be expanded once more in a Wick-like way. For this we introduce the expectation of two normally ordered operators

$$G_N(x_1, x_2) \equiv \frac{\text{Tr} \left[e^{-H_G/k_B T} N \left(\psi^\dagger(x_1) \psi(x_2) \right) \right]}{\text{Tr} [e^{-H_G/k_B T}]}. \quad (7.870)$$

This quantity can be calculated by inserting (7.853) and (7.854), as well as intermediate states, with the result

$$G_{\hat{N}}(x_1, x_2) = \int d^3p e^{i[\mathbf{p}(\mathbf{x}_2 - \mathbf{x}_1) + i\xi(\mathbf{p})(\tau_1 - \tau_2)]/\hbar} n_{\xi(\mathbf{p})}, \quad (7.871)$$

where n_{ξ} is the particle distribution function for bosons and fermions, respectively:

$$n_{\xi} = \frac{1}{e^{\xi/k_B T} \pm 1}. \quad (7.872)$$

It can now be shown that the thermal expectation value of an arbitrary normal product can be expanded into expectation values of the one-particle normal products (7.870). This happens in the same way as the decomposition of the τ -ordered products into the expectations of one-particle τ -ordered propagators. The proof is most easily given functionally. We consider the generating functional

$$N[j, j^{\dagger}] \equiv \text{Tr} \left(e^{-H_G/k_B T} N e^{i \int d^4x (\psi^{\dagger}(x) j(x) + j^{\dagger}(x) \psi(x))} \right) / \text{Tr} \left(e^{-H_G/k_B T} \right) \quad (7.873)$$

and differentiate this with respect to $j^{\dagger}(x)$:

$$\frac{\delta N[j, j^{\dagger}]}{i \delta j^{\dagger}(x)} = \text{Tr} \left[e^{-H_G/k_B T} N \left(\psi(x) e^{i \int d^4x (\psi^{\dagger} j + j^{\dagger} \psi)} \right) \right] / \text{Tr} \left[e^{-H_G/k_B T} \right]. \quad (7.874)$$

Applying to this the field equation

$$\left(-\partial_{\tau} + \frac{\nabla^2}{2M} + \mu \right) \psi(x) = 0, \quad (7.875)$$

we see that $\hat{N}[j, j^{\dagger}]$ satisfies

$$\left(-\partial_{\tau} + \frac{\nabla^2}{2M} + \mu \right) \frac{\delta}{\delta j^{\dagger}} N[j, j^{\dagger}] = 0. \quad (7.876)$$

This is solved by

$$\hat{N}[j, j^{\dagger}] = e^{-\int d^4x_1 d^4x_2 j^{\dagger}(x_1) G_N(x_1, x_2) j(x_2)}, \quad (7.877)$$

where $G_N(x_1, x_2)$ is a solution of the homogeneous differential equation. To obtain the correct result for the ordinary imaginary-time propagator, we expand both sides in $j, j^{\dagger}$ and see that $G_N(x_1, x_2)$ coincides with (7.870), (7.871).

Appendix 7A Euler-Maclaurin Formula

The Euler-Maclaurin formula serves to calculate discrete sums such as those in Eqs. (7.693), (7.702), and (7.693). It can be derived from a fundamental summation formula due to Bernoulli. Starting point is the observation that a power n^p may be integrated over a real variable n to

$$\int_N^M dn n^p = \frac{b_{p+1}(M) - b_{p+1}(N)}{p+1}, \quad (7A.1)$$

where $b_{p+1}(x) \equiv x^{p+1}$. The corresponding summation formula produces *Bernoulli polynomials* $B_p(x)$ as follows:

$$\sum_{n=N}^M n^p = \frac{B_{p+1}(M+1) - B_{p+1}(N)}{p+1}. \quad (7A.2)$$

Here $B_p(x)$ denote the Bernoulli polynomials:

$$\begin{aligned} B_0(x) &\equiv 1, \\ B_1(x) &= -\frac{1}{2} + x, \\ B_2(x) &= \frac{1}{6} - x + x^2, \\ B_3(x) &= \frac{1}{2}x - \frac{3}{2}x^2 + x^3, \\ B_4(x) &= -\frac{1}{30} + x^2 - 2x^3 + x^4, \\ B_5(x) &= -\frac{1}{6}x + \frac{5}{3}x^3 - \frac{5}{2}x^4 + x^5, \\ &\vdots \end{aligned} \quad (7A.3)$$

The more general integral

$$\int_N^M dn (n+x)^p = \frac{b_{p+1}(M+x) - b_{p+1}(N+x)}{p+1} \quad (7A.4)$$

goes into the sum:

$$\sum_{n=N}^M (n+x)^p = \frac{B_{p+1}(M+1+x) - B_{p+1}(N+x)}{p+1}. \quad (7A.5)$$

The values of the polynomials $B_p(x)$ at $x=0$ are called *Bernoulli numbers* B_p :

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = 0, \quad B_4 = -\frac{1}{30}, \quad B_5 = 0, \quad B_6 = \frac{1}{42}, \quad \dots \quad (7A.6)$$

Except for B_1 , all odd Bernoulli numbers vanish.

The close correspondence between integrals and sums has its counterpart in differential versus difference equations: By differentiating $b_p(x) = x^p$, we find:

$$b'_p(x) = px^{p-1}, \quad (7A.7)$$

whose discrete counterpart is the difference equation

$$B_p(x+1) - B_p(x) = px^{p-1}, \quad (7A.8)$$

and the initial condition

$$B_0(x) \equiv 1. \quad (7A.9)$$

The differential relation

$$b'_p(x) = pb_{p-1}(x) \quad (7A.10)$$

is completely shared by $B_p(x)$:

$$B'_p(x) = pB_{p-1}(x). \quad (7A.11)$$

There is another important property of the function $b_p(x) = x^p$. The binomial expansion of $(x+h)^p$,

$$b_p(x+h) = \sum_{q=0}^p \binom{p}{q} b_q(x) h^{p-q}, \quad (7A.12)$$

goes over into

$$B_p(x+h) = \sum_{n=0}^p \binom{p}{n} B_n(x) h^{p-n}. \quad (7A.13)$$

A useful property of the Bernoulli polynomials is caused by the discrete nature of the sum and reads

$$B_p(1-x) = (-1)^p B_p(x). \quad (7A.14)$$

There exists a simple generating function for the Bernoulli polynomials which ensures the fundamental property (7A.8):

$$\frac{te^{xt}}{e^t - 1} = \sum_{p=0}^{\infty} B_p(x) \frac{t^p}{p!}. \quad (7A.15)$$

The property (7A.5) can directly be used to calculate the difference between an integral and a discrete sum over a function $F(t)$. If an interval $t \in (a, b)$ is divided into m slices of width $h = (b-a)/N$, we obviously have

$$h \sum_{n=0}^{N-1} F(a + (n+x)h) - \int_a^b dt F(t) = \sum_{p=1}^{\infty} \frac{h^p}{p!} [B_p(N+x) - B_p(x)] F^{(p-1)}(a). \quad (7A.16)$$

This follows from expanding the left-hand side into powers of h . After this, the binomial expansion (7A.28) leads to

$$\begin{aligned} \sum_{p=1}^{\infty} \frac{h^p}{p!} B_p(x+N+1) F^{(p-1)}(a) &= \sum_{p=1}^{\infty} \sum_{l=0}^p \frac{h^p}{p!} \binom{p}{l} B_l(x) N^{p-l} F^{(p-1)}(a) \\ &= \sum_{l=0}^p \frac{h^l}{l!} B_l(x) \sum_{p=l}^{\infty} \frac{1}{(p-l)!} (hN)^{p-l} F^{(p-1)}(a) \\ &= \sum_{l=0}^p \frac{h^l}{l!} B_l(x) F^{(l-1)}(b), \end{aligned} \quad (7A.17)$$

which brings (7A.16) to *Euler's formula*

$$h \sum_{n=0}^{N-1} F(a + (n+x)h) - \int_a^b dt F(t) = \sum_{p=1}^{\infty} \frac{h^p}{p!} B_p(x) [F^{(p-1)}(b) - F^{(p-1)}(a)]. \quad (7A.18)$$

Since all odd Bernoulli numbers vanish except for $B_1 = -1/2$, it is useful to remove the $p = 1$ -term from the right-hand side and rewrite (7A.25) as

$$\begin{aligned} h \sum_{n=0}^{N-1} F(a + (n+x)h) - \int_a^b dt F(t) &= (-1/2 + x) [F(b) - F(a)] \\ &+ \sum_{p=1}^{\infty} \frac{h^{2p}}{(2p)!} B_{2p}(x) [F^{(2p-1)}(b) - F^{(2p-1)}(a)]. \end{aligned} \quad (7A.19)$$

For $x = 0$ we may extend the sum on the left-hand side to $n = N$ and obtain the *Euler-Maclaurin formula*:²⁷

$$\begin{aligned} h \sum_{n=0}^N F(a + nh) - \int_a^b dt F(t) &= \frac{1}{2} [F(b) + F(a)] \\ &+ \sum_{p=1}^{\infty} \frac{h^{2p}}{(2p)!} B_{2p}(x) [F^{(2p-1)}(b) - F^{(2p-1)}(a)]. \end{aligned} \quad (7A.20)$$

²⁷See M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Eqs. 23.1.30 and 23.1.32.

If the sums (7A.5) are carried to infinity, they diverge. These infinities may, however, be removed by considering such sums as analytic continuations of convergent sums

$$\zeta(z, x) \equiv \sum_{n=0}^{\infty} \frac{1}{(n+x)^z}, \quad \operatorname{Re} z > 1, \quad (7A.21)$$

known as *Riemann's zeta functions*. A continuation is possible by an appropriate deformation of the contour in the integral representation

$$\zeta(z, x) = \frac{1}{\Gamma(z)} \int_0^{\infty} \frac{t^{z-1} e^{-xt}}{1 - e^{-t}} dt. \quad (7A.22)$$

This yields the relation:

$$\zeta(-p, x) = -\frac{B_{p+1}(x)}{p+1}. \quad (7A.23)$$

Thus the finite sum (7A.5) can be understood as the difference between the regularized infinite sums

$$\sum_{n=0}^{\infty} (n+x)^p = \zeta(-p, x) = -\frac{B_{p+1}(x)}{p+1}, \quad (7A.24)$$

and

$$\sum_{n=m+1}^{\infty} (n+x)^p = \zeta(-p, m+x) = -\frac{B_{p+1}(m+1+x)}{p+1}.$$

With the help of these regularized infinite sums we can derive Euler's formula (7A.25) by considering the left-hand side as a difference between the infinite sum

$$\left[h \sum_{n=0}^{\infty} F(a + (n+x)h) - \int_a^{\infty} dt F(t) \right] \quad (7A.25)$$

and a corresponding sum for b instead of a . By expanding each sum in powers of h and using the formula (7A.24), we find directly (7A.25).

For completeness, let us mention that alternating sums are governed quite similarly by *Euler polynomials*²⁸

$$\sum_{n=N}^M (-1)^{m-n} (n+x)^n = \frac{E_{n+1}(M+1+x) + (-1)^m E_{n+1}(p+x)}{2}. \quad (7A.26)$$

The Euler polynomials satisfy

$$E_p(x+1) + E_p(x) = 2x^{p-2}, \quad E'_p(x) = pE_{p-1}(x), \quad E_p(1-x) = (-1)^p E_p(x), \quad (7A.27)$$

and

$$E_p(x+h) = \sum_{n=0}^p \binom{p}{n} E_n(x) h^{p-n}. \quad (7A.28)$$

The generating function of the Euler polynomials is²⁹

$$\frac{2e^{xt}}{e^t + 1} = \sum_{n=0}^{\infty} E_p(x) \frac{t^n}{n!}. \quad (7A.29)$$

²⁸Note the difference with respect to the definition of the Bernoulli numbers (7A.6) which are defined by the values of $B_n(x)$ at $x = 0$.

²⁹Further properties of these polynomials can be found in M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Chapter 23.

The values $E_p(0)$ are related to the Bernoulli numbers by

$$E_p(0) = -2(2^{p+1} - 1)B_{p+1}/(p+1). \quad (7A.30)$$

The quantities $E_n \equiv 2^n E_n(1/2)$ are called *Euler numbers*. Their values are

$$E_0 = 1, \quad E_1 = 0, \quad E_2 = -1, \quad E_3 = 0, \quad E_4 = 5, \quad E_5 = 0, \quad E_6 = -61, \quad \dots \quad (7A.31)$$

Note that all odd Euler numbers vanish.

Appendix 7B Liénard-Wiechert Potential

Let us calculate the field around a point source with a time-dependent position $\bar{\mathbf{x}}(t)$, whose current is

$$j(t', \mathbf{x}') = \int d\tau \delta^{(4)}(x' - \bar{x}(\tau)) = \frac{1}{d\bar{x}_0/d\tau} \delta^{(3)}(\mathbf{x}' - \bar{\mathbf{x}}(t')), \quad (7B.1)$$

where τ is the proper time, and $d\bar{x}^0/d\tau = \sqrt{1 - \bar{\mathbf{v}}^2(t)} = \gamma(t)$, with $\bar{\mathbf{v}}(t)$ being the velocity along the trajectory $\bar{\mathbf{x}}(t)$:

$$\bar{\mathbf{v}}(t) \equiv \dot{\bar{\mathbf{x}}}(t). \quad (7B.2)$$

After performing the spatial integral in (7.191), we obtain

$$\phi(\mathbf{x}, t) = \int dt' \Theta(t - t') \frac{1}{4\pi R} \frac{1}{\gamma} \delta(t - t' - R(t')), \quad (7B.3)$$

where $R(t)$ is the distance from the moving source position at the time t :

$$R(t') = |\mathbf{x} - \bar{\mathbf{x}}(t')|. \quad (7B.4)$$

The integral over t' gives a contribution only for $t' = t_R$ determined from t by the retardation condition

$$t - t_R - R(t_R) = 0. \quad (7B.5)$$

At that point, the δ -function can be rewritten as

$$\delta(t - t' - R(t')) = \frac{1}{|d[t' + R(t')]/dt'|_{t'=t_R}} \delta(t' - t_R) = \frac{1}{1 - \mathbf{n}(t_R) \cdot \bar{\mathbf{v}}(t_R)} \delta(t' - t_R), \quad (7B.6)$$

where $\mathbf{n}(t)$ is the direction of the distance vector from the charge.

$$\mathbf{n}(t) \equiv \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|}. \quad (7B.7)$$

Thus we find the Liénard-Wiechert-like potential:

$$\phi(\mathbf{x}, t) = - \left[\frac{1}{\gamma(1 - \mathbf{n} \cdot \bar{\mathbf{v}})R} \right]_{\text{ret}}, \quad (7B.8)$$

and the *retarded distance* from the point source

$$R_{\text{ret}}(t) = |\mathbf{x} - \bar{\mathbf{x}}(t_R)|. \quad (7B.9)$$

Appendix 7C Equal-Time Commutator from Time-Ordered Products

As an exercise in handling the functions in Section 7.2, consider the relationship between the commutator at equal-times and the time-ordered product. The first can be obtained from the latter by forming the difference

$$[\phi(x), \phi(x')]_{x^0=x'^0} = \hat{T}(\phi(x)\phi(x'))|_{x^0=x'^0=\epsilon} - \hat{T}(\phi(x)\phi(x'))|_{x^0=x'^0=-\epsilon}, \quad (7C.1)$$

where ϵ is an infinitesimal positive time. Thus, the Fourier representation of the equal-time commutator is obtained from that of the Feynman propagator by replacing the exponential $e^{-ip^0(x^0-x'^0)}$ in the p^0 -integral of (7.66) by $e^{-ip^0\epsilon} - e^{ip^0\epsilon}$. Thus we should get, for the commutator function at equal times, the energy-momentum integral:

$$C(x-x')|_{x^0=x'^0} = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \int \frac{dp^0}{2\pi} (e^{-ip^0\epsilon} - e^{ip^0\epsilon}) \frac{i}{p^2 - M^2 + i\eta}. \quad (7C.2)$$

The p^0 -integral can now be performed by closing the contour in the first term by a semicircle in the lower half-plane, in the second term by one in the upper half-plane. To do this, we express the Feynman propagator via the first of the rules (7.212) [see also (7.199)] as

$$\frac{i}{p^2 - M^2 + i\eta} = \pi\delta_-(p^2 - M^2) = \pi\delta_-(p^0^2 - \omega_{\mathbf{p}}^2), \quad (7C.3)$$

and use the simple integrals

$$\int_{-\infty}^{\infty} \frac{dp^0}{2\pi} e^{-ip^0\epsilon} \pi\delta_-(p^0 - \omega_{\mathbf{p}}) = 1, \quad \int_{-\infty}^{\infty} \frac{dp^0}{2\pi} e^{-ip^0\epsilon} \pi\delta_+(p^0 + \omega_{\mathbf{p}}) = 0, \quad (7C.4)$$

$$\int_{-\infty}^{\infty} \frac{dp^0}{2\pi} e^{ip^0\epsilon} \pi\delta_-(p^0 - \omega_{\mathbf{p}}) = 0, \quad \int_{-\infty}^{\infty} \frac{dp^0}{2\pi} e^{ip^0\epsilon} \pi\delta_+(p^0 + \omega_{\mathbf{p}}) = 1, \quad (7C.5)$$

to find a vanishing commutator function.

For its time derivative, these imply that exponentials $e^{\mp ip^0\epsilon}$ together with $\delta_-(p^0 - \omega_{\mathbf{p}})$ and $\delta_+(p^0 + \omega_{\mathbf{p}})$ have the same effect as Heaviside functions $\Theta(\pm p^0)$ accompanied by $2\pi\delta_{\pm}(p^0 - \omega_{\mathbf{p}})$ and $2\pi\delta_{\pm}(p^0 + \omega_{\mathbf{p}})$, respectively. We can therefore make the following replacements in the p^0 -integrals of the Fourier representation (7C.2) of the commutator function:

$$\int \frac{dp^0}{2\pi} (e^{-ip^0\epsilon} - e^{ip^0\epsilon}) \frac{i}{p^2 - M^2 + i\eta} \rightarrow \int \frac{dp^0}{2\pi} [\Theta(p^0) - \Theta(-p^0)] 2\pi\delta(p^2 - M^2). \quad (7C.6)$$

The result is the same as the p^0 -integral in Eq. (7.206) for $C(x-x')$ at equal times, which vanishes.

For the time derivative of the commutator function $C(x-x')$, the integrand carries an extra factor $-p^0$, and (7C.6) becomes

$$\int \frac{dp^0}{2\pi} (-ip^0) (e^{-ip^0\epsilon} - e^{ip^0\epsilon}) \frac{i}{p^2 - M^2 + i\eta} \rightarrow -i \int \frac{dp^0}{2\pi} \omega_{\mathbf{p}} 2\pi\delta(p^2 - M^2) = -i, \quad (7C.7)$$

so that we find the correct result $\dot{C}(-x')_{x^0=x'^0} = -i\delta^{(3)}(x-x')$.

With the same formalism one may also check the consistency of the photon propagator (7.539) with the commutation rules (7.542)–(7.545). As in (7C.2), we write in the p^0 -integral of (7.66):

$$[A^\mu(x), A^\nu(x')]_{x^0=x'^0} = \int \frac{d^4k}{(2\pi)^4} (e^{-ik^0\epsilon} - e^{ik^0\epsilon}) e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \frac{i}{k^2 + i\eta} \left[-g^{\mu\nu} + (1-\alpha) \frac{k^\mu k^\nu}{k^2 + i\eta} \right]. \quad (7C.8)$$

The contribution of $-g^{\mu\nu}$ in the brackets yields the commutator function $C(x-x')$ of the scalar field. The second contribution proportional to $k^\mu k^\nu$ is nontrivial. First we insert

$$\frac{1}{k^2 + i\eta} = \delta_+(k^2) = \frac{1}{2\omega_{\mathbf{k}}} [\delta_+(k^0 - \omega_{\mathbf{k}}) + \delta_+(k^0 + \omega_{\mathbf{k}})],$$

with $\omega_{\mathbf{k}} = |\mathbf{k}|$. By forming the derivative ∂_μ and taking $\nu = 0$, the first term gives

$$i\delta^{(3)}(\mathbf{x} - \mathbf{x}').$$

The second term is equal to

$$-i(1 - \alpha) \int \frac{d^4 k}{(2\pi)^4} (e^{-ik^0 \epsilon} - e^{ik^0 \epsilon}) e^{i\mathbf{k}(\mathbf{x} - \mathbf{x}')} \frac{1}{2\omega_{\mathbf{k}}} [\delta_+(k^0 - \omega_{\mathbf{k}}) + \delta_+(k^0 + \omega_{\mathbf{k}})] k^0. \quad (7C.9)$$

Since k^0 changes the relative sign of the two pole contributions, the k -integration gives

$$-i(1 - \alpha)\delta^{(3)}(\mathbf{x} - \mathbf{x}'),$$

leading to the equal-time commutator

$$[\partial_\mu A^\mu(x), A^0(x')]|_{x_0=x'^0} = i\alpha\delta^{(3)}(\mathbf{x} - \mathbf{x}') \quad (7C.10)$$

in agreement with (7.542), provided that

$$[\partial_i A^i(x), A^0(x')]|_{x_0=x'^0} = 0. \quad (7C.11)$$

This commutator has a spectral decomposition coming from the second term in (7C.8): It is equal to

$$\begin{aligned} -i(1 - \alpha) \int \frac{d^4 k}{(2\pi)^4} (e^{-ik^0 \epsilon} - e^{ik^0 \epsilon}) e^{i\mathbf{k}(\mathbf{x} - \mathbf{x}')} \frac{1}{2k^0} [\delta_+(k^0 - \omega_{\mathbf{k}}) + \delta_+(k^0 + \omega_{\mathbf{k}})] \\ \times \mathbf{k}^2 k^0 \frac{1}{2\omega_{\mathbf{k}}} [\delta_+(k^0 - \omega_{\mathbf{k}}) + \delta_+(k^0 + \omega_{\mathbf{k}})]. \end{aligned} \quad (7C.12)$$

By writing

$$k^0 \frac{1}{2\omega_{\mathbf{k}}} [\delta_+(k^0 - \omega_{\mathbf{k}}) + \delta_+(k^0 + \omega_{\mathbf{k}})] = k^0 \frac{1}{2\omega_{\mathbf{k}}} [\delta_+(k^0 - \omega_{\mathbf{k}}) - \delta_+(k^0 + \omega_{\mathbf{k}})],$$

we see that the δ_+ -functions appear in the combination $[\delta_+(k^0 - \omega_{\mathbf{k}})]^2 - [\delta_+(k^0 + \omega_{\mathbf{k}})]^2$. When closing the integration contours in the upper or lower k^0 -plane, the double poles give no contribution. Hence

$$[\partial_i A^i(x), A^0(x')]|_{x_0=x'^0} = 0. \quad (7C.13)$$

For the same reason, the commutators $[\dot{A}^i(x), \dot{A}^j(x')]|_{x_0=x'^0}$ receive only a contribution from the first term and yield $-i\delta_{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}')$. Other commutators are

$$\begin{aligned} [D(x), \dot{A}^i(x')]|_{x_0=x'^0} &= -[D(x), \partial_i A^0(x')]|_{x_0=x'^0} \\ &= \int \frac{d^4 k}{(2\pi)^4} (e^{-ik^0 \epsilon} - e^{ik^0 \epsilon}) e^{i\mathbf{k}(\mathbf{x} - \mathbf{x}')} \frac{i}{k^2 + i\eta} \alpha k^i k^0, \end{aligned} \quad (7C.14)$$

yielding

$$\alpha i\delta^{(3)}(\mathbf{x} - \mathbf{x}'),$$

which shows that $D(x)$ commutes with $E^i(x)$ at equal times. Together with the previous result we recover the third of the canonical commutators (7.542)–(7.545).

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8

Continuous Symmetries and Conservation Laws. Noether's Theorem

In many physical systems, the action is invariant under some continuous set of transformations. In such systems, there exist local and global *conservation laws* analogous to current and charge conservation in electrodynamics. The analogs of the charges can be used to generate the symmetry transformation, from which they were derived, with the help of Poisson brackets, or after quantization, with the help of commutators.

8.1 Point Mechanics

Consider a simple mechanical system with a generic action

$$\mathcal{A} = \int_{t_a}^{t_b} dt L(q(t), \dot{q}(t), t). \quad (8.1)$$

8.1.1 Continuous Symmetries and Conservation Law

Suppose $\mathcal{A}$ is invariant under a continuous set of transformations of the dynamical variables:

$$q(t) \rightarrow q'(t) = f(q(t), \dot{q}(t)), \quad (8.2)$$

where $f(q(t), \dot{q}(t))$ is some functional of $q(t)$. Such transformations are called symmetry transformations. Thereby it is important that the equations of motion are not used when establishing the invariance of the action under (8.2).

If the action is subjected successively to two *symmetry transformations*, the result is again a symmetry transformation. Thus, symmetry transformations form a group called the *symmetry group* of the system. For infinitesimal symmetry transformations (8.2), the difference

$$\delta_s q(t) \equiv q'(t) - q(t) \quad (8.3)$$

will be called a *symmetry variation*. It has the general form

$$\delta_s q(t) = \epsilon \Delta(q(t), \dot{q}(t), t). \quad (8.4)$$

Symmetry variations must not be confused with ordinary variations $\delta q(t)$ used in Section 1.1 to derive the Euler-Lagrange equations (1.8). While the ordinary variations $\delta q(t)$ vanish at initial and final times, $\delta q(t_b) = \delta q(t_a) = 0$ [recall (1.4)], the symmetry variations $\delta_s q(t)$ are usually nonzero at the ends.

Let us calculate the change of the action under a symmetry variation (8.4). Using the chain rule of differentiation and an integration by parts, we obtain

$$\delta_s \mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{\partial L}{\partial q(t)} - \partial_t \frac{\partial L}{\partial \dot{q}(t)} \right] \delta_s q(t) + \frac{\partial L}{\partial \dot{q}(t)} \delta_s q(t) \Big|_{t_a}^{t_b}. \quad (8.5)$$

For orbits $q(t)$ that satisfy the Euler-Lagrange equations (1.8), only boundary terms survive, and we are left with

$$\delta_s \mathcal{A} = \epsilon \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) \Big|_{t_b}^{t_a}. \quad (8.6)$$

Under the symmetry assumption, $\delta_s \mathcal{A}$ vanishes for *any* orbit $q(t)$, implying that the quantity

$$Q(t) \equiv \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) \quad (8.7)$$

is the same at times $t = t_a$ and $t = t_b$. Since t_b is arbitrary, $Q(t)$ is *independent* of the time t , i.e., it satisfies

$$Q(t) \equiv Q. \quad (8.8)$$

It is a *conserved quantity*, a *constant of motion*. The expression on the right-hand side of (8.7) is called *Noether charge*.

The statement can be generalized to transformations $\delta_s q(t)$ for which the action is not directly invariant but its symmetry variation is equal to an arbitrary boundary term:

$$\delta_s \mathcal{A} = \epsilon \Lambda(q, \dot{q}, t) \Big|_{t_a}^{t_b}. \quad (8.9)$$

In this case,

$$Q(t) = \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) - \Lambda(q, \dot{q}, t) \quad (8.10)$$

is a conserved Noether charge.

It is also possible to derive the constant of motion (8.10) without invoking the action, but starting from the Lagrangian. For it we evaluate the symmetry variation as follows:

$$\delta_s L \equiv L(q + \delta_s q, \dot{q} + \delta_s \dot{q}) - L(q, \dot{q}) = \left[\frac{\partial L}{\partial q(t)} - \partial_t \frac{\partial L}{\partial \dot{q}(t)} \right] \delta_s q(t) + \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{q}(t)} \delta_s q(t) \right]. \quad (8.11)$$

On account of the Euler-Lagrange equations (1.8), the first term on the right-hand side vanishes as before, and only the last term survives. The assumption of invariance of the action up to a possible surface term in Eq. (8.9) is equivalent to assuming that the symmetry variation of the Lagrangian is a *total time derivative* of some function $\Lambda(q, \dot{q}, t)$:

$$\delta_s L(q, \dot{q}, t) = \epsilon \frac{d}{dt} \Lambda(q, \dot{q}, t). \quad (8.12)$$

Inserting this into the left-hand side of (8.11), we find

$$\epsilon \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) - \Lambda(q, \dot{q}, t) \right] = 0, \quad (8.13)$$

thus recovering again the conserved Noether charge (8.8).

The existence of a conserved quantity for every continuous symmetry is the content of *Noether's theorem* [1].

8.1.2 Alternative Derivation

Let us do the substantial variation in Eq. (8.5) explicitly, and change a classical orbit $q_c(t)$, that extremizes the action, by an *arbitrary variation* $\delta_a q(t)$. If this does *not* vanish at the boundaries, the action changes by a pure boundary term that follows directly from (8.5):

$$\delta_a \mathcal{A} = \left. \frac{\partial L}{\partial \dot{q}} \delta_a q \right|_{t_a}^{t_b}. \quad (8.14)$$

From this equation we can derive Noether's theorem in yet another way. Suppose we subject a classical orbit to a new type of symmetry variation, to be called *local symmetry transformations*, which generalizes the previous symmetry variations (8.4) by making the parameter ϵ time-dependent:

$$\delta_s^t q(t) = \epsilon(t) \Delta(q(t), \dot{q}(t), t). \quad (8.15)$$

The superscript t of $\delta_s^t q(t)$ indicates the new time dependence in the parameter $\epsilon(t)$. These variations may be considered as a special set of the general variations $\delta_a q(t)$ introduced above. Thus also $\delta_s^t \mathcal{A}$ must be a pure boundary term of the type (8.14). For the subsequent discussion it is useful to introduce the infinitesimally transformed orbit

$$q^\epsilon(t) \equiv q(t) + \delta_s^t q(t) = q(t) + \epsilon(t) \Delta(q(t), \dot{q}(t), t), \quad (8.16)$$

and the associated Lagrangian:

$$L^\epsilon \equiv L(q^\epsilon(t), \dot{q}^\epsilon(t)). \quad (8.17)$$

Using the time-dependent parameter $\epsilon(t)$, the local symmetry variation of the action can be written as

$$\delta_s^t \mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{\partial L^\epsilon}{\partial \epsilon(t)} - \frac{d}{dt} \frac{\partial L^\epsilon}{\partial \dot{\epsilon}(t)} \right] \epsilon(t) + \left. \frac{\partial L^\epsilon}{\partial \dot{\epsilon}} \epsilon(t) \right|_{t_a}^{t_b}. \quad (8.18)$$

Along the classical orbits, the action is extremal and satisfies the equation

$$\frac{\delta \mathcal{A}}{\delta \epsilon(t)} = 0, \quad (8.19)$$

which translates for a local action to an Euler-Lagrange type of equation:

$$\frac{\partial L^\epsilon}{\partial \epsilon(t)} - \frac{d}{dt} \frac{\partial L^\epsilon}{\partial \dot{\epsilon}(t)} = 0. \quad (8.20)$$

This can also be checked explicitly by differentiating (8.17) according to the chain rule of differentiation:

$$\frac{\partial L^\epsilon}{\partial \epsilon(t)} = \frac{\partial L^\epsilon}{\partial q(t)} \Delta(q, \dot{q}, t) + \frac{\partial L^\epsilon}{\partial \dot{q}(t)} \dot{\Delta}(q, \dot{q}, t); \quad (8.21)$$

$$\frac{\partial L^\epsilon}{\partial \dot{\epsilon}(t)} = \frac{\partial L^\epsilon}{\partial \dot{q}(t)} \Delta(q, \dot{q}, t), \quad (8.22)$$

and inserting on the right-hand side the ordinary Euler-Lagrange equations (1.8).

We now invoke the symmetry assumption that the action is a pure surface term under the time-independent transformations (8.15). This implies that

$$\frac{\partial L^\epsilon}{\partial \epsilon} = \frac{d}{dt} \Lambda. \quad (8.23)$$

Combining this with (8.20), we derive a conservation law for the charge:

$$Q = \frac{\partial L^\epsilon}{\partial \dot{\epsilon}} - \Lambda. \quad (8.24)$$

Inserting here Eq. (8.22), we find that this is the same charge as that derived by the previous method.

8.2 Displacement and Energy Conservation

As a simple but physically important example consider the case that the Lagrangian does not depend explicitly on time, i.e., that $L(q, \dot{q}, t) \equiv L(q, \dot{q})$. Let us perform a time translation on the coordinate frame:

$$t' = t - \epsilon. \quad (8.25)$$

In the new coordinate frame, the *same* orbit has the new description

$$\dot{q}(t') = q(t), \quad (8.26)$$

i.e., the orbit $\dot{q}(t)$ at the translated time t' is precisely the same as the orbit $q(t)$ at the original time t . If we replace the argument of $\dot{q}(t)$ in (8.26) by t' , we describe a

time-translated orbit in terms of the original coordinates. This implies the symmetry variation of the form (8.4):

$$\begin{aligned}\delta_s q(t) &= q'(t) - q(t) = q(t' + \epsilon) - q(t) \\ &= q(t') + \epsilon \dot{q}(t') - q(t) = \epsilon \dot{q}(t).\end{aligned}\quad (8.27)$$

The symmetry variation of the Lagrangian is in general

$$\delta_s L = L(q'(t), \dot{q}(t)) - L(q(t), \dot{q}(t)) = \frac{\partial L}{\partial q} \delta_s q(t) + \frac{\partial L}{\partial \dot{q}} \delta_s \dot{q}(t). \quad (8.28)$$

Inserting $\delta_s q(t)$ from (8.27) we find, without using the Euler-Lagrange equation,

$$\delta_s L = \epsilon \left(\frac{\partial L}{\partial \dot{q}} \dot{q} + \frac{\partial L}{\partial \ddot{q}} \ddot{q} \right) = \epsilon \frac{d}{dt} L. \quad (8.29)$$

This has precisely the form of Eq. (8.12), with $\Lambda = L$ as expected, since time translations are symmetry transformations. Here the function Λ in (8.12) happens to coincide with the Lagrangian.

According to Eq. (8.10), we find the Noether charge

$$Q = \frac{\partial L}{\partial \dot{q}} \dot{q} - L(q, \dot{q}) \quad (8.30)$$

to be a constant of motion. This is recognized as the *Legendre transform* of the Lagrangian which is, of course, the *Hamiltonian* of the system. $\square$

Let us briefly check how this Noether charge is obtained from the alternative formula (8.10). The time-dependent symmetry variation is here

$$\delta_s^t q(t) = \epsilon(t) \dot{q}(t), \quad (8.31)$$

under which the Lagrangian is changed by

$$\delta_s^t L = \frac{\partial L}{\partial q} \epsilon \dot{q} + \frac{\partial L}{\partial \dot{q}} (\dot{\epsilon} \dot{q} + \epsilon \ddot{q}) = \frac{\partial L^\epsilon}{\partial \epsilon} \epsilon + \frac{\partial L^\epsilon}{\partial \dot{\epsilon}} \dot{\epsilon}, \quad (8.32)$$

with

$$\frac{\partial L^\epsilon}{\partial \dot{\epsilon}} = \frac{\partial L}{\partial \dot{q}} \dot{q} \quad (8.33)$$

and

$$\frac{\partial L^\epsilon}{\partial \epsilon} = \frac{\partial L}{\partial q} \dot{q} + \frac{\partial L}{\partial \ddot{q}} \epsilon \ddot{q} = \frac{d}{dt} L. \quad (8.34)$$

This shows that time translations fulfill the symmetry condition (8.23), and that the Noether charge (8.24) coincides with the Hamiltonian found in Eq. (8.10).

8.3 Momentum and Angular Momentum

While the conservation law of energy follows from the symmetry of the action under time translations, conservation laws of momentum and angular momentum are found if the action is invariant under translations and rotations.

Consider a Lagrangian of a point particle in a euclidean space

$$L = L(x^i(t), \dot{x}^i(t), t). \quad (8.35)$$

In contrast to the previous discussion of time translation invariance, which was applicable to systems with arbitrary Lagrange coordinates $q(t)$, we denote the coordinates here by x^i to emphasize that we now consider cartesian coordinates. If the Lagrangian does depend only on the velocities $\dot{x}^i$ and not on the coordinates x^i themselves, the system is *translationally invariant*. If it depends, in addition, only on $\dot{\mathbf{x}}^2 = \dot{x}^i \dot{x}^i$, it is also rotationally invariant.

The simplest example is the Lagrangian of a point particle of mass m in euclidean space:

$$L = \frac{m}{2} \dot{\mathbf{x}}^2. \quad (8.36)$$

It exhibits both invariances, leading to conserved Noether charges of momentum and angular momentum, as we now demonstrate.

8.3.1 Translational Invariance in Space

Under a spatial translation, the coordinates x^i change to

$$x'^i = x^i + \epsilon^i, \quad (8.37)$$

where ϵ^i are small numbers. The infinitesimal translations of a particle path are [compare (8.4)]

$$\delta_s x^i(t) = \epsilon^i. \quad (8.38)$$

Under these, the Lagrangian changes by

$$\begin{aligned} \delta_s L &= L(x'^i(t), \dot{x}'^i(t), t) - L(x^i(t), \dot{x}^i(t), t) \\ &= \frac{\partial L}{\partial x^i} \delta_s x^i = \frac{\partial L}{\partial x^i} \epsilon^i = 0. \end{aligned} \quad (8.39)$$

By assumption, the Lagrangian is independent of x^i , so that the right-hand side vanishes. This has to be compared with the symmetry variation of the Lagrangian around the classical orbit, calculated via the chain rule, and using the Euler-Lagrange equation:

$$\begin{aligned} \delta_s L &= \left(\frac{\partial L}{\partial x^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}^i} \right) \delta_s x^i + \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}^i} \delta_s x^i \right] \\ &= \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}^i} \right] \epsilon^i. \end{aligned} \quad (8.40)$$

This has the form (8.6), from which we extract a conserved Noether charge (8.7) for each coordinate x^i :

$$p^i = \frac{\partial L}{\partial \dot{x}^i}. \quad (8.41)$$

These are simply the canonical momenta of the system.

8.3.2 Rotational Invariance

Under rotations, the coordinates x^i change to

$$x'^i = R^i_j x^j, \quad (8.42)$$

where R^i_j is an orthogonal 3×3 -matrix. Infinitesimally, this can be written as

$$R^i_j = \delta^i_j - \omega_k \epsilon_{kij}, \quad (8.43)$$

where ω is an infinitesimal rotation vector. The corresponding rotation of a particle path is

$$\delta_s x^i(t) = x'^i(t) - x^i(t) = -\omega^k \epsilon_{kij} x^j(\tau). \quad (8.44)$$

It is useful to introduce the antisymmetric infinitesimal rotation tensor

$$\omega_{ij} \equiv \omega_k \epsilon_{kij}, \quad (8.45)$$

in terms of which

$$\delta_s x^i = -\omega_{ij} x^j. \quad (8.46)$$

Then we can write the change of the Lagrangian under $\delta_s x^i$,

$$\begin{aligned} \delta_s L &= L(x'^i(t), \dot{x}'^i(t), t) - L(x^i(t), \dot{x}^i(t), t) \\ &= \frac{\partial L}{\partial x^i} \delta_s x^i + \frac{\partial L}{\partial \dot{x}^i} \delta_s \dot{x}^i, \end{aligned} \quad (8.47)$$

as

$$\delta_s L = - \left(\frac{\partial L}{\partial x^i} x^j + \frac{\partial L}{\partial \dot{x}^i} \dot{x}^j \right) \omega_{ij} = 0. \quad (8.48)$$

If the Lagrangian depends only on the rotational invariants $\mathbf{x}^2, \dot{\mathbf{x}}^2, \mathbf{x} \cdot \dot{\mathbf{x}}$, and on powers thereof, the right-hand side vanishes on account of the antisymmetry of ω_{ij} . This ensures the rotational symmetry.

We now calculate once more the symmetry variation of the Lagrangian via the chain rule and find, using the Euler-Lagrange equations,

$$\begin{aligned} \delta_s L &= \left(\frac{\partial L}{\partial x^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}^i} \right) \delta_s x^i + \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}^i} \delta_s x^i \right] \\ &= - \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}^i} x^j \right] \omega_{ij} = \frac{1}{2} \frac{d}{dt} \left[x_i \frac{\partial L}{\partial \dot{x}^j} - (i \leftrightarrow j) \right] \omega_{ij}. \end{aligned} \quad (8.49)$$

The right-hand side yields the conserved Noether charges of type (8.7), one for each antisymmetric pair i, j :

$$L^{ij} = x^i \frac{\partial L}{\partial \dot{x}^j} - x^j \frac{\partial L}{\partial \dot{x}^i} \equiv x^i p^j - x^j p^i. \quad (8.50)$$

These are the antisymmetric components of angular momentum.

Had we worked with the original vector form of the rotation angles ω^k , we would have found the angular momentum in the more common form:

$$L_k = \frac{1}{2} \epsilon_{kij} L^{ij} = (\mathbf{x} \times \mathbf{p})^k. \quad (8.51)$$

The quantum-mechanical operators associated with these, after replacing $p^i \rightarrow -i\partial/\partial x^i$, have the well-known commutation rules

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k. \quad (8.52)$$

In the tensor notation (8.50), these become

$$[\hat{L}_{ij}, \hat{L}_{kl}] = -i \left(\delta_{ik} \hat{L}_{jl} - \delta_{il} \hat{L}_{jk} + \delta_{jl} \hat{L}_{ik} - \delta_{jk} \hat{L}_{il} \right). \quad (8.53)$$

8.3.3 Center-of-Mass Theorem

Consider now the transformations corresponding to a uniform motion of the coordinate system. We shall study the behavior of a set of free massive point particles in euclidean space described by the Lagrangian

$$L(\dot{x}^i) = \sum_n \frac{m_n}{2} \dot{\mathbf{x}}_n^2. \quad (8.54)$$

Under Galilei transformations, the spatial coordinates and the time are changed to

$$\begin{aligned} \dot{x}^i(t) &= \dot{x}^i(t) - v^i t, \\ t' &= t, \end{aligned} \quad (8.55)$$

where v^i is the relative velocity along the i th axis. The infinitesimal symmetry variations are

$$\delta_s x^i(t) = \dot{x}^i(t) - x^i(t) = -v^i t, \quad (8.56)$$

which change the Lagrangian by

$$\delta_s L = L(\dot{x}^i - v^i t, \dot{x}^i - v^i) - L(\dot{x}^i, \dot{x}^i). \quad (8.57)$$

Inserting the explicit form (8.54), we find

$$\delta_s L = \sum_n \frac{m_n}{2} \left[(\dot{x}_n^i - v^i)^2 - (\dot{x}_n^i)^2 \right]. \quad (8.58)$$

This can be written as a total time derivative:

$$\delta_s L = \frac{d}{dt} \Lambda = \frac{d}{dt} \sum_n m_n \left[-\dot{x}_n^i v^i + \frac{v^2}{2} t \right], \quad (8.59)$$

proving that Galilei transformations are symmetry transformations in the Noether sense. By assumption, the velocities v^i in (8.55) are infinitesimal, so that the second term can be ignored.

By calculating $\delta_s L$ once more via the chain rule with the help of the Euler-Lagrange equations, and by equating the result with (8.59), we find the conserved Noether charge

$$\begin{aligned} Q &= \sum_n \frac{\partial L}{\partial \dot{x}^i} \delta_s x^i - \Lambda \\ &= \left(-\sum_n m_n \dot{x}_n^i t + \sum_n m_n x_n^i \right) v^i. \end{aligned} \quad (8.60)$$

Since the direction of the velocity v^i is arbitrary, each component is separately a constant of motion:

$$N^i = -\sum_n m_n \dot{x}_n^i t + \sum_n m_n x_n^i = \text{const.} \quad (8.61)$$

This is the well-known *center-of-mass theorem* [2]. Indeed, introducing the center-of-mass coordinates

$$x_{\text{CM}}^i \equiv \frac{\sum_n m_n x_n^i}{\sum_n m_n}, \quad (8.62)$$

and the associated velocities

$$v_{\text{CM}}^i = \frac{\sum_n m_n \dot{x}_n^i}{\sum_n m_n}, \quad (8.63)$$

the conserved charge (8.61) can be written as

$$N^i = \sum_n m_n (-v_{\text{CM}}^i t + x_{\text{CM}}^i). \quad (8.64)$$

The time-independence of N^i implies that the center-of-mass moves with uniform velocity according to the law

$$x_{\text{CM}}^i(t) = x_{0\text{CM}}^i + v_{\text{CM}}^i t, \quad (8.65)$$

where

$$x_{0\text{CM}}^i = \frac{N^i}{\sum_n m_n} \quad (8.66)$$

is the position of the center of mass at $t = 0$.

Note that in non-relativistic physics, the center-of-mass theorem is a consequence of momentum conservation since momentum $\equiv$ mass $\times$ velocity. In relativistic physics, this is no longer true.

8.3.4 Conservation Laws Resulting from Lorentz Invariance

In relativistic physics, particle orbits are described by functions in spacetime

$$x^\mu(\tau), \quad (8.67)$$

where τ is an arbitrary Lorentz-invariant parameter. The action is an integral over some Lagrangian:

$$\mathcal{A} = \int d\tau L(x^\mu(\tau), \dot{x}^\mu(\tau), \tau), \quad (8.68)$$

where $\dot{x}^\mu(\tau)$ denotes the derivative with respect to the parameter τ . If the Lagrangian depends only on invariant scalar products $x^\mu x_\mu, x^\mu \dot{x}_\mu, \dot{x}^\mu \dot{x}_\mu$, then it is invariant under Lorentz transformations

$$x^\mu \rightarrow \dot{x}^\mu = \Lambda^\mu{}_\nu x^\nu, \quad (8.69)$$

where $\Lambda^\mu{}_\nu$ is a 4×4 matrix satisfying

$$\Lambda g \Lambda^T = g, \quad (8.70)$$

with the Minkowski metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \quad (8.71)$$

For a free massive point particle in spacetime, the Lagrangian is

$$L(\dot{x}(\tau)) = -Mc\sqrt{g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}. \quad (8.72)$$

It is reparametrization invariant under $\tau \rightarrow f(\tau)$, with an arbitrary function $f(\tau)$. Under translations

$$\delta_s x^\mu(\tau) = x^\mu(\tau) - \epsilon^\mu(\tau), \quad (8.73)$$

the Lagrangian is obviously invariant, satisfying $\delta_s \mathcal{L} = 0$. Calculating this variation once more via the chain rule with the help of the Euler-Lagrange equations, we find

$$\begin{aligned} 0 &= \int_{\tau_\mu}^{\tau_\nu} d\tau \left(\frac{\partial L}{\partial x^\mu} \delta_s x^\mu + \frac{\partial L}{\partial \dot{x}^\mu} \delta_s \dot{x}^\mu \right) \\ &= -\epsilon^\mu \int_{\tau_\mu}^{\tau_\nu} d\tau \frac{d}{d\tau} \left(\frac{\partial L}{\partial \dot{x}^\mu} \right). \end{aligned} \quad (8.74)$$

From this we obtain the Noether charges

$$p_\mu \equiv -\frac{\partial L}{\partial \dot{x}^\mu} = Mc \frac{\dot{x}_\mu(\tau)}{\sqrt{g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}} = Mc u^\mu, \quad (8.75)$$

which satisfy the conservation law

$$\frac{d}{d\tau}p_\mu(t) = 0. \quad (8.76)$$

They are the conserved four-momenta of a free relativistic particle. The quantity

$$u^\mu \equiv \frac{\dot{x}^\mu}{\sqrt{g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}} \quad (8.77)$$

is the dimensionless relativistic four-velocity of the particle. It has the property $u^\mu u_\mu = 1$, and it is reparametrization invariant. By choosing for τ the physical time $t = x^0/c$, we can express u^μ in terms of the physical velocities $v^i = dx^i/dt$ as

$$u^\mu = \gamma(1, v^i/c), \quad \text{with} \quad \gamma \equiv \sqrt{1 - v^2/c^2}. \quad (8.78)$$

Note the minus sign in the definition (8.75) of the canonical momentum with respect to the nonrelativistic case. It is necessary to write Eq. (8.75) covariantly. The derivative with respect to $\dot{x}^\mu$ transforms like a covariant vector with a subscript μ , whereas the physical momenta are p^μ .

For small Lorentz transformations near the identity we write

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu, \quad (8.79)$$

where

$$\omega^\mu{}_\nu = g^{\mu\lambda}\omega_{\lambda\nu} \quad (8.80)$$

is an arbitrary infinitesimal antisymmetric matrix. An infinitesimal Lorentz transformation of the particle path is

$$\begin{aligned} \delta_s x^\mu(\tau) &= \dot{x}^\mu(\tau) - x^\mu(\tau) \\ &= \omega^\mu{}_\nu x^\nu(\tau). \end{aligned} \quad (8.81)$$

Under it, the symmetry variation of a Lorentz-invariant Lagrangian vanishes:

$$\delta_s L = \left(\frac{\partial L}{\partial x^\mu} x^\nu + \frac{\partial L}{\partial \dot{x}^\mu} \dot{x}^\nu \right) \omega^\mu{}_\nu = 0. \quad (8.82)$$

This has to be compared with the symmetry variation of the Lagrangian calculated via the chain rule with the help of the Euler-Lagrange equation

$$\begin{aligned} \delta_s L &= \left(\frac{\partial L}{\partial x^\mu} - \frac{d}{d\tau} \frac{\partial L}{\partial \dot{x}^\mu} \right) \delta_s x^\mu + \frac{d}{d\tau} \left[\frac{\partial L}{\partial \dot{x}^\mu} \delta_s x^\mu \right] \\ &= \frac{d}{d\tau} \left[\frac{\partial L}{\partial \dot{x}^\mu} \dot{x}^\nu \right] \omega^\mu{}_\nu \\ &= \frac{1}{2} \omega^\mu{}_\nu \frac{d}{d\tau} \left(x^\mu \frac{\partial L}{\partial \dot{x}_\nu} - x^\nu \frac{\partial L}{\partial \dot{x}_\mu} \right). \end{aligned} \quad (8.83)$$

By equating this with (8.82), we obtain the conserved rotational Noether charges [containing again a minus sign as in (8.75)]:

$$L^{\mu\nu} = -x^\mu \frac{\partial L}{\partial \dot{x}_\nu} + x^\nu \frac{\partial L}{\partial \dot{x}_\mu} = x^\mu p^\nu - x^\nu p^\mu. \quad (8.84)$$

They are four-dimensional generalizations of the angular momenta (8.50). The quantum-mechanical operators

$$\hat{L}^{\mu\nu} \equiv i(x^\mu \partial^\nu - x^\nu \partial^\mu) \quad (8.85)$$

obtained after the replacement $p^\mu \rightarrow i\partial/\partial x_\mu$ satisfy the four-dimensional spacetime generalization of the commutation relations (8.53):

$$[\hat{L}^{\mu\nu}, \hat{L}^{\kappa\lambda}] = i(g^{\mu\kappa} \hat{L}^{\nu\lambda} - g^{\mu\lambda} \hat{L}^{\nu\kappa} + g^{\nu\lambda} \hat{L}^{\mu\kappa} - g^{\nu\kappa} \hat{L}^{\mu\lambda}). \quad (8.86)$$

The quantities L^{ij} coincide with the earlier-introduced angular momenta (8.50). The conserved components

$$L^{0i} = x^0 p^i - x^i p^0 \equiv M_i \quad (8.87)$$

yield the relativistic generalization of the center-of-mass theorem (8.61):

$$M_i = \text{const.} \quad (8.88)$$

8.4 Generating the Symmetry Transformations

As mentioned in the introduction to this chapter, the relation between invariances and conservation laws has a second aspect. With the help of Poisson brackets, the charges associated with continuous symmetry transformations can be used to generate the symmetry transformation from which they were derived. Explicitly,

$$\delta_s \hat{x} = -i\epsilon[\hat{Q}, \hat{x}(t)]. \quad (8.89)$$

The charge derived in Section 7.2 from the invariance of the system under time displacement is the most famous example for this property. The charge (8.30) is by definition the *Hamiltonian*,

$$Q \equiv H,$$

whose operator version generates infinitesimal time displacements by the *Heisenberg equation of motion*:

$$\dot{\hat{x}}(t) = -i[\hat{H}, \hat{x}(t)]. \quad (8.90)$$

This equation is obviously the same as (8.89).

To quantize the system canonically, we may assume the Lagrangian to have the standard form

$$L(x, \dot{x}) = \frac{M}{2} \dot{x}^2 - V(x), \quad (8.91)$$

so that the *Hamiltonian operator* becomes, with the canonical momentum $p \equiv \dot{x}$:

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(\hat{x}). \quad (8.92)$$

Equation (8.90) is then a direct consequence of the canonical equal-time commutation rules

$$[\hat{p}(t), \hat{x}(t)] = -i, \quad [\hat{p}(t), \hat{p}(t)] = 0, \quad [\hat{x}(t), \hat{x}(t)] = 0. \quad (8.93)$$

The charges (8.41), derived in Section 7.3 from translational symmetry, are another famous example. After quantization, the commutation rule (8.89) becomes, with (8.38),

$$\epsilon^j = i\epsilon^i [\hat{p}^i(t), \hat{x}^j(t)]. \quad (8.94)$$

This coincides with one of the canonical commutation relations (here it appears only for time-independent momenta, since the system is translationally invariant).

The relativistic charges (8.75) of spacetime generate translations via

$$\delta_s \hat{x}^\mu = \epsilon^\mu = -i\epsilon^\nu [\hat{p}_\nu(t), \hat{x}^\mu(\tau)], \quad (8.95)$$

in agreement with the relativistic canonical commutation rules (29.27).

Similarly we find that the quantized versions of the conserved charges L_i in Eq. (8.51) generate infinitesimal rotations:

$$\delta_s \hat{x}^j = -\omega^i \epsilon_{ijk} \hat{x}^k(t) = i\omega^i [\hat{L}_i, \hat{x}^j(t)], \quad (8.96)$$

whereas the quantized conserved charges N^i of Eq. (8.61) generate infinitesimal Galilei transformations, and that the charges M_i of Eq. (8.87) generate pure rotational Lorentz transformations:

$$\begin{aligned} \delta_s \hat{x}^j &= \epsilon_i \hat{x}^0 = i\epsilon_i [M_i, \hat{x}^j], \\ \delta_s \hat{x}^0 &= \epsilon_i \hat{x}^i = i\epsilon_i [M_i, \hat{x}^0]. \end{aligned} \quad (8.97)$$

Since the quantized charges generate the rotational symmetry transformations, they form a *representation* of the generators of the symmetry group. When commuted with each other, they obey the same commutation rules as the generators of the symmetry group. The charges (8.51) associated with rotations, for example, have the commutation rules

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k, \quad (8.98)$$

which are the same as those between the 3×3 generators of the three-dimensional rotations $(L_i)_{jk} = -i\epsilon_{ijk}$.

The quantized charges of the generators (8.84) of the Lorentz group satisfy the commutation rules (8.86) of the 4×4 generators (8.85)

$$[\hat{L}^{\mu\nu}, \hat{L}^{\mu\lambda}] = -ig^{\mu\mu} \hat{L}^{\nu\lambda}. \quad (8.99)$$

This follows directly from the canonical commutation rules (8.95) [i.e., (29.27)].

8.5 Field Theory

A similar relation between continuous symmetries and constants of motion holds in field theory.

8.5.1 Continuous Symmetry and Conserved Currents

Let $\mathcal{A}$ be the action of an arbitrary field $\varphi(x)$,

$$\mathcal{A} = \int d^4x \mathcal{L}(\varphi, \partial\varphi, x), \quad (8.100)$$

and suppose that a transformation of the field

$$\delta_s \varphi(x) = \epsilon \Delta(\varphi, \partial\varphi, x) \quad (8.101)$$

changes the Lagrangian density $\mathcal{L}$ merely by a total derivative

$$\delta_s \mathcal{L} = \epsilon \partial_\mu \Lambda^\mu, \quad (8.102)$$

or equivalently, that it changes the action $\mathcal{A}$ by a surface term

$$\delta_s \mathcal{A} = \epsilon \int d^4x \partial_\mu \Lambda^\mu. \quad (8.103)$$

Then $\delta_s \mathcal{L}$ is called a *symmetry transformation*.

Given such a symmetry transformation, we can find a current four-vector

$$j^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \Delta - \Lambda^\mu \quad (8.104)$$

that has no four-divergence

$$\partial_\mu j^\mu(x) = 0. \quad (8.105)$$

The expression on the right-hand side of (8.104) is called a *Noether current*, and (8.105) is referred to as the associated *current conservation law*. It is a *local conservation law*.

The proof of (8.105) is just as simple as that of the time-independence of the charge (8.10) associated with the corresponding symmetry of the mechanical action (8.1) in Section 8.1. We calculate the symmetry variation of $\mathcal{L}$ under the symmetry transformation in a similar way as in Eq. (8.11), and find

$$\begin{aligned} \delta_s \mathcal{L} &= \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \right) \delta_s \varphi + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \delta_s \varphi \right) \\ &= \epsilon \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \right) \Delta + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \Delta \right). \end{aligned} \quad (8.106)$$

Then we invoke the Euler-Lagrange equation to remove the first term. Equating the second term with (8.102), we obtain

$$\partial_\mu j^\mu \equiv \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \Delta - \Lambda^\mu \right) = 0. \quad (8.107)$$

The relation between continuous symmetries and conservation is called *Noether's theorem* [1].

Assuming all fields to vanish at spatial infinity, we can derive from the local law (8.107) a *global conservation law* for the charge that is obtained from the spatial integral over the *charge density* j^0 :

$$Q(t) = \int d^3x j^0(\mathbf{x}, t). \quad (8.108)$$

Indeed, we may write the time derivative of the charge as an integral

$$\frac{d}{dt}Q(t) = \int d^3x \partial_0 j^0(\mathbf{x}, t) \quad (8.109)$$

and adding on the right-hand side a spatial integral over a total three-divergence, which vanishes due to the boundary conditions, we find

$$\frac{d}{dt}Q(t) = \int d^3x \partial_0 j^0(\mathbf{x}, t) = \int d^3x [\partial_0 j^0(\mathbf{x}, t) + \partial_i j^i(\mathbf{x}, t)] = 0. \quad (8.110)$$

Thus the charge is conserved:

$$\frac{d}{dt}Q(t) = 0. \quad (8.111)$$

8.5.2 Alternative Derivation

There is again an alternative derivation of the conserved current that is analogous to Eqs. (8.15)–(8.24). It is based on a variation of the fields under symmetry transformations whose parameter ϵ is made artificially spacetime-dependent $\epsilon \rightarrow \epsilon(x)$, thus extending (8.15) to

$$\delta_s^x \varphi(x) = \epsilon(x) \Delta(\varphi(x), \partial_\mu \varphi(x), x). \quad (8.112)$$

As before in Eq. (8.17), we calculate the Lagrangian density for a slightly transformed field

$$\varphi^\epsilon(x) \equiv \varphi(x) + \delta_s^x \varphi(x), \quad (8.113)$$

calling it

$$L^\epsilon \equiv L(\varphi^\epsilon(t), \partial \varphi^\epsilon(t)). \quad (8.114)$$

The corresponding action differs from the original one by

$$\delta_s^x \mathcal{A} = \int dx \left\{ \left[\frac{\partial \mathcal{L}^\epsilon}{\partial \epsilon(x)} - \partial_\mu \frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)} \right] \delta \epsilon(x) + \partial_\mu \left[\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)} \delta \epsilon(x) \right] \right\}. \quad (8.115)$$

From this we obtain the Euler-Lagrange-like equation

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \epsilon(x)} - \partial_\mu \frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)} = 0. \quad (8.116)$$

By assumption, the action is a pure surface term under x -independent transformations, implying that

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \epsilon(x)} = \partial_\mu \Lambda^\mu. \quad (8.117)$$

Together with (8.116), we see that

$$j^\mu = \frac{\partial \delta_s^x \mathcal{L}}{\partial \partial_\mu \epsilon(x)} - \Lambda^\mu \quad (8.118)$$

has no four-divergence. By the chain rule of differentiation we calculate

$$\delta_s^t \mathcal{L} = \frac{\partial \mathcal{L}(x)}{\partial \varphi} \epsilon \Delta + \frac{\partial \mathcal{L}}{\partial \partial_\nu \varphi} \partial_\nu \epsilon \Delta, \quad (8.119)$$

and see that

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \Delta(\varphi, \partial \varphi, x), \quad (8.120)$$

so that the current (8.118) coincides with (8.104).

8.5.3 Local Symmetries

If we apply the alternative derivation of a conserved current to a local symmetry, such as a local gauge symmetry, the current density (8.118) vanishes identically. Let us illuminate the symmetry origin of this phenomenon.

To be specific, we consider directly the field theory of electrodynamics. The theory does have a conserved charge resulting from the global U(1)-symmetry of the matter Lagrangian. There is a conserved current which is the source of a massless particle, the photon. This is described by a gauge field which is minimally coupled to the conserved current. A similar structure exists for many internal symmetries giving rise to nonabelian versions of the photon, such as gluons, whose exchange causes the strong interactions, and W - and Z -vector mesons, which mediate the weak interactions. It is useful to reconsider Noether's derivation of conservation laws in such theories.

The conserved matter current in a locally gauge-invariant theory cannot be found any more by the rule (8.118), which was so useful in the globally invariant theory. For the gauge transformation of quantum electrodynamics, the derivative with respect to the local field transformation $\epsilon(x)$ would simply be given by

$$j_\mu = \frac{\delta \mathcal{L}}{\partial \partial_\mu \Lambda}. \quad (8.121)$$

This would be identically equal to zero, due to local gauge invariance. We may, however, subject *just* the matter field to a local gauge transformation at *fixed* gauge fields. Then we obtain the correct current

$$j_\mu \equiv \left. \frac{\partial \mathcal{L}}{\partial \partial_\mu \Lambda} \right|_{\text{em}}. \quad (8.122)$$

Since the complete change under local gauge transformations $\delta_s^x \mathcal{L}$ vanishes identically, we can alternatively vary *only* the gauge fields and keep the particle orbit fixed:

$$j_\mu = - \left. \frac{\partial \mathcal{L}}{\partial \partial_\mu \Lambda} \right|_{\text{m}}. \quad (8.123)$$

This is done most simply by forming the functional derivative with respect to the gauge field, thereby omitting the contribution of $\mathcal{L}^{\text{em}}$:

$$j_\mu = - \frac{\partial \mathcal{L}^{\text{m}}}{\partial \partial_\mu \Lambda}. \quad (8.124)$$

An interesting consequence of local gauge invariance can be found for the gauge field itself. If we form the variation of the pure gauge field action

$$\delta_s^{\text{em}} \mathcal{A} = \int d^4x \, \text{tr} \left[\delta_s^x A_\mu \frac{\delta \mathcal{A}^{\text{em}}}{\delta A_\mu} \right], \quad (8.125)$$

and insert for $\delta_s^x A$ an infinitesimal pure gauge field configuration

$$\delta_s^x A_\mu = -i \partial_\mu \Lambda(x), \quad (8.126)$$

the right-hand side must vanish for all $\Lambda(x)$. After a partial integration this implies the local conservation law $\partial_\mu j^\mu(x) = 0$ for the current:

$$j^\mu(x) = -i \frac{\delta \mathcal{A}^{\text{em}}}{\delta A_\mu}. \quad (8.127)$$

In contrast to the earlier conservation laws derived for matter fields, which were valid only if the matter fields obey the Euler-Lagrange equations, the current conservation law for gauge fields is valid for *all* field configurations. It is an *identity* which we may call *Bianchi identity* due to its close analogy with the Bianchi identities in Riemannian geometry.

To verify the conservation of (12.63), we insert the Lagrangian (12.3) into (12.63) and find $j^\nu = \partial_\mu F^{\mu\nu}/2$. This current is trivially conserved for any field configuration due to the antisymmetry of $F^{\mu\nu}$.

8.6 Canonical Energy-Momentum Tensor

As an important example for the field theoretic version of the theorem, consider the usual case that the Lagrangian density does not depend explicitly on the spacetime coordinates x :

$$\mathcal{L} = \mathcal{L}(\varphi, \partial\varphi). \quad (8.128)$$

We then perform a translation along an arbitrary direction $\nu = 0, 1, 2, 3$ of spacetime

$$x'^\mu = x^\mu - \epsilon^\mu, \quad (8.129)$$

under which field $\varphi(x)$ transforms as

$$\varphi'(x') = \varphi(x). \quad (8.130)$$

This equation expresses the fact that the field has the same value at the same absolute point in space and time, which in one coordinate system is labeled by the coordinates x^μ and in the other by x'^μ .

Under an infinitesimal translation of the field configuration coordinate, the Lagrangian density undergoes the following symmetry variation

$$\begin{aligned} \delta_s \mathcal{L} &\equiv \mathcal{L}(\varphi'(x), \partial\varphi'(x)) - \mathcal{L}(\varphi(x), \partial\varphi(x)) \\ &= \frac{\partial \mathcal{L}}{\partial \varphi(x)} \delta_s \varphi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \partial_\mu \delta_s \varphi(x), \end{aligned} \quad (8.131)$$

where

$$\delta_s \varphi(x) = \varphi'(x) - \varphi(x) \quad (8.132)$$

is the symmetry variation of the fields. For the particular transformation (8.130) the symmetry variation becomes simply

$$\delta_s \varphi(x) = \epsilon^\nu \partial_\nu \varphi(x). \quad (8.133)$$

The Lagrangian density (8.128) changes by

$$\delta_s \mathcal{L}(x) = \epsilon^\nu \partial_\nu \mathcal{L}(x). \quad (8.134)$$

Hence the requirement (8.103) is satisfied and $\delta_s \varphi(x)$ is a symmetry transformation. The function Λ happens to coincide with the Lagrangian density

$$\Lambda = \mathcal{L}. \quad (8.135)$$

We can now define a set of currents $j_\nu{}^\mu$, one for each ϵ^ν . In the particular case at hand, the currents $j_\nu{}^\mu$ are denoted by $\Theta_\nu{}^\mu$, and read:

$$\Theta_\nu{}^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \partial_\nu \varphi - \delta_\nu{}^\mu \mathcal{L}. \quad (8.136)$$

They have no four-divergence

$$\partial_\mu \Theta_\nu{}^\mu(x) = 0. \quad (8.137)$$

As a consequence, the *total four-momentum* of the system, defined by

$$P^\mu = \int d^3x \Theta^{\mu 0}(x), \quad (8.138)$$

is independent of time.

The alternative derivation of the currents goes as follows. Introducing

$$\delta_s^x \varphi(x) = \epsilon^\nu(x) \partial_\nu \varphi(x), \quad (8.139)$$

we see that

$$\delta_s^x \varphi(x) = \varphi^\nu(x) \partial_\nu \varphi(x). \quad (8.140)$$

On the other hand, the chain rule of differentiation yields

$$\delta_s^x \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \varphi(x)} \epsilon^\nu(x) \partial_\nu \varphi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi(x)} \{ [\partial_\mu \epsilon^\nu(x)] \partial_\nu \varphi + \epsilon^\nu \partial_\mu \partial_\nu \varphi(x) \}. \quad (8.141)$$

Hence

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon^\nu(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \partial_\nu \varphi, \quad (8.142)$$

and we obtain once more the energy-momentum tensor (8.136).

Note that (8.142) can also be written as

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon^\nu(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \frac{\partial \delta_s^x \varphi}{\partial \epsilon^\nu(x)}. \quad (8.143)$$

Since ν is a contravariant vector index, the set of currents $\Theta_\nu{}^\mu$ forms a Lorentz tensor called the *canonical energy-momentum tensor*. The component

$$\Theta_0{}^0 = \frac{\partial \mathcal{L}}{\partial \partial_0 \varphi} \partial_0 \varphi - \mathcal{L} \quad (8.144)$$

is recognized to be the Hamiltonian density in the canonical formalism.

8.6.1 Electromagnetism

As an important physical application of the field theoretic Noether theorem, consider the free electromagnetic field with the action

$$\mathcal{L} = -\frac{1}{4c} F_{\lambda\kappa} F^{\lambda\kappa}, \quad (8.145)$$

where $F_{\lambda\kappa}$ are the components of the field strength $F_{\lambda\kappa} \equiv \partial_\lambda A_\kappa - \partial_\kappa A_\lambda$. Under a translation in space and time from x^μ to $x^\mu - \epsilon \delta_\nu^\mu$, the vector potential undergoes a similar change as in (8.130):

$$A'^\mu(x') = A^\mu(x). \quad (8.146)$$

As before, this equation expresses the fact that at the same absolute spacetime point, which in the two coordinate frames is labeled once by x' and once by x , the field components have the same numerical values. The equation transformation law (8.146) can be rewritten in an infinitesimal form as

$$\begin{aligned}\delta_s A^\lambda(x^\mu) &\equiv A'^\lambda(x^\mu) - A^\lambda(x^\mu) \\ &= A'^\lambda(x'^\mu + \epsilon \delta_\nu^\mu) - A^\lambda(x^\mu) \\ &= \epsilon \partial_\nu A^\lambda(x^\mu).\end{aligned}\tag{8.147}$$

$$\tag{8.148}$$

Under it, the field tensor changes as follows

$$\delta_s F^{\lambda\kappa} = \epsilon \partial_\nu F^{\lambda\kappa}, \tag{8.149}$$

so that the Lagrangian density is a total four-divergence:

$$\delta_s \mathcal{L} = -\epsilon \frac{1}{2c} F_{\lambda\kappa} \partial_\nu F^{\lambda\kappa} = \epsilon \partial_\nu \mathcal{L} \tag{8.150}$$

Thus, the spacetime translations (8.148) are symmetry transformations, and the currents

$$\Theta_\nu{}^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu A^\lambda} \partial_\nu A^\lambda - \delta_\nu{}^\mu \mathcal{L} \tag{8.151}$$

are conserved:

$$\partial_\mu \Theta_\nu{}^\mu(x) = 0. \tag{8.152}$$

Using $\partial \mathcal{L} / \partial \partial_\mu A^\lambda = -F^\mu{}_\lambda$, the currents (8.151) become more explicitly

$$\Theta_\nu{}^\mu = -\frac{1}{c} \left(F^\mu{}_\lambda \partial_\nu A^\lambda - \frac{1}{4} \delta_\nu{}^\mu F^{\lambda\kappa} F_{\lambda\kappa} \right). \tag{8.153}$$

They form the *canonical energy-momentum tensor* of the electromagnetic field.

8.6.2 Dirac Field

We now turn to the Dirac field which has the well-known action

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \bar{\psi}(x) (i \gamma^\mu \overleftrightarrow{\partial}_\mu - M) \psi(x), \tag{8.154}$$

where γ^μ are the Dirac matrices

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix}. \tag{8.155}$$

Here σ^μ , $\tilde{\sigma}^\mu$ are four 2×2 matrices

$$\sigma^\mu \equiv (\sigma^0, \sigma^i), \tilde{\sigma}^\mu \equiv (\sigma^0, -\sigma^i), \tag{8.156}$$

whose zeroth component is the unit matrix

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (8.157)$$

and whose spatial components consist of the *Pauli spin matrices*

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.158)$$

On behalf of the algebraic properties of the Pauli matrices

$$\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk} \sigma^k, \quad (8.159)$$

the Dirac matrices (8.155) satisfy the anticommutation rules

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \quad (8.160)$$

Under spacetime translations

$$x'^\mu = x^\mu - \epsilon^\mu, \quad (8.161)$$

the Dirac field transforms in the same way as the previous scalar and vector fields:

$$\psi'(x') = \psi(x), \quad (8.162)$$

or infinitesimally:

$$\delta_s \psi(x) = \epsilon^\mu \partial_\mu \psi(x). \quad (8.163)$$

The same is true for the Lagrangian density, where

$$\mathcal{L}'(x') = \mathcal{L}(x), \quad (8.164)$$

and

$$\delta_s \mathcal{L}(x) = \epsilon^\mu \partial_\mu \mathcal{L}(x). \quad (8.165)$$

Thus we obtain the Noether current

$$\Theta_\nu{}^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu \psi^\lambda} \partial_\nu \psi^\lambda + \text{c.c.} - \delta_\nu{}^\mu \mathcal{L}, \quad (8.166)$$

with the local conservation law

$$\partial_\mu \Theta_\nu{}^\mu(x) = 0. \quad (8.167)$$

From (8.154), we see that

$$\frac{\partial \mathcal{L}}{\partial \partial_\mu \psi^\lambda} = \frac{1}{2} \bar{\psi} \gamma^\mu, \quad (8.168)$$

so that we obtain the *canonical energy-momentum tensor* of the Dirac field:

$$\Theta_\nu{}^\mu = \frac{1}{2} \bar{\psi} \gamma^\mu \partial_\nu \psi^\lambda + \text{c.c.} - \delta_\nu{}^\mu \mathcal{L} \quad (8.169)$$

8.7 Angular Momentum

Let us now turn to angular momentum in field theory. Consider first the case of a scalar field $\varphi(\dot{x})$. Under a rotation of the coordinates,

$$x'^i = R^i_j x^j, \quad (8.170)$$

the field does not change, if considered at the same space point, i.e.,

$$\varphi'(x'^i) = \varphi(x^i). \quad (8.171)$$

The infinitesimal symmetry variation is:

$$\delta_s \varphi(x) = \varphi'(x) - \varphi(x). \quad (8.172)$$

Using the infinitesimal form (8.46) of (8.170),

$$\delta x^i = -\omega_{ij} x^j, \quad (8.173)$$

we see that

$$\begin{aligned} \delta_s \varphi(x) &= \varphi'(x^0, x'^i - \delta x^i) - \varphi(x) \\ &= \partial_i \varphi(x) x^j \omega_{ij}. \end{aligned} \quad (8.174)$$

Suppose we are dealing with a Lorentz-invariant Lagrangian density that has no explicit x -dependence:

$$\mathcal{L} = \mathcal{L}(\varphi(x), \partial\varphi(x)). \quad (8.175)$$

Then the symmetry variation is

$$\begin{aligned} \delta_s \mathcal{L} &= \mathcal{L}(\varphi'(x), \partial\varphi'(x)) - \mathcal{L}(\varphi(x), \partial\varphi(x)) \\ &= \frac{\partial \mathcal{L}}{\partial \varphi(x)} \delta_s \varphi(x) + \frac{\partial \mathcal{L}}{\partial \partial \varphi(x)} \partial_\mu \delta_s \varphi(x). \end{aligned} \quad (8.176)$$

For a Lorentz-invariant $\mathcal{L}$, the derivative $\partial \mathcal{L} / \partial \partial_\mu \varphi$ is a vector proportional to $\partial_\mu \varphi$.

For the Lagrangian density, the rotational symmetry variation Eq. (8.174) becomes

$$\begin{aligned} \delta_s \mathcal{L} &= \left[\frac{\partial \mathcal{L}}{\partial \varphi} \partial_i \varphi x^j + \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \partial_\mu (\partial_i \mathcal{L} x^j) \right] \omega_{ij} \\ &= \left[(\partial_i \mathcal{L}) x^j + \frac{\partial \mathcal{L}}{\partial \partial_j \varphi} \partial_i \varphi \right] \omega_{ij} = \partial_i (\mathcal{L} x^j \omega_{ij}). \end{aligned} \quad (8.177)$$

The right-hand side is a total derivative. In arriving at this result, the antisymmetry of φ_{ij} has been used twice: first for dropping the second term in the brackets, which

is possible since $\partial\mathcal{L}/\partial\partial_i\varphi$ is proportional to $\partial_i\varphi$ as a consequence of the assumed rotational invariance¹ of $\mathcal{L}$. Second it is used to pull x^j inside the last parentheses.

Calculating $\delta_s\mathcal{L}$ once more with the help of the Euler-Lagrange equations gives

$$\begin{aligned}\delta_s\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\mathcal{L}}\delta_s\varphi + \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\mu\delta_s\varphi \\ &= \left(\frac{\partial\mathcal{L}}{\partial\varphi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\right)\delta_s\varphi + \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\delta_s\varphi\right) \\ &= \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_i\varphi x^j\right)\omega_{ij}.\end{aligned}\tag{8.178}$$

Thus the Noether charges

$$L^{ij,\mu} = \left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_i\varphi x^j - \delta_i^\mu\mathcal{L} x^j\right) - (i \leftrightarrow j)\tag{8.179}$$

have no four-divergence

$$\partial_\mu L^{ij,\mu} = 0.\tag{8.180}$$

The associated charges

$$L^{ij} = \int d^3x L^{ij,\mu}\tag{8.181}$$

are called the *total angular momenta* of the field system. In terms of the canonical energy-momentum tensor

$$\Theta_\nu^\mu = \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\nu\varphi - \delta_\nu^\mu\mathcal{L},\tag{8.182}$$

the current density $L^{ij,\mu}$ can also be rewritten as

$$L^{ij,\mu} = x^i\Theta^{j\mu} - x^j\Theta^{i\mu}.\tag{8.183}$$

8.8 Four-Dimensional Angular Momentum

A similar procedure can be applied to pure Lorentz transformations. An infinitesimal boost to rapidity ζ^i produces a coordinate change

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu = x^\mu + \delta^\mu{}_i \zeta^i x^\nu + \delta^\mu{}_0 \zeta^i x^i.\tag{8.184}$$

This can be written as

$$\delta x^\mu = \omega^\mu{}_\nu x^\nu,\tag{8.185}$$

¹Recall the similar argument after Eq. (8.48)

where

$$\begin{aligned}\omega_{ij} &= 0, \\ \omega_{0i} &= -\omega_{i0} = \zeta^i.\end{aligned}\tag{8.186}$$

With the tensor $\omega^\mu{}_\nu$, the restricted Lorentz transformations and the infinitesimal rotations can be treated on the same footing. The rotations have the form (8.185) for the particular choice

$$\begin{aligned}\omega_{ij} &= \epsilon_{ijk}\omega^k, \\ \omega_{0i} &= \omega_{i0} = 0.\end{aligned}\tag{8.187}$$

We can now identify the symmetry variations of the field as being

$$\begin{aligned}\delta_s\varphi(x) &= \varphi'(x'^\mu - \delta x^\mu) - \varphi(x) \\ &= -\partial_\mu\varphi(x)x^\nu\omega^\mu{}_\nu.\end{aligned}\tag{8.188}$$

Just as in (8.177), the Lagrangian density transforms as the total derivative

$$\delta_s\varphi = -\partial_\mu(\mathcal{L}x^\nu)\omega^\mu{}_\nu,\tag{8.189}$$

and we obtain the Noether currents

$$L^{\mu\nu,\lambda} = -\left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda\varphi}\partial^\lambda\varphi x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) + (\mu \leftrightarrow \nu).\tag{8.190}$$

The right-hand side can be expressed in terms of the canonical energy-momentum tensor (8.136), so that we find

$$\begin{aligned}L^{\mu\nu,\lambda} &= -\left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda\varphi}\partial^\lambda\varphi x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) + (\mu \leftrightarrow \nu) \\ &= x^\mu\Theta^{\nu\lambda} - x^\nu\Theta^{\mu\lambda}.\end{aligned}\tag{8.191}$$

These currents have no four-divergence

$$\partial_\lambda L^{\mu\nu,\lambda} = 0.\tag{8.192}$$

The associated charges

$$L^{\mu\nu} \equiv \int d^3x L^{\mu\nu,0}\tag{8.193}$$

are independent of time.

For the particular form of $\omega_{\mu\nu}$ in (8.186), we find time-independent components L^{i0} . The components L^{ij} coincide with the previously-derived angular momenta.

The constancy of L^{i0} is the relativistic version of the *center-of-mass theorem* (8.65). Indeed, since

$$L^{i0} = \int d^3x (x^i\Theta^{00} - x^0\Theta^{i0}),\tag{8.194}$$

we can define the relativistic center of mass

$$x_{\text{CM}}^i = \frac{\int d^3x \Theta^{00} x^i}{\int d^3x \Theta^{00}}, \quad (8.195)$$

and the average velocity

$$v_{\text{CM}}^i = c \frac{\int d^3x \Theta^{i0}}{\int d^3x \Theta^{00}} = c \frac{P^i}{P^0}. \quad (8.196)$$

Since $\int d^3x \Theta^{i0} = P^i$ is the constant momentum of the system, also v_{CM}^i is a constant. Thus, the constancy of L^{0i} implies the center-of-mass moves with the constant velocity

$$x_{\text{CM}}^i(t) = x_{0\text{CM}}^i + v_{0\text{CM}}^i t, \quad (8.197)$$

with $x_{0\text{CM}}^i = L^{0i}/P^0$. The quantities $L^{\mu\nu}$ are referred to as four-dimensional orbital angular momenta.

It is important to point out that the vanishing divergence of $L^{\mu\nu,\lambda}$ makes $\Theta^{\nu\mu}$ symmetric:

$$\begin{aligned} \partial_\lambda L^{\mu\nu,\lambda} &= \partial_\lambda (x^\mu \Theta^{\nu\lambda} - x^\nu \Theta^{\mu\lambda}) \\ &= \Theta^{\nu\mu} - \Theta^{\mu\nu} = 0. \end{aligned} \quad (8.198)$$

Thus, translationally invariant field theories whose orbital angular momentum is conserved have always a symmetric canonical energy-momentum tensor.

$$\Theta^{\mu\nu} = \Theta^{\nu\mu}. \quad (8.199)$$

8.9 Spin Current

If the field $\varphi(x)$ is no longer a scalar but carries spin degrees of freedom, the derivation of the four-dimensional angular momentum becomes slightly more involved.

8.9.1 Electromagnetic Fields

Consider first the case of electromagnetism where the relevant field is the four-vector potential $A^\mu(x)$. When going to a new coordinate frame

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu, \quad (8.200)$$

the vector field at the same point remains unchanged in absolute spacetime. However, since the components A^μ refer to two different basic vectors in the different frames, they must be transformed accordingly. Indeed, since A^μ is a vector and transforms like x^μ , it must satisfy the relation characterizing a *vector field*:

$$A'^\mu(x') = \Lambda^\mu{}_\nu A^\nu(x). \quad (8.201)$$

For an infinitesimal transformation

$$\delta_s x^\mu = \omega^\mu{}_\nu x^\nu, \quad (8.202)$$

this implies a symmetry variation

$$\begin{aligned} \delta_s A^\mu(x) &= A'^\mu(x) - A^\mu(x) = A'^\mu(x - \delta x) - A^\mu(x) \\ &= \omega^\mu{}_\nu A^\nu(x) - \omega^\lambda{}_\nu x^\nu \partial_\lambda A^\mu. \end{aligned} \quad (8.203)$$

The first term is a *spin transformation*, the other an *orbital transformation*. The orbital transformation can also be written in terms of the generators $\hat{L}_{\mu\nu}$ of the Lorentz group defined in (8.84) as

$$\delta_s^{\text{orb}} A^\mu(x) = -i\omega^{\mu\nu} \hat{L}_{\mu\nu} A(x). \quad (8.204)$$

It is convenient to introduce 4×4 spin transformation matrices $L_{\mu\nu}$ with the matrix elements:

$$(L_{\mu\nu})_{\lambda\kappa} \equiv i(g_{\mu\lambda}g_{\nu\kappa} - g_{\mu\kappa}g_{\nu\lambda}). \quad (8.205)$$

They satisfy the same commutation relations (8.86) as the differential operators $\hat{L}_{\mu\nu}$ defined in Eq. (8.85). By adding together the two generators $\hat{L}_{\mu\nu}$ and $L_{\mu\nu}$, we form the operator of total four-dimensional angular momentum

$$\hat{J}_{\mu\nu} \equiv \hat{L}_{\mu\nu} + L_{\mu\nu}, \quad (8.206)$$

and can write the symmetry variation (8.203) as

$$\delta_s^{\text{orb}} A^\mu(x) = -i\omega^{\mu\nu} \hat{J}_{\mu\nu} A(x). \quad (8.207)$$

If the Lagrangian density involves only scalar combinations of four-vectors A^μ , and if it has no explicit x -dependence, it changes under Lorentz transformations like a scalar field:

$$\mathcal{L}'(x') \equiv \mathcal{L}(A'(x'), \partial' A'(x')) = \mathcal{L}(A(x), \partial A(x)) \equiv \mathcal{L}(x). \quad (8.208)$$

Infinitesimally, this makes the symmetry variation a pure gradient term:

$$\delta_s \mathcal{L} = -(\partial_\mu \mathcal{L} x^\nu) \omega^\mu{}_\nu. \quad (8.209)$$

Thus Lorentz transformations are symmetry transformations in the Noether sense. Following Noether's construction (8.179), we calculate the *current of total four-dimensional angular momentum*:

$$J^{\mu\nu,\lambda} = \frac{\partial \mathcal{L}}{\partial \partial_\lambda A_\mu} A^\nu - \left(\frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} \partial^\mu A^\kappa x^\nu - \delta^{\mu\lambda} \mathcal{L} x^\nu \right) - (\mu \leftrightarrow \nu). \quad (8.210)$$

The last two terms have the same form as the current $L^{\mu\nu,\lambda}$ of the four-dimensional angular momentum of the scalar field. Here they are the *currents of the four-dimensional orbital angular momentum*:

$$L^{\mu\nu,\lambda} = - \left(\frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} \partial^\mu A^\kappa x^\nu - \delta^{\mu\lambda} \mathcal{L} x^\nu \right) + (\mu \leftrightarrow \nu). \quad (8.211)$$

Note that this current has the form

$$L^{\mu\nu,\lambda} = -i \frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} \hat{L}^{\mu\nu} A^\kappa + \left[\delta^{\mu\lambda} \mathcal{L} x^\nu - (\mu \leftrightarrow \nu) \right], \quad (8.212)$$

where $\hat{L}^{\mu\nu}$ are the differential operators of four-dimensional angular momentum in the commutation rules (8.86).

Just as the scalar case (8.191), the currents (8.211) can be expressed in terms of the canonical energy-momentum tensor as

$$L^{\mu\nu,\lambda} = x^\mu \Theta^{\nu\lambda} - x^\nu \Theta^{\mu\lambda}. \quad (8.213)$$

The first term in (8.210),

$$\Sigma^{\mu\nu,\lambda} = \left[\frac{\partial \mathcal{L}}{\partial \partial_\lambda A_\nu} A^\nu - (\mu \leftrightarrow \nu) \right], \quad (8.214)$$

is referred to as the *spin current*. It can be written in terms of the 4×4 -generators (8.205) of the Lorentz group as

$$\Sigma^{\mu\nu,\lambda} = -i \frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} (L^{\mu\nu})_{\kappa\sigma} A^\sigma. \quad (8.215)$$

The two currents together,

$$J^{\mu\nu,\lambda}(x) \equiv L^{\mu\nu,\lambda}(x) + \Sigma^{\mu\nu,\lambda}(x), \quad (8.216)$$

are conserved, satisfying $\partial_\lambda J^{\mu\nu,\lambda}(x) = 0$. Individually, they are not conserved.

The total angular momentum is given by the charge

$$J^{\mu\nu} = \int d^3x J^{\mu\nu,0}(x). \quad (8.217)$$

It is a constant of motion. Using the conservation law of the energy-momentum tensor we find, just as in (8.198), that the orbital angular momentum satisfies

$$\partial_\lambda L^{\mu\nu,\lambda}(x) = - [\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)]. \quad (8.218)$$

From this we find the divergence of the spin current

$$\partial_\lambda \Sigma^{\mu\nu,\lambda}(x) = - [\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)]. \quad (8.219)$$

For the charges associated with orbital and spin currents

$$L^{\mu\nu}(t) \equiv \int d^3x L^{\mu\nu,0}(x), \quad \Sigma^{\mu\nu}(t) \equiv \int d^3x \Sigma^{\mu\nu,0}(x), \quad (8.220)$$

this implies the following time dependence:

$$\begin{aligned} \dot{L}^{\mu\nu}(t) &= - \int d^3x [\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)], \\ \dot{\Sigma}^{\mu\nu}(t) &= \int d^3x [\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)]. \end{aligned} \quad (8.221)$$

Thus fields with a nonzero spin density have always a non-symmetric energy momentum tensor.

In general, the current density $J^{\mu\nu,\lambda}$ of total angular momentum reads

$$J^{\mu\nu,\lambda} = \left(\frac{\partial \delta_s^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} - \delta^{\mu\lambda} \mathcal{L} x^\nu \right) - (\mu \leftrightarrow \nu). \quad (8.222)$$

By the chain rule of differentiation, the derivative with respect to $\partial_\lambda \omega_{\mu\nu}(x)$ can come only from field derivatives, for a scalar field

$$\frac{\partial \delta_s^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\lambda \varphi} \frac{\partial \delta_s^x \varphi}{\partial \omega_{\mu\nu}(x)}, \quad (8.223)$$

and for a vector field

$$\frac{\partial \delta_s^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} \frac{\partial \delta_s^x A^\kappa}{\partial \omega_{\mu\nu}}. \quad (8.224)$$

The alternative rule of calculating angular momenta is to introduce spacetime-dependent transformations

$$\delta^x x = \omega^\mu{}_\nu(x) x^\nu, \quad (8.225)$$

under which the scalar fields transform as

$$\delta_s \varphi = -\partial_\lambda \varphi \omega^\lambda{}_\nu(x) x^\nu, \quad (8.226)$$

and the Lagrangian density as

$$\delta_s^x \varphi = -\partial_\lambda \mathcal{L} \omega^\lambda{}_\nu(x) x^\nu = -\partial_\lambda (x^\nu \mathcal{L}) \omega^\lambda{}_\nu(x). \quad (8.227)$$

By separating spin and orbital transformations of $\delta_s^x A^\kappa$, we find the two contributions $\sigma^{\mu\nu,\lambda}$ and $L^{\mu\nu,\lambda}$ to the current $J^{\mu\nu,\lambda}$ of the total angular momentum, the latter receiving a contribution from the second term in (8.222).

8.9.2 Dirac Field

We now turn to the Dirac field. Under a Lorentz transformation (8.200), this transforms according to the law

$$\psi(x') \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda) \psi(x), \quad (8.228)$$

where $D(\Lambda)$ are the 4×4 spinor representation matrices of the Lorentz group. Their matrix elements can most easily be specified for infinitesimal transformations. For an infinitesimal Lorentz transformation

$$\Lambda_\mu{}^\nu = \delta_\mu{}^\nu + \omega_\mu{}^\nu, \quad (8.229)$$

under which the coordinates are changed by

$$\delta_s x^\mu = \omega^\mu{}_\nu x^\nu, \quad (8.230)$$

the spin components transform under the representation matrix

$$D(\delta_\mu{}^\nu + \omega_\mu{}^\nu) = \left(1 - i\frac{1}{2}\omega_{\mu\nu}\sigma^{\mu\nu}\right), \quad (8.231)$$

where $\sigma_{\mu\nu}$ are the 4×4 matrices acting on the spinor space

$$\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]. \quad (8.232)$$

From the anticommutation rules (8.160), it is easy to verify that the spin matrices $S_{\mu\nu} \equiv \sigma_{\mu\nu}/2$ satisfy the same commutation rules (8.86) as the previous orbital and spin-1 generators $\hat{L}_{\mu\nu}$ and $L_{\mu\nu}$ of Lorentz transformations.

The field has the symmetry variation [compare (8.203)]:

$$\begin{aligned} \delta_s \psi(x) &= \psi'(x) - \psi(x) = D(\delta_\mu{}^\nu + \omega_\mu{}^\nu)\psi(x - \delta x) - \psi(x) \\ &= -i\frac{1}{2}\omega_{\mu\nu}\sigma^{\mu\nu}\psi(x) - \omega^\lambda{}_\nu x^\nu \partial_\lambda \psi(x) \\ &= -i\frac{1}{2}\omega_{\mu\nu}(S^{\mu\nu} + \hat{L}^{\mu\nu})\psi(x) \equiv -i\frac{1}{2}\omega_{\mu\nu}\hat{J}^{\mu\nu}\psi(x), \end{aligned} \quad (8.233)$$

the last line showing the separation into spin and orbital transformation for a Dirac particle.

Since the Dirac Lagrangian is Lorentz-invariant, it changes under Lorentz transformations like a scalar field [compare (8.208)]:

$$\mathcal{L}'(x') = \mathcal{L}(x). \quad (8.234)$$

Infinitesimally, this amounts to

$$\delta_s \mathcal{L} = -(\partial_\mu \mathcal{L} x^\mu)_{,\nu}. \quad (8.235)$$

With the Lorentz transformations being symmetry transformations in the Noether sense, we calculate the *current of total four-dimensional angular momentum* extending the formulas (8.191) and (8.210) for scalar field and vector potential. The result is

$$J^{\mu\nu,\lambda} = \left(-i\frac{\partial \mathcal{L}}{\partial \partial_\lambda \psi}\sigma^{\mu\nu}\psi - i\frac{\partial \mathcal{L}}{\partial \partial_\lambda \psi}\hat{L}^{\mu\nu}\psi + \text{c.c.}\right) + [\delta^{\mu\lambda}\mathcal{L}x^\nu - (\mu \leftrightarrow \nu)]. \quad (8.236)$$

As before in (8.211) and (8.191), the orbital part of (8.236) can be expressed in terms of the canonical energy-momentum tensor as

$$L^{\mu\nu,\lambda} = x^\mu \Theta^{\nu\lambda} - x^\nu \Theta^{\mu\lambda}. \quad (8.237)$$

The first term in (8.236) is the *spin current*

$$\Sigma^{\mu\nu,\lambda} = \frac{1}{2} \left(-i \frac{\partial \mathcal{L}}{\partial \partial_\lambda \psi} \sigma^{\mu\nu} \psi + \text{c.c.} \right). \quad (8.238)$$

Inserting (8.168), this becomes explicitly

$$\Sigma^{\mu\nu,\lambda} = -\frac{i}{2} \bar{\psi} \gamma^\lambda \sigma^{\mu\nu} \psi = \frac{1}{2} \bar{\psi} \gamma^{[\mu} \gamma^\nu \gamma^{\lambda]} \psi = \frac{1}{2} \epsilon^{\mu\nu\lambda\kappa} \bar{\psi} \gamma^\kappa \psi. \quad (8.239)$$

The spin density is completely antisymmetric in the three indices [3].

The conservation properties of the three currents are the same as in Eqs. (8.217)–(8.221).

Due to the presence of spin, the energy-momentum tensor is nonsymmetric.

8.10 Symmetric Energy-Momentum Tensor

Since the presence of spin is the cause of asymmetry of the canonical energy-momentum tensor, it is suggestive that an appropriate use of the spin current should help to construct a new modified momentum tensor

$$T^{\mu\nu} = \Theta^{\mu\nu} + \Delta \Theta^{\nu\mu}, \quad (8.240)$$

that is symmetric, while still having the fundamental property of $\Theta^{\mu\nu}$ that its spatial integral $P^\mu = \int d^3x T^{\mu 0}$ yields the total energy-momentum vector of the system. This is ensured by the fact that $\Delta \Theta^{\mu 0}$ being a three-divergence of a spatial vector. Such a construction was found in 1939 by Belinfante [4]. He introduced the tensor

$$T^{\mu\nu} = \Theta^{\mu\nu} - \frac{1}{2} \partial_\lambda (\Sigma^{\mu\nu,\lambda} - \Sigma^{\nu\lambda,\mu} + \Sigma^{\lambda\mu,\nu}), \quad (8.241)$$

whose symmetry is manifest, due to (8.219) and the symmetry of the last two terms under the exchange $\mu \leftrightarrow \nu$. Moreover, the relation (8.241) for the $\mu 0$ -components of (8.241),

$$T^{\mu 0} = \Theta^{\mu 0} - \frac{1}{2} \partial_\lambda (\Sigma^{\mu 0,\lambda} - \Sigma^{0\lambda,\mu} + \Sigma^{\lambda\mu,0}), \quad (8.242)$$

ensures that the spatial integral over $J^{\mu\nu,0} \equiv x^\mu T^{\nu 0} - x^\nu T^{\mu 0}$ leads to the same total angular momentum

$$J^{\mu\nu} = \int d^3x J^{\mu\nu,0} \quad (8.243)$$

as the canonical expression (8.216). Indeed, the zeroth component of (8.242) is

$$x^\mu \Theta^{\nu 0} - x^\nu \Theta^{\mu 0} - \frac{1}{2} \left[\partial_k (\Sigma^{\mu 0, k} - \Sigma^{0k, \mu} + \Sigma^{k\mu, 0}) x^\nu - (\mu \leftrightarrow \nu) \right]. \quad (8.244)$$

Integrating the second term over d^3x and performing a partial integration gives, for $\mu = 0, \nu = i$:

$$-\frac{1}{2} \int d^3x \left[x^0 \partial_k (\Sigma^{i0, k} - \Sigma^{0k, i} + \Sigma^{ki, 0}) - x^i \partial_k (\Sigma^{00, k} - \Sigma^{0k, 0} + \Sigma^{k0, 0}) \right] = \int d^3x \Sigma^{0i, 0}, \quad (8.245)$$

and for $\mu = i, \nu = j$:

$$-\frac{1}{2} \int d^3x \left[x^i \partial_k (\Sigma^{j0, k} - \Sigma^{0k, j} + \Sigma^{kj, 0}) - (i \leftrightarrow j) \right] = \int d^3x \Sigma^{ij, 0}. \quad (8.246)$$

The right-hand sides are the contributions of spin to the total angular momentum.

For the electromagnetic field, the spin current (8.214) reads explicitly

$$\Sigma^{\mu\nu, \lambda} = -\frac{1}{c} \left[F^{\lambda\mu} A^\nu - (\mu \leftrightarrow \nu) \right]. \quad (8.247)$$

From this we calculate the Belinfante correction

$$\begin{aligned} \Delta\Theta^{\mu\nu} &= \frac{1}{2c} [\partial_\lambda (F^{\lambda\mu} A^\nu - F^{\lambda\nu} A^\mu) - \partial_\lambda (F^{\mu\nu} A^\lambda - F^{\mu\lambda} A^\nu) + \partial_\lambda (F^{\nu\lambda} A^\mu - F^{\nu\mu} A^\lambda)] \\ &= \frac{1}{c} \partial_\lambda (F^{\nu\lambda} A^\mu). \end{aligned} \quad (8.248)$$

Adding this to the canonical energy-momentum tensor (8.153)

$$\Theta^{\mu\nu} = -\frac{1}{c} (F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa}), \quad (8.249)$$

we find the symmetric energy-momentum tensor

$$T^{\mu\nu} = -\frac{1}{c} (F^\nu{}_\lambda F^{\mu\lambda} - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa}) + \frac{1}{c} (\partial_\lambda F^{\nu\lambda}) A^\mu. \quad (8.250)$$

The last term vanishes due to the free Maxwell field equations, $\partial_\lambda F^{\mu\nu} = 0$. Therefore it can be dropped. Note that the proof of the symmetry of $T^{\mu\nu}$ involves the field equations via the divergence equation (8.219).

It is useful to see what happens to Belinfante's energy-momentum tensor in the presence of an external current, i.e., if $T^{\mu\nu}$ is calculated from the Lagrangian

$$\mathcal{L} = -\frac{1}{4c} F_{\mu\nu} F^{\mu\nu} - \frac{1}{c^2} j^\mu A_\mu, \quad (8.251)$$

with an external current. The energy-momentum tensor is

$$\Theta^{\mu\nu} = \frac{1}{c} \left(F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa} \right) + \frac{1}{c^2} g^{\mu\nu} j^\lambda A_\lambda, \quad (8.252)$$

generalizing (8.25).

The spin current is the same as before, and we find Belinfante's energy-momentum tensor [4]:

$$\begin{aligned} T^{\mu\nu} &= \Theta^{\mu\nu} + \frac{1}{c} \partial_\lambda (F^{\nu\lambda} A^\mu) \\ &= -\frac{1}{c} (F^\nu{}_\lambda F^{\mu\lambda} - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa}) + \frac{1}{c^2} g^{\mu\nu} j^\lambda A_\lambda + \frac{1}{c} (\partial_\lambda F^{\nu\lambda}) A^\mu. \end{aligned} \quad (8.253)$$

Using Maxwell's equations $\partial_\lambda F^{\nu\lambda} = -j^\nu$, the last term can also be rewritten as

$$-\frac{1}{c} j^\nu A^\nu. \quad (8.254)$$

This term prevents $T^{\mu\nu}$ from being symmetric, unless the current j^λ vanishes.

8.10.1 Gravitational Field

The derivation of the canonical energy-momentum tensor $\Theta^{\mu\nu}$ for the gravitational field is similar to that for the electromagnetic field in Subsection 8.9.1. We start from the quadratic action of the gravitational field (4.372),

$$\mathcal{A}^f = -\frac{1}{8\kappa} \int d^4x (\partial_\mu h^{\nu\lambda} \partial^\mu h_{\nu\lambda} - 2\partial_\lambda h_{\mu\nu} \partial^\mu h^{\nu\lambda} + 2\partial_\mu h^{\mu\nu} \partial_\nu h - \partial_\mu h \partial^\mu h), \quad (8.255)$$

and identify the canonically conjugate field $\pi_{\lambda\mu\nu}$,

$$\pi_{\lambda\mu\nu} \equiv \frac{\partial \mathcal{L}^f}{\partial \partial^\lambda h^{\mu\nu}}, \quad (8.256)$$

as being

$$\pi_{\lambda\mu\nu} = \frac{1}{8\kappa} [(\partial_\lambda h_{\mu\nu} - \partial_\mu h_{\lambda\nu})(\eta_{\lambda\nu} \partial_\mu h - \eta_{\mu\nu} \partial_\lambda h) - \eta_{\lambda\nu} \partial^\sigma h_{\sigma\mu} + \eta_{\mu\nu} \partial^\sigma h_{\sigma\lambda}] + (\mu \leftrightarrow \nu). \quad (8.257)$$

It is antisymmetric under the exchange $\lambda \leftrightarrow \mu$, and symmetric under $\mu \leftrightarrow \nu$. From the integrand in (8.255) we calculate, according to the general expression (8.136),

$$\begin{aligned} \Theta^{\mu}{}_{\nu}^f &= \frac{\partial \mathcal{L}}{\partial \partial^\nu h^{\lambda\kappa}} \partial^\mu h^{\lambda\kappa} - \eta^{\mu\nu} \mathcal{L} = \pi_{\nu\lambda\kappa} \partial^\mu h^{\lambda\kappa} - \eta^{\mu}{}_{\nu} \mathcal{L} \\ &= \frac{1}{2\kappa} (\partial_\nu h_{\lambda\kappa} - \partial_\kappa h_{\delta\lambda} + \eta_{\nu\kappa} \partial_\lambda h - \eta_{\nu\lambda} \partial_\kappa h - \eta_{\nu\kappa} \partial^\sigma h_{\sigma\lambda} + \eta_{\nu\kappa} \partial^\sigma h_{\sigma\nu}) \partial^\mu h^{\lambda\kappa} \\ &\quad - \frac{\eta^{\mu}{}_{\nu}}{8\kappa} (\partial_\kappa h^{\sigma\lambda} \partial^\kappa h_{\sigma\lambda} - 2\partial_\lambda h_{\sigma\nu} \partial^\sigma h^{\nu\lambda} + 2\partial_\sigma h^{\sigma\nu} \partial_\nu h - \partial_\sigma h \partial^\sigma h). \end{aligned} \quad (8.258)$$

In order to find the symmetric energy-momentum tensor $\overset{f}{T}^{\mu\nu}$, we follow Belinfante's construction rule. The spin current density is calculated as in Subsection 8.9.1, starting from the substantial derivative of the tensor field

$$\delta_s h^{\mu\nu} = \omega^\mu{}_\kappa h^{\kappa\nu} + \omega^\nu{}_\kappa h^{\mu\kappa}. \quad (8.259)$$

Following the Noether rules, we find, as in (8.215),

$$\Sigma^{\mu\nu,\lambda} = 2 \frac{\partial \phi}{\partial \partial_\lambda h_{\mu\kappa}} - (\mu \leftrightarrow \nu) = 2 [\pi_{\lambda\mu\kappa} h^{\nu\kappa} - (\mu \leftrightarrow \nu)]. \quad (8.260)$$

Combining the two results according to Belinfante's formula (4.57), we obtain the symmetric energy-momentum tensor

$$\overset{\text{f}}{T}^{\mu\nu} = \pi^{\nu\lambda\kappa} \partial^\mu h_{\lambda\kappa} - \partial_c (\pi^{\lambda\mu\kappa} h^\nu_{\kappa} - \pi^{\lambda\nu\kappa} h^\mu_{\kappa} - \pi^{\mu\nu\kappa} h^c_d + \pi^{\mu\lambda\kappa} h^\nu_{\kappa} \pi^{\nu\lambda\kappa} h^\mu_{\kappa} - \pi^{\nu\mu\kappa} h_{\lambda\kappa}) - \eta^{\mu\nu} \mathcal{L}. \quad (8.261)$$

Using the field equation $\partial_\mu \pi^{\mu\nu\lambda} = 0$ and the Hilbert gauge (4.399) with $\partial_\mu \phi^{\mu\nu} = 0$, this takes the simple form in $\phi^{\mu\nu}$:

$$\overset{\text{f}}{T}^{\mu\nu} = \frac{1}{8\kappa} \left[2\partial^\mu \phi^{\lambda\kappa} \partial^\nu \phi_{\lambda\kappa} - \partial^\mu \phi \partial^\nu \phi - \eta^{\mu\nu} \left(\partial_\lambda \phi^{\kappa\sigma} \partial^\lambda \phi_{\kappa\sigma} - \frac{1}{2} \partial_\lambda \phi \partial^\lambda \phi \right) \right]. \quad (8.262)$$

8.11 Internal Symmetries

In quantum field theory, an important role is played by *internal symmetries*. They do not involve any change in the spacetime coordinate of the fields, whose symmetry transformations have the simple form

$$\phi'(x) = e^{-i\alpha G} \phi(x), \quad (8.263)$$

where G are the generators of some Lie group and α the associated transformation parameters. The field ϕ may have several indices on which the generators G act as a matrix. The symmetry variation associated with (8.263) is obviously

$$\delta_s \phi'(x) = -i\alpha G \phi(x). \quad (8.264)$$

The most important example is that of a complex field ϕ and a generator $G = 1$, where (8.263) is simply a multiplication by a constant phase factor. One also speaks of U(1)-symmetry. Other important examples are those of a triplet or an octet of fields ϕ_i with G being the generators of an SU(2) vector representation or an SU(3) octet representation (the adjoint representations of these groups). The first case is associated with charge conservation in electromagnetic interactions, the other two with isospin and SU(3) invariance in strong interactions. The latter symmetries are, however, not exact.

8.11.1 U(1)-Symmetry and Charge Conservation

Suppose that a Lagrangian density $\mathcal{L}(x) = \mathcal{L}(\phi(x), \partial\phi(x), x)$ depends only on the absolute squares $|\phi|^2, |\partial\phi|^2, |\phi\partial\phi|$. Then $\mathcal{L}(x)$ is invariant under U(1)-transformations

$$\delta_s \phi(x) = -i\phi(x). \quad (8.265)$$

Indeed:

$$\delta_s \mathcal{L} = 0. \quad (8.266)$$

On the other hand, we find by the chain rule of differentiation:

$$\delta_s \mathcal{L} = \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial_\mu \phi} \right) \delta_s \phi + \left[\partial_\mu \frac{\partial \mathcal{L}}{\partial_\mu \phi} \right] \delta_s \phi = 0. \quad (8.267)$$

The Euler-Lagrange equation removes the first part of this, and inserting (8.265) we find by comparison with (8.266) that

$$j_\mu = -\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} \phi \quad (8.268)$$

is a conserved current.

For a free relativistic complex scalar field with a Lagrangian density

$$\mathcal{L}(x) = \partial_\mu \varphi^* \partial_\mu \varphi - m^2 \varphi^* \varphi \quad (8.269)$$

we have to add the contributions of real and imaginary parts of the field ϕ in formula (8.268). Then we obtain the conserved current

$$j_\mu = -i \varphi^* \overleftrightarrow{\partial}_\mu \varphi \quad (8.270)$$

where $\varphi^* \overleftrightarrow{\partial}_\mu \varphi$ denotes the left-minus-right derivative:

$$\varphi^* \overleftrightarrow{\partial}_\mu \varphi \equiv \varphi^* \partial_\mu \varphi - (\partial_\mu \varphi^*) \varphi. \quad (8.271)$$

For a free Dirac field, we find from (8.268) the conserved current

$$j^\mu(x) = \bar{\psi}(x) \gamma^\mu \psi(x). \quad (8.272)$$

8.11.2 SU(N)-Symmetry

For more general internal symmetry groups, the symmetry variations have the form

$$\delta_s \varphi = -i \alpha_i G_i \varphi, \quad (8.273)$$

and the conserved currents are

$$j_i^\mu = -i \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} G_i \varphi. \quad (8.274)$$

8.11.3 Broken Internal Symmetries

The physically important symmetries $SU(2)$ of isospin and $SU(3)$ are not exact. The Lagrange density is not strictly zero. In this case we remember the alternative derivation of the conservation law from (8.116). We introduce the spacetime-dependent parameters $\alpha(x)$ and conclude from the extremality property of the action that

$$\partial_\mu \frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \alpha_i(x)} = \frac{\partial \mathcal{L}^\epsilon}{\partial \alpha_i(x)}. \quad (8.275)$$

This implies the divergence law for the above derived current

$$\partial_\mu j_i^\mu(x) = \frac{\partial \mathcal{L}^\epsilon}{\partial \alpha_i}. \quad (8.276)$$

8.12 Generating the Symmetry Transformations of Quantum Fields

As in quantum mechanical systems, the charges associated with the conserved currents of the previous section can be used to generate the transformations of the fields from which they were derived. One merely has to invoke the canonical field commutation rules.

As an important example, consider the currents (8.274) of an internal $U(N)$ -symmetry. Their charges

$$Q^i = -i \int d^3x \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} G_i \varphi \quad (8.277)$$

can be written as

$$Q^i = -i \int d^3x \pi G_i \varphi, \quad (8.278)$$

where $\pi(x) \equiv \partial \mathcal{L}(x) / \partial \partial_\mu \varphi(x)$ is the canonical momentum of the field $\varphi(x)$. After quantization, these fields satisfy the canonical commutation rules:

$$\begin{aligned} [\pi(\mathbf{x}, t), \varphi(\mathbf{x}', t)] &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\ [\varphi(\mathbf{x}, t), \varphi(\mathbf{x}', t)] &= 0, \\ [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] &= 0. \end{aligned} \quad (8.279)$$

From this we derive directly the commutation rule between the quantized charges (8.278) and the field $\varphi(x)$:

$$[Q^i, \hat{\varphi}(x)] = -\alpha^i G_i \varphi(x). \quad (8.280)$$

We also find that the commutation rules among the quantized charges are

$$[\hat{Q}^i, \hat{Q}^j] = [G^i, G^j]. \quad (8.281)$$

Since these coincide with those of the matrices G_i , the operators Q^i are seen to form a representation of the generators of the symmetry group in the Fock space.

It is important to realize that the commutation relations (8.280) and (8.281) remain also valid in the presence of symmetry breaking terms, as long as these do not contribute to the canonical momentum of the theory. Such terms are called *soft symmetry breaking terms*. The charges are no longer conserved, so that we must attach a time argument to the commutation relations (8.280) and (8.281). All times in these relations must be the same, in order to invoke the equal-time canonical commutation rules.

The most important example is the canonical commutation relation (8.95) itself, which holds also in the presence of any potential $V(q)$ in the Hamiltonian. This breaks translational symmetry, but does not contribute to the canonical momentum $p = \partial L / \partial \dot{q}$. In this case, the relation generalizes to

$$\epsilon^j = i\epsilon^i [\hat{p}^i(t), \hat{x}^j(t)], \quad (8.282)$$

which is correct thanks to the validity of the canonical commutation relations (8.93) at arbitrary equal times, also in the presence of a potential.

Other important examples are the commutation rules of the conserved charges associated with the Lorentz generators (8.237):

$$J^{\mu\nu} \equiv \int d^3x J^{\mu\nu,0}(x), \quad (8.283)$$

which are the same as those of the 4×4 -matrices (8.205), and those of the quantum mechanical generators (8.85):

$$[\hat{J}^{\mu\nu}, \hat{J}^{\mu\lambda}] = -ig^{\mu\mu} \hat{J}^{\nu\lambda}. \quad (8.284)$$

The generators $J^{\mu\nu} \equiv \int d^3x J^{\mu\nu,0}(x)$ are sums $J^{\mu\nu} = L^{\mu\nu}(t) + \Sigma^{\mu\nu}(t)$ of charges (8.220) associated with orbital and spin rotations. According to (8.221), the individual charges are time-dependent. Only their sum is conserved. Nevertheless, they both generate Lorentz transformations: $L^{\mu\nu}(t)$ on the spacetime argument of the fields, and $\Sigma^{\mu\nu}(t)$ on the spin indices. As a consequence, they both satisfy the commutation relations (8.284):

$$\begin{aligned} [\hat{L}^{\mu\nu}, \hat{L}^{\mu\lambda}] &= -ig^{\mu\mu} \hat{L}^{\nu\lambda}, \\ [\hat{\Sigma}^{\mu\nu}, \hat{\Sigma}^{\mu\lambda}] &= -ig^{\mu\mu} \hat{\Sigma}^{\nu\lambda}. \end{aligned} \quad (8.285)$$

The commutators (8.281) have played an important role in developing a theory of strong interactions, where they first appeared in the form of a *charge algebra* of the broken symmetry $SU(3) \times SU(3)$ of weak and electromagnetic charges. This symmetry will be discussed in more detail in Chapter 10.

8.13 Energy Momentum Tensor of a Relativistic Massive Point Particle

If we want to study energy and momentum of charged relativistic point particles in an electromagnetic field, it is useful to consider the action (8.68) with (8.72) as a spacetime integral over a *Lagrangian density*:

$$\mathcal{A} = \int d^4x \mathcal{L}(x), \quad \text{with} \quad \mathcal{L}(x) = \int_{\tau_\mu}^{\tau_b} L(\dot{x}^\mu(\tau)) \delta^{(4)}(x - x(\tau)). \quad (8.286)$$

We can then derive for point particles local conservation laws that look very similar to those for fields. Instead of doing this from scratch, however, we shall simply take the already known global conservation laws and convert them into the local ones by inserting appropriate δ -functions with the help of the trivial identity

$$\int d^4x \delta^{(4)}(x - x(\tau)) = 1. \quad (8.287)$$

Consider for example the conservation law (8.74) for the momentum (8.75). With the help of (8.287) this becomes

$$0 = - \int d^4x \int_{-\infty}^{\infty} d\tau \left[\frac{d}{d\tau} p_\lambda(\tau) \right] \delta^{(4)}(x - x(\tau)). \quad (8.288)$$

Note that the boundaries of the four volume in this expression contain the information on initial and final times. We now perform a partial integration in τ , and rewrite (8.288) as

$$0 = - \int d^4x \int_{-\infty}^{\infty} d\tau \frac{d}{d\tau} \left[p_\lambda(\tau) \delta^{(4)}(x - x(\tau)) \right] + \int d^4x \int_{-\infty}^{\infty} d\tau p_\lambda(\tau) \partial_\tau \delta^{(4)}(x - x(\tau)). \quad (8.289)$$

The first term vanishes if the orbits come from and disappear into infinity. The second term can be rewritten as

$$0 = - \int d^4x \partial_\nu \left[\int_{-\infty}^{\infty} d\tau p_\lambda(\tau) \dot{x}^\nu(\tau) \delta^{(4)}(x - x(\tau)) \right]. \quad (8.290)$$

This shows that the tensor

$$\Theta^{\lambda\nu}(x) \equiv \int_{-\infty}^{\infty} d\tau p^\lambda(\tau) \dot{x}^\nu(\tau) \delta^{(4)}(x - x(\tau)) \quad (8.291)$$

satisfies the local conservation law

$$\partial_\nu \Theta^{\lambda\nu}(x) = 0. \quad (8.292)$$

This is the conservation law of the energy-momentum tensor of a massive point particle.

The total momenta are obtained from the spatial integrals over $\Theta^{\lambda 0}$:

$$P^\mu(t) \equiv \int d^3x \Theta^{\lambda 0}(x). \quad (8.293)$$

For point particles, they coincide with the canonical momenta $p^\mu(t)$. If the Lagrangian depends only on the velocity $\dot{x}^\mu(t)$ and not on the position $x^\mu(t)$, the momenta $p^\mu(t)$ are constants of motion: $p^\mu(t) \equiv p^\mu$.

The Lorentz invariant quantity

$$M^2 = P^2 = g_{\mu\nu} P^\mu P^\nu \quad (8.294)$$

is called the *total mass* of the system. For a single particle it coincides with the mass of the particle.

Subjecting the orbits $x^\mu(\tau)$ to Lorentz transformations according to the rules of the last section we find the currents of the total angular momentum

$$L^{\mu\nu,\lambda} \equiv x^\mu \Theta^{\nu\lambda} - x^\nu \Theta^{\mu\lambda}, \quad (8.295)$$

to satisfy the conservation law:

$$\partial_\lambda L^{\mu\nu,\lambda} = 0. \quad (8.296)$$

A spatial integral over the zeroth component of the current $L^{\mu\nu,\lambda}$ yields the conserved charges:

$$L^{\mu\nu}(t) \equiv \int d^3x L^{\mu\nu,0}(x) = x^\mu p^\nu(t) - x^\nu p^\mu(t). \quad (8.297)$$

8.14 Energy Momentum Tensor of a Massive Charged Particle in a Maxwell Field

Let us consider an important combination of a charged point particle and an electromagnetic field Lagrangian

$$\mathcal{A} = -mc \int_{\tau_\mu}^{\tau_\nu} d\tau \sqrt{g_{\mu\nu} \dot{x}^\mu(\tau) \dot{x}^\nu(\tau)} - \frac{1}{4c} \int d^4x F_{\mu\nu} F^{\mu\nu} - \frac{e}{c^2} \int_{\tau_\mu}^{\tau_\nu} d\tau \dot{x}^\mu(\tau) A_\mu(x(\tau)). \quad (8.298)$$

By varying the action in the particle orbits, we obtain the Lorentz equation of motion

$$\frac{dp^\mu}{d\tau} = \frac{e}{c} F^\mu{}_\nu \dot{x}^\nu(\tau). \quad (8.299)$$

We now vary the action in the vector potential, and find the Maxwell-Lorentz equation

$$-\partial_\nu F^{\mu\nu} = \frac{e}{c} \dot{x}^\mu(\tau). \quad (8.300)$$

The action (8.298) is invariant under translations of the particle orbits and the electromagnetic fields. The first term is obviously invariant, since it depends only

on the derivatives of the orbital variables $x^\mu(\tau)$. The second term changes under translations by a pure divergence [recall (8.134)]. The interaction term also changes by a pure divergence, which is seen as follows: Since the symmetry variation changes the coordinates as $x^\nu(\tau) \rightarrow x^\nu(\tau) - \epsilon^\nu$, and the field $A_\mu(x^\nu)$ is transformed as follows:

$$A_\mu(x^\nu) \rightarrow A'_\mu(x^\nu) = A_\mu(x^\nu + \epsilon^\nu) = A_\mu(x^\nu) + \epsilon^\nu \partial_\mu A_\mu(x^\nu), \quad (8.301)$$

we have altogether the symmetry variation

$$\delta_s \mathcal{L} = \epsilon^\nu \partial_\nu \overset{\text{m}}{\mathcal{L}}. \quad (8.302)$$

We now calculate the same variation once more using the equations of motion. This gives

$$\delta_s \mathcal{A} = \int d\tau \frac{d}{d\tau} \frac{\partial L^{\text{m}}}{\partial x'^\mu} \delta_s x^\mu + \int d^4x \frac{\partial \overset{\text{em}}{\mathcal{L}}}{\partial \partial_\lambda A^\mu} \delta_s A^\mu. \quad (8.303)$$

The first term can be treated as in (8.289)–(8.290), after which it acquires the form

$$\begin{aligned} - \int_{\tau_\mu}^{\tau_\nu} d\tau \frac{d}{d\tau} \left(p_\mu + \frac{e}{c} A_\mu \right) &= - \int d^4x \int_{-\infty}^{\infty} d\tau \frac{d}{d\tau} \left[\left(p_\mu + \frac{e}{c} A_\mu \right) \delta^{(4)}(x - x(\tau)) \right] \\ &\quad + \int d^4x \int_{-\infty}^{\infty} d\tau \left(p_\mu + \frac{e}{c} A_\mu \right) \frac{d}{d\tau} \delta^{(4)}(x - x(\tau)), \end{aligned} \quad (8.304)$$

and thus, after dropping boundary terms,

$$- \int_{\tau_\mu}^{\tau_\nu} d\tau \frac{d}{d\tau} \left(p_\mu + \frac{e}{c} A_\mu \right) = \partial_\lambda \int d^4x \int_{-\infty}^{\infty} d\tau \left(p_\mu + \frac{e}{c} A_\mu \right) \frac{dx^\lambda}{d\tau} \delta^{(4)}(x - x(\tau)). \quad (8.305)$$

The electromagnetic part is the same as before, since the interaction contains no derivative of the gauge field. In this way we find the canonical energy-momentum tensor

$$\begin{aligned} \Theta^{\mu\nu}(x) &= \int d\tau \left(p^\mu + \frac{e}{c} A^\mu \right) \dot{x}^\nu(\tau) \delta^{(4)}(x - x(\tau)) \\ &\quad - \frac{1}{c} \left(F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa} \right). \end{aligned} \quad (8.306)$$

Let us check its conservation by calculating the divergence:

$$\begin{aligned} \partial_\nu \Theta^{\mu\nu}(x) &= \int d\tau \left(p + \frac{e}{c} A_\mu \right) \dot{x}^\nu(\tau) \partial_\nu \delta^{(4)}(x - x(\tau)) \\ &\quad - \frac{1}{c} \partial_\nu F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{c} \left[F^\nu{}_\lambda \partial_\nu \partial^\mu A^\lambda - \frac{1}{4} \partial^\mu (F^{\lambda\kappa} F_{\lambda\kappa}) \right]. \end{aligned} \quad (8.307)$$

The first term is, up to a boundary term, equal to

$$- \int d\tau \left(p^\mu + \frac{e}{c} A^\mu \right) \frac{d}{d\tau} \delta^{(4)}(x - x(\tau)) = \int d\tau \left[\frac{d}{d\tau} \left(p^\mu + \frac{e}{c} A^\mu \right) \right] \delta^{(4)}(x - x(\tau)). \quad (8.308)$$

Using the Lorentz equation of motion (8.299), this becomes

$$\frac{e}{c} \int_{-\infty}^{\infty} d\tau \left(F^{\mu}{}_{\nu} \dot{x}^{\nu}(\tau) + \frac{d}{d\tau} A^{\mu} \right) \delta^{(4)}(x - x(\tau)). \quad (8.309)$$

Inserting the Maxwell equation

$$\partial_{\nu} F^{\mu\nu} = -e \int d\tau (dx^{\mu}/d\tau) \delta^{(4)}(x - x(\tau)), \quad (8.310)$$

the second term in Eq. (8.307) can be rewritten as

$$-\frac{e}{c} \int_{-\infty}^{\infty} d\tau \frac{dx_{\lambda}}{d\tau} \partial^{\mu} A^{\lambda} \delta^{(4)}(x - x(\tau)), \quad (8.311)$$

which is the same as

$$-\frac{e}{c} \int d\tau \left(\frac{dx_{\mu}}{d\tau} F^{\mu\lambda} + \frac{dx_{\lambda}}{d\tau} \partial^{\lambda} A^{\mu} \right) \delta^{(4)}(x - x(\tau)), \quad (8.312)$$

thus canceling (8.309). The third term in (8.307) is finally equal to

$$-\frac{1}{c} \left[F^{\nu}{}_{\lambda} \partial^{\mu} F_{\nu}{}^{\lambda} - \frac{1}{4} \partial^{\mu} (F^{\lambda\kappa} F_{\lambda\kappa}) \right], \quad (8.313)$$

due to the antisymmetry of $F^{\nu\lambda}$. With the help of the homogeneous Maxwell equation we verify the *Bianchi identity*

$$\partial_{\lambda} F_{\mu\nu} + \partial_{\mu} F_{\nu\lambda} + \partial_{\nu} F_{\lambda\mu} = 0. \quad (8.314)$$

is identically guaranteed.

It is easy to construct from (8.306) Belinfante's symmetric energy-momentum tensor. We merely observe that the spin density comes entirely from the vector potential, and is hence the same as before in (8.247). Hence the additional piece to be added to the canonical energy-momentum tensor is again [see (8.248)]

$$\begin{aligned} \Delta\Theta^{\mu\nu} &= \frac{1}{c} \partial_{\lambda} (F^{\mu\nu} A^{\lambda}) \\ &= \frac{1}{2} (\partial_{\lambda} F^{\nu\lambda} A^{\mu} + F^{\nu\lambda} \partial_{\lambda} A^{\mu}). \end{aligned} \quad (8.315)$$

The second term in this expression serves to symmetrize the electromagnetic part of the canonical energy-momentum tensor and brings it to the Belinfante form:

$$\overset{\text{em}}{T}{}^{\mu\nu} = -\frac{1}{c} \left(F^{\nu}{}_{\lambda} F^{\mu\lambda} - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa} \right). \quad (8.316)$$

The first term in (8.315), which in the absence of charges vanishes, is now just what is needed to symmetrize the matter part of $\Theta^{\mu\nu}$. Indeed, using once more Maxwell's equation, it becomes

$$-\frac{e}{c} \int d\tau \dot{x}^{\nu}(\tau) A^{\mu} \delta^{(4)}(x - x(\tau)), \quad (8.317)$$

thus canceling the corresponding term in (8.306). In this way we find that the total energy-momentum tensor of charged particles plus electromagnetic fields is simply the sum of the two symmetric energy-momentum tensors:

$$\begin{aligned} T^{\mu\nu} &= \overset{\text{m}}{T}{}^{\mu\nu} + \overset{\text{em}}{T}{}^{\mu\nu} \\ &= \frac{1}{m} \int_{-\infty}^{\infty} d\tau u^\mu u^\nu \delta^{(4)}(x - x(\tau)) - \frac{1}{c} \left(F^\nu{}_\lambda F^{\mu\lambda} - \frac{1}{4} g^{\mu\nu} F^{\lambda\kappa} F_{\lambda\kappa} \right). \end{aligned} \quad (8.318)$$

For completeness, let us also cross-check its conservation:

$$\partial_\nu T^{\mu\nu} = 0. \quad (8.319)$$

Indeed, forming the divergence of the first term gives [in contrast to (8.309)]

$$\frac{e}{c} \int d\tau \dot{x}^\nu(\tau) F^\mu{}_\nu(x(\tau)), \quad (8.320)$$

which is canceled by the divergence in the second term [in contrast to (8.312)]

$$-\frac{1}{c} \partial_\nu F^\nu{}_\lambda F^{\mu\lambda} = -\frac{e}{c} \int d\tau \dot{x}_\lambda(\tau) F^{\mu\lambda}(x(\tau)). \quad (8.321)$$

Notes and References

For more details see

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*All human things are subject to decay,
and when fate summons, monarchs must obey.*

JOHN DRYDEN (1631-1700)

9

Scattering and Decay of Particles

So far we have discussed only free particles. If we want to detect the presence and detailed properties of any of them, it is necessary to perform scattering experiments or to observe their decay products. In this chapter, we shall develop an appropriate quantum mechanical description of such processes.

9.1 Quantum-Mechanical Description

We begin by developing the appropriate quantum-mechanical tools for describing the scattering process.

9.1.1 Schrödinger Picture

Consider a quantum mechanical system whose Schrödinger equation

$$\hat{H}|\psi_S(t)\rangle = i\partial_t|\psi_S(t)\rangle \quad (9.1)$$

cannot be solved analytically (here we use natural units with $\hbar=1$). The standard method of deriving information on such a system comes from perturbation theory: The Hamilton operator is separated into a time-independent part $\hat{H}_0$, whose Schrödinger equation

$$\hat{H}_0|\psi_S(t)\rangle = i\partial_t|\psi_S(t)\rangle \quad (9.2)$$

is solvable, plus a remainder $\hat{V}$, to be called interaction. The operator $\hat{H}_0$ is also called the *unperturbed Hamiltonian*, and the interaction $\hat{V}$ is often called the *perturbation*. For the sake of a simple notation we have omitted the hats on top of all operators without danger of confusion. The time-dependent state $|\psi_S(t)\rangle$ carries a subscript S to indicate the fact that we are dealing with the Schrödinger picture. Observables are operators $\hat{O}_S(\mathbf{p}, \mathbf{x}, t)$ whose matrix elements between states yield transition amplitudes. The interaction will be assumed to be of finite range. This excludes, for the moment, the most important interaction potential, the Coulomb

potential. As an example, we may assume the unperturbed Hamiltonian to describe a particle in a Rosen-Morse potential well:

$$\langle \mathbf{x} | \hat{V} | \mathbf{x} \rangle = V(\mathbf{x}) = \frac{\text{const}}{\cosh^2 |\mathbf{x}|}. \quad (9.3)$$

If the constant is sufficiently negative, the system has one or more discrete bound states. The important Coulomb potential does not fall directly into the class of potentials under consideration. It must first be modified by multiplying it with a very small exponential screening factor. The consequences of an infinite range that would be present in the absence of screening will have to be discussed separately. The interaction $\hat{V}$ may in general depend explicitly on time.

The results will later be applied to quantum field theory. Then $\hat{H}_0$ will be a sum of the second-quantized Hamilton operator of all particles involved, and $\hat{V}$ will be some as yet unspecified short-range interaction between them. If the particles are all massive, all forces are of short range. Moreover, the vacuum state is a discrete state which is well separated from all other states by an energy gap. The lowest excited state contains a single particle with the smallest mass at rest. This mass is the energy gap.

9.1.2 Heisenberg Picture

The other, equivalent, description of the system is due to Heisenberg. It is based on *time-independent* states which are equal to the Schrödinger states $|\psi_S(t)\rangle$ at a certain fixed time $t = t_0$:

$$|\psi_H\rangle \equiv |\psi_S(0)\rangle = \hat{U}(t, t_0)^{-1} |\psi_S(t)\rangle. \quad (9.4)$$

For simplicity, we choose $t_0 = 0$. When using these states, the time dependence of the system is carried by *time-dependent* Heisenberg operators

$$\hat{O}_H(t) = \hat{U}(t, 0)^{-1} \hat{O}_S \hat{U}(t, 0). \quad (9.5)$$

Here $\hat{U}(t, 0)$ is the unitary time evolution operator introduced in Section 1.6 which governs the motion of the Schrödinger state. It has the explicit form [recall (1.269)]

$$\hat{U}(t, 0) = \hat{T} \left(e^{-i \int_0^t dt' \hat{H}(t')} \right). \quad (9.6)$$

If $\hat{H}$ has no explicit time dependence, which we shall assume from now on, then $\hat{U}(t, 0)$ has the explicit form $\hat{U}(t, 0) = e^{-i\hat{H}t/\hbar}$ and satisfies the *unitarity relations*

$$\hat{U}^{-1}(t, 0) = \hat{U}^\dagger(t, 0) = \hat{U}(0, t). \quad (9.7)$$

Then the relation (9.5) becomes

$$\hat{O}_H(t) = e^{i\hat{H}t/\hbar} \hat{O}_S e^{-i\hat{H}t/\hbar}. \quad (9.8)$$

9.1.3 Interaction Picture

As far as perturbation theory is concerned it is useful to introduce yet a third description called the *Dirac* or *interaction picture*. Its states are related to the previous ones by

$$|\psi_I(t)\rangle = e^{i\hat{H}_0 t} |\psi_S(t)\rangle = e^{i\hat{H}_0 t} \hat{U}(t, 0) |\psi_H\rangle. \quad (9.9)$$

In the absence of interactions, they become time *independent* and coincide with the Heisenberg states (9.4). The interactions, however, drive $\psi_I(t)$ away from $\psi_H(t)$.

When using such states, the observables in the interaction picture are

$$\hat{O}_I(t) = e^{i\hat{H}_0 t} \hat{O}_S e^{-i\hat{H}_0 t} = e^{i\hat{H}_0 t} e^{-i\hat{H} t} \hat{O}_H e^{i\hat{H} t} e^{-i\hat{H}_0 t}. \quad (9.10)$$

These operators coincide, of course, with those of the Heisenberg picture in the absence of interactions. By definition, the unperturbed Schrödinger equation $\hat{H}_0 |\psi(t)\rangle$ can be solved explicitly implying that the time dependence of the operators $\hat{O}_I(t)$,

$$\frac{d}{dt} \hat{O}_I(t) = [\hat{H}_0, \hat{O}_I(t)], \quad (9.11)$$

is completely known. If the Schrödinger operator $\hat{O}_S$ is explicitly time-dependent, this becomes

$$\frac{d}{dt} \hat{O}_I(t) = [\hat{H}_0, \hat{O}_I(t)] + [\dot{\hat{O}}_S(t)]_I, \quad (9.12)$$

where

$$[\dot{\hat{O}}_S(t)]_I \equiv e^{i\hat{H}_0 t} \dot{\hat{O}}_S(t) e^{-i\hat{H}_0 t}. \quad (9.13)$$

9.1.4 Neumann-Liouville Expansion

A state vector in the interaction picture moves according to the following equation of motion:

$$\begin{aligned} i\partial_t |\psi_I(t)\rangle &= i\partial_t e^{i\hat{H}_0 t} |\psi_S(t)\rangle \\ &= -\hat{H}_0 |\psi_I(t)\rangle + e^{i\hat{H}_0 t} \hat{H} e^{-i\hat{H}_0 t} |\psi_I(t)\rangle \\ &= \hat{V}_I(t) |\psi_I(t)\rangle, \end{aligned} \quad (9.14)$$

where

$$\hat{V}_I(t) \equiv e^{i\hat{H}_0 t} \hat{V}_S e^{-i\hat{H}_0 t} \quad (9.15)$$

is the interaction picture of the potential $\hat{V}_S$. It is useful to introduce a unitary time evolution operator also for the interaction picture. It determines the evolution of the states by

$$|\psi_I(t)\rangle = \hat{U}_I(t, t_0) |\psi_I(t_0)\rangle. \quad (9.16)$$

Obviously, $\hat{U}_I(t, t_0)$ satisfies the same composition law as the previously introduced time translation operator $\hat{U}(t, t_0)$ in the Schrödinger picture:

$$\hat{U}_I(t, t_0) = \hat{U}_I(t, t')\hat{U}_I(t', t_0). \quad (9.17)$$

Using the differential equation (9.14) for the states we see that the operator $\hat{U}_I(t, t_0)$ satisfies the equation of motion

$$i\partial_t \hat{U}_I(t, t_0) = \hat{V}_I(t)\hat{U}_I(t, t_0). \quad (9.18)$$

The equation of motion (9.18) can be integrated, resulting in the *Neumann-Liouville expansion* [recall (1.200), (1.201)]:

$$\begin{aligned} \hat{U}_I(t, t_0) &= 1 - i \int_{t_0}^t dt_1 \hat{V}_I(t_1) + \frac{(-i)^2}{2!} \hat{T} \int_{t_0}^t dt_1 dt_2 \hat{V}_I(t_1) \hat{V}_I(t_2) + \dots \\ &\equiv \hat{T} \exp \left[-i \int_{t_0}^t dt' \hat{V}_I(t') \right]. \end{aligned} \quad (9.19)$$

The expansion holds for $t > t_0$ and respects the initial condition $\hat{U}_I(t_0, t_0) = 1$.

Note that the differential equation (9.18) for $\hat{U}_I(t, t_0)$ implies that $\hat{U}_I(t, t_0)$ satisfies an integral equation:

$$\hat{U}_I(t, t_0) = 1 - i \int_{t_0}^t dt' \hat{V}_I(t') \hat{U}_I(t', t_0). \quad (9.20)$$

Indeed, we may solve this equation by iteration, starting with $\hat{U}_I(t', t_0) = 1$ which yields the lowest approximation:

$$\hat{U}_I(t, t_0) = 1 - i \int_{t_0}^t dt_1 \hat{V}_I(t_1). \quad (9.21)$$

Reinserting this into (9.2), we obtain the second approximation

$$\hat{U}_I(t, t_0) = 1 - i \int_{t_0}^t dt_1 \hat{V}_I(t_1) + \frac{(-i)^2}{2!} \hat{T} \int_{t_0}^t dt_1 dt_2 \hat{V}_I(t_1) \hat{V}_I(t_2). \quad (9.22)$$

Continuing this iteration we recover the full Neumann-Liouville expansion (9.19).

For $t < t_0$, we may use the relation (9.7) according to which $\hat{U}(t, t_0)$ is simply the inverse $\hat{U}^{-1}(t_0, t)$, and an expansion is again applicable. The time-ordering operator T makes sure that the operators $\hat{V}_I(t_i)$ in the expansion appear in chronological order, with all later $\hat{V}_I(t_i)$ standing to the left of earlier ones.

If $\hat{V}$ and therefore $\hat{H}$ has no explicit time dependence, the Schrödinger state is governed by the simple exponential time evolution operator:

$$|\psi_S(t)\rangle = \hat{U}(t, t_0)|\psi_S(t_0)\rangle = e^{-i\hat{H}(t-t_0)}|\psi_S(t_0)\rangle. \quad (9.23)$$

Combining this with (9.9), we see that

$$\hat{U}_I(t, t_0) = e^{i\hat{H}_0 t} e^{-i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}. \quad (9.24)$$

If the potential $\hat{V}$ depends explicitly on time, this has to be replaced by [recall (9.6)]

$$\begin{aligned}\hat{U}_I(t, t_0) &= e^{i\hat{H}_0 t} \hat{T} \left(e^{-i \int_{t_0}^t dt' \hat{H}(t')} \right) e^{-i\hat{H}_0 t_0} \\ &= e^{i\hat{H}_0 t} \hat{U}(t, t_0) e^{-i\hat{H}_0 t_0}.\end{aligned}\quad (9.25)$$

For a time-independent $\hat{H}$, this relation shows that $\hat{U}_I(t, t_0)$ satisfies the same unitarity relations (9.7) as $\hat{U}(t, t_0)$:

$$\hat{U}_I^{-1}(t, 0) = \hat{U}_I^\dagger(t, 0) = \hat{U}_I(0, t). \quad (9.26)$$

The Heisenberg representation (9.5) of an arbitrary operator is obtained from the interaction representation (9.10) via

$$\begin{aligned}\hat{O}_{\hat{H}}(t) &= \hat{U}^{-1}(t, 0) e^{-i\hat{H}_0 t} \hat{O}_I(t) e^{i\hat{H}_0 t} \hat{U}(t, 0) \\ &= \hat{U}_I^{-1}(t, 0) \hat{O}_I(t) \hat{U}_I(t, 0).\end{aligned}\quad (9.27)$$

We have observed above that the operator in the interaction picture $\hat{O}_I(t)$ has a particularly simple time dependence. Its movement is determined by the unperturbed equation of motion (9.11). Thus (9.27) establishes a relation between the complicated time dependence of the Heisenberg operator $\hat{O}_H(t)$ in the presence of interaction and the simple time dependence of $\hat{O}_I(t)$ which reduces to the Heisenberg operator in the absence of an interaction.

9.1.5 Møller Operators

Consider now a scattering process in which two initial particles approach each other from a large distance outside the range of their interactions. This implies that at a very early time $t \rightarrow -\infty$, their states obey the unperturbed Schrödinger equation, i.e., that their wave function $\psi_I(t)$ is time-independent. The same thing will be true a very long time after the scattering has taken place. Let us study the behavior of the operator $\hat{U}_I(t, t_0)$ in the two limits of large positive and negative time arguments. In order to make all expressions well defined mathematically it is convenient to introduce a simple modification of the potential by multiplying it with a switching factor $e^{-\eta|t|}$:

$$\hat{V} \rightarrow e^{-\eta|t|} \hat{V} \equiv \hat{V}^\eta(t), \quad \hat{V}_I(t) \rightarrow e^{-\eta|t|} \hat{V}_I(t) \equiv \hat{V}_I^\eta(t), \quad (9.28)$$

with an infinitesimal parameter η . As far as physical observations are concerned, such a factor must have little relevance since η can be chosen so that $\hat{V}$ remains unchanged over any finite interval of time. However, an immediate consequence of the prescription (9.28) is that for $t \rightarrow \pm\infty$, the state vector in the interaction picture becomes time-independent, due to (9.14): Let us denote the limiting states by $|\psi_{\text{out}}^{\text{in}}\rangle$, i.e.,

$$|\psi_I(t)\rangle \xrightarrow{t \rightarrow \mp\infty} |\psi_{\text{out}}^{\text{in}}\rangle. \quad (9.29)$$

Using the time evolution operator, the limit (9.29) may be written as

$$\hat{U}_I(t, 0)|\psi_I(0)\rangle \xrightarrow{t \rightarrow \mp\infty} |\psi_{\text{out}}^{\text{in}}\rangle, \quad (9.30)$$

i.e., the operator $\hat{U}_I$ becomes a constant in the limit $t \rightarrow \mp\infty$. Inverting this relation we may write

$$|\psi_I(0)\rangle = \hat{U}_I(0, \mp\infty)|\psi_{\text{out}}^{\text{in}}\rangle \equiv \hat{\Omega}^{(\pm)}|\psi_{\text{out}}^{\text{in}}\rangle. \quad (9.31)$$

The operators

$$\hat{\Omega}^{(\pm)} \equiv \hat{U}_I(0, \mp\infty) \quad (9.32)$$

were first studied extensively by Møller¹ and are named after him. Their most important property is the following:

$$\hat{H}\hat{\Omega}^{(\pm)} = \hat{\Omega}^{(\pm)}\hat{H}_0, \quad \hat{\Omega}^{(\pm)\dagger}\hat{H} = \hat{H}_0\hat{\Omega}^{(\pm)\dagger}. \quad (9.33)$$

To derive this, we consider, for simplicity, only the most common situation that $\hat{V}$ has no explicit time dependence except for the very slow switching factor (9.28). Then we multiply the explicit representation (9.24) of the time-evolution operator by a factor $e^{-it\hat{H}}$ and find

$$e^{-it\hat{H}}\hat{U}(0, t_a) = e^{-it\hat{H}}e^{it_a\hat{H}}e^{-it_a\hat{H}_0} = e^{-i(t-t_a)\hat{H}}e^{-i(t_a-t)\hat{H}_0}e^{-it\hat{H}_0} = \hat{U}(0, t_a - t)e^{-it\hat{H}_0}. \quad (9.34)$$

In the limit $t_a \rightarrow \pm\infty$, this yields

$$e^{-it\hat{H}}\hat{U}(0, \mp\infty) = \hat{U}(0, \mp\infty)e^{-it\hat{H}_0}. \quad (9.35)$$

The time derivative of this at $t = 0$ yields precisely the first equation in (9.33). The second follows by Hermitian conjugation.

Let $|\psi_{\text{out}}^{\text{in}}\rangle$ be a steady-state solution of the time-independent unperturbed Schrödinger equation:

$$\hat{H}_0|\psi_{\text{out}}^{\text{in}}\rangle = E|\psi_{\text{out}}^{\text{in}}\rangle. \quad (9.36)$$

Then due to (9.33) [or directly (9.35)], the interacting state $|\psi_I(0)\rangle$ solves the full Schrödinger equation with the *same energy*:

$$\hat{H}|\psi_I(0)\rangle = E|\psi_I(0)\rangle. \quad (9.37)$$

In the laboratory, one does not really observe steady states but wave packets, which can be obtained from superpositions of steady-state solutions with different momenta. The packets of free particles approach each other and enter into the range

¹C. Møller, Kgl. Danske Vidensk. Selsk. Mat.Fys. Medd 23, No. 1, (1945).

of the interaction potential. Also there, the total energy remains the same, due to energy conservation.

The amplitude for the scattering process is found as follows. Let $|a_{\text{in}}\rangle$ be a complete set of incoming eigenstates of the unperturbed Schrödinger equation

$$\hat{H}_0|a_{\text{in}}\rangle = E_a|a_{\text{in}}\rangle, \quad (9.38)$$

where a denotes the collection of all quantum numbers of these states. By applying the interaction operator $\hat{U}_I(t, -\infty)$ to the states $|a_{\text{in}}\rangle$, these are transformed into the time-dependent $|a_I(t)\rangle$. After a long time, these develop into time-independent states $|a_{\text{out}}\rangle$. The energies E_a remain, of course, unchanged.

Let us analyze the outgoing states

$$|a_{\text{out}}\rangle = \hat{U}_I(\infty, -\infty)|a_{\text{in}}\rangle \quad (9.39)$$

with respect to the incoming waves $|b_{\text{in}}\rangle$. The scalar products $\langle b_{\text{in}}|a_{\text{out}}\rangle$ are obviously equal to the matrix elements of $\hat{U}_I(\infty, -\infty)$:

$$\langle b_{\text{in}}|a_{\text{out}}\rangle = \langle b_{\text{in}}|\hat{U}_I(\infty, -\infty)|a_{\text{in}}\rangle. \quad (9.40)$$

The right-hand side is defined as the *scattering matrix* or *S-matrix*:

$$S_{ba} = \langle b_{\text{in}}|\hat{U}_I(\infty, -\infty)|a_{\text{in}}\rangle. \quad (9.41)$$

The same name is also often used sloppily for the scattering operator

$$\hat{S} \equiv \hat{U}_I(\infty, -\infty) \quad (9.42)$$

itself, which can be written as a product of the two Møller operators (9.32):

$$S = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}. \quad (9.43)$$

Since $\hat{U}_I(t, t_0)$ is a unitary operator, the *S-matrix* is also unitary and satisfies

$$SS^\dagger = S^\dagger S = 1. \quad (9.44)$$

The Møller operators, however, are not unitary. As we shall see in the next section, the operators $\hat{\Omega}^{(\pm)\dagger}$ are inverse to $\hat{\Omega}^{(\pm)}$ if $\hat{H}_0$ has no bound states. Under multiplication of the states from the left-hand side one has

$$\hat{\Omega}^{(\pm)\dagger}\hat{\Omega}^{(\pm)} = 1. \quad (9.45)$$

In contrast, under multiplication from the right-hand side, the product yields a projection operator onto the subspace of continuous states of the Hamiltonian $\hat{H}$:

$$\hat{\Omega}^{(\pm)}\hat{\Omega}^{(\pm)\dagger} = \hat{P}_{\text{continuum}}. \quad (9.46)$$

Note that only in an infinite-dimensional Hilbert space can it happen that the left-inverse is not equal to the right-inverse.

9.1.6 Lippmann-Schwinger Equation

The solution (9.31) of Eq. (9.37) can usually not be given analytically but only in form of a perturbation series. This is found by inserting the Neumann-Liouville expansion (9.19) into Eq. (9.31):

$$|\psi_I(0)\rangle = |\psi_{\text{in}}\rangle - i \int_{-\infty}^0 dt' \hat{V}_I(t') |\psi_{\text{in}}\rangle + (-i)^2 \int_{-\infty}^0 dt' \int_{-\infty}^t dt'' \hat{V}_I(t') \hat{V}_I(t'') |\psi_{\text{in}}\rangle + \dots \quad (9.47)$$

With the help of (9.15), and the damping factor as in Eq. (9.28), we see that the second term is equal to

$$-i \int_{-\infty}^0 dt e^{\eta t} e^{i\hat{H}_0 t} \hat{V} e^{-i\hat{H}_0 t} |\psi_{\text{in}}\rangle. \quad (9.48)$$

By assumption, $|\psi_{\text{in}}\rangle$ is an eigenstate of $\hat{H}_0$ with energy E , and $\hat{V}$ is independent of time. Thus we can perform the integration and obtain

$$-i \int_{-\infty}^0 dt e^{\eta t} e^{i(\hat{H}_0 - E)t} \hat{V} |\psi_{\text{in}}\rangle = \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} |\psi_{\text{in}}\rangle. \quad (9.49)$$

Treating the other expansion terms in (9.47) likewise, we arrive at the expansion

$$|\psi_I(0)\rangle = |\psi_{\text{in}}\rangle + \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} |\psi_{\text{in}}\rangle + \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} |\psi_{\text{in}}\rangle + \dots \quad (9.50)$$

In the second denominator we have replaced $2i\eta$ by $i\eta$ since η is infinitesimally small and its actual size is irrelevant. The infinite sum is recognized as an iterative solution of the so-called *Lippmann-Schwinger equation*²

$$|\psi_I(0)\rangle = |\psi_{\text{in}}\rangle + \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} |\psi_I(0)\rangle. \quad (9.51)$$

The fact that this state solves the Schrödinger equation (9.37) is easily verified by multiplying both sides by $E - \hat{H}_0$, to obtain

$$(E - \hat{H}_0) |\psi_I(0)\rangle = (E - \hat{H}_0) |\psi_{\text{in}}\rangle + \hat{V} |\psi_I(0)\rangle. \quad (9.52)$$

The first term on the right-hand side vanishes, due to (9.36). The remaining equation coincides with Eq. (9.37).

Comparing (9.51) with (9.31), we identify the Møller operator as

$$\hat{\Omega}^{(+)} = \hat{U}_I(0, -\infty) = 1 + \frac{1}{E - \hat{H}_0 + i\eta} \hat{V}. \quad (9.53)$$

²For a discussion see M. Gell-Mann and M.L. Goldberger, Phys. Rev. *91*, 398 (1953).

Making use of this relation, one often writes the scattering state $|\psi_I(0)\rangle$ in (9.51) as $|\psi^{(+)}\rangle$ and the equation itself as

$$|\psi^{(+)}\rangle = |\psi_{\text{in}}\rangle + \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} |\psi^{(+)}\rangle. \quad (9.54)$$

There also exists a Lippmann-Schwinger equation yielding a different set of interacting states $|\psi^{(-)}\rangle$ from the outgoing free state $|\psi_{\text{out}}\rangle$:

$$|\psi^{(-)}\rangle = |\psi_{\text{out}}\rangle + \frac{1}{E - \hat{H}_0 - i\eta} \hat{V} |\psi^{(-)}\rangle, \quad (9.55)$$

where the Møller operator is

$$\hat{\Omega}^{(-)} = \hat{U}_I(0, \infty) = 1 + \frac{1}{E - \hat{H}_0 - i\eta} \hat{V}. \quad (9.56)$$

The only difference with respect to (9.53) is the sign of the $i\eta$ -term.

The operators

$$\hat{G}_0(E) \equiv \frac{i\hbar}{E - \hat{H}_0 + i\eta}, \quad \hat{G}(E) \equiv \frac{i\hbar}{E - \hat{H} + i\eta} \quad (9.57)$$

are the *resolvents* of the free and interacting Hamiltonians, respectively [recall (11.8)]. The second is related to the first by the equation

$$\hat{G}(E) = \hat{G}_0(E) - \frac{i}{\hbar} \hat{G}_0(E) \hat{V} \hat{G}(E). \quad (9.58)$$

This can easily be verified by multiplying (9.58) with $[\hat{G}(E)]^{-1} = (E - \hat{H})/i\hbar$ from the right:

$$1 = \left[\hat{G}_0(E) - \frac{i}{\hbar} \hat{G}_0(E) \hat{V} \hat{G}(E) \right] [\hat{G}(E)]^{-1} = -\frac{i}{\hbar} \hat{G}_0(E) (E - \hat{H}) - \frac{i}{\hbar} \hat{G}_0(E) \hat{V}. \quad (9.59)$$

The equation (9.58) for $\hat{G}(E)$ can be solved iteratively by the geometric series

$$\hat{G}(E) = \hat{G}_0(E) - \frac{i}{\hbar} \hat{G}_0(E) \hat{V} \hat{G}_0(E) + \left(\frac{i}{\hbar} \right)^2 \hat{G}_0(E) \hat{V} \hat{G}_0(E) \hat{V} \hat{G}_0(E) + \dots \quad (9.60)$$

The Møller operators (9.53) and (9.56) can be expressed with the help of the free resolvent as

$$\hat{\Omega}^{(+)} = 1 - \frac{i}{\hbar} \hat{G}_0(E) \hat{V}, \quad \hat{\Omega}^{(-)} = 1 - \frac{i}{\hbar} \hat{G}_0(E^*) \hat{V}. \quad (9.61)$$

9.1.7 Discrete States

The Møller operators have interesting nontrivial properties with respect to the discrete spectrum of the unperturbed Hamiltonian $\hat{H}_0$ and the perturbed Hamiltonian $\hat{H}$. Let us first understand the difference between the quasi-unitarity relations (9.45) and (9.46). We denote by $|\varphi_a\rangle$ the continuum, and by $|\varphi_\beta\rangle$ the bound states of $\hat{H}_0$, similarly by $|\psi_a^{(\pm)}\rangle$ the continuum and by $|\psi_\beta\rangle$ the bound states of $\hat{H}$ which solve the Lippmann-Schwinger equations (9.54) or (9.55), respectively. These states satisfy the completeness relations

$$\sum_a |\varphi_a\rangle\langle\varphi_a| + \sum_\beta |\varphi_\beta\rangle\langle\varphi_\beta| = 1, \quad \sum_a |\psi_a^{(\pm)}\rangle\langle\psi_a^{(\pm)}| + \sum_\beta |\psi_\beta\rangle\langle\psi_\beta| = 1. \quad (9.62)$$

Only the continuum states carry the distinctive label $(\pm)$, since only these depend on the sign of the small quantity η in the Lippmann-Schwinger equations (9.54) and (9.55). The bound states are uniquely determined by the condition of quadratic integrability.

The Møller operators $\hat{\Omega}^{(\pm)}$ transform the continuum states $|\varphi_a\rangle$ into scattering states $|\psi^{(\pm)}\rangle$. Thus we can expand

$$\hat{\Omega}^{(\pm)} = \hat{U}_I(0, \mp\infty) = \sum_a |\psi_a^{(\pm)}\rangle\langle\varphi_a|, \quad \hat{\Omega}^{(\pm)\dagger} = \hat{U}_I^\dagger(0, \mp\infty) = \sum_a |\varphi_a\rangle\langle\psi_a^{(\pm)}|. \quad (9.63)$$

From these expansions, we extract the following important properties of the Møller operators:

$$\hat{\Omega}^{(\pm)\dagger}|\psi_a^{(\pm)}\rangle = |\varphi_a\rangle, \quad \hat{\Omega}^{(\pm)\dagger}|\psi_\beta\rangle = 0. \quad (9.64)$$

The second relation implies that

$$\hat{\Omega}^{(\pm)\dagger}P_{\text{bd}} = 0. \quad (9.65)$$

We further find

$$\hat{\Omega}^{(\pm)\dagger}\hat{\Omega}^{(\pm)} = \sum_{a,b} |\varphi_a\rangle\langle\psi_a^{(\pm)}|\psi_b^{(\pm)}\rangle\langle\varphi_b| = 1 - \sum_\beta |\varphi_\beta\rangle\langle\varphi_\beta| = 1 - P_{\text{bd}}^0. \quad (9.66)$$

The operator on the right-hand side is the projection on the bound states of $\hat{H}_0$. In the opposite order, the product yields

$$\hat{\Omega}^{(\pm)}\hat{\Omega}^{(\pm)\dagger} = \sum_{a,b} |\psi_a^{(\pm)}\rangle\langle\varphi_a|\varphi_b\rangle\langle\psi_b^{(\pm)}| = 1 - \sum_\beta |\psi_\beta\rangle\langle\psi_\beta| = 1 - \hat{P}_{\text{bd}}, \quad (9.67)$$

where $\hat{P}_{\text{bd}}$ projects onto the bound states of $\hat{H}$. The different orders of the products differ by the projection onto the bound states of $\hat{H}$.

For the S -matrix, on the other hand, this dependence on the order disappears and we find

$$\begin{aligned} S^\dagger S &= [\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}]^\dagger[\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}] = \hat{\Omega}^{(+)\dagger}\hat{\Omega}^{(-)}\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)} = \hat{\Omega}^{(+)\dagger}(1 - \hat{P}_{\text{bd}})\hat{\Omega}^{(+)} \\ &= 1 - P_{\text{bd}}^0, \end{aligned} \quad (9.68)$$

and

$$SS^\dagger = \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(+)} \hat{\Omega}^{(+)\dagger} \hat{\Omega}^{(-)} = \hat{\Omega}^{(-)\dagger} (1 - \hat{P}_{\text{bd}}) \hat{\Omega}^{(-)} = \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(-)} = 1. \quad (9.69)$$

The projection operator $\hat{P}_{\text{bd}}$ has dropped out because of (9.65).

By definition, the S -matrix is calculated only between states in the subspace of the Hilbert space formed by the continuous eigenstates of $\hat{H}_0$. In this subspace, the projection operator P_{bd}^0 vanishes and we find $S^\dagger S = 1$ and $SS^\dagger = 1$, in either order, showing that the S -matrix is unitary.

From the property (9.33) of the Møller operator we derive immediately that S does not change the energy of the incoming continuum states since $[\hat{H}_0, S] = 0$:

$$\hat{H}_0 S = \hat{H}_0 \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(+)} = \hat{\Omega}^{(-)\dagger} \hat{H} \hat{\Omega}^{(+)} = \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(+)} \hat{H}_0 = S \hat{H}_0. \quad (9.70)$$

For scattering states which all lie in the continuum of $\hat{H}_0$, the size of η is irrelevant as long as it is very small and has a fixed sign. In contrast, a discrete eigenstate of $\hat{H}_0$ has a singular η -dependence in the limit of small η . In order to understand this we observe that, for any short-range potential, the two scattering particles lie practically all the time outside of each other's range. Only for a small time interval do they interact. The potential has no effect for large positive and negative times where the wave packets are separated by a large distance. The switching factor is therefore physically irrelevant for sufficiently small η . It cannot influence the physics of the system. For bound states, however, the particles interact with each other *all the time* with the same strength. In order to understand this consider a specific discrete state, assuming it to be well separated from the lower and higher states by a finite energy gap Δ . Then, for $\eta \ll \Delta$, the time dependence of $\hat{V}^\eta(t) = e^{-\eta|t|} \hat{V}$ is so slow that the interaction is, over a long time interval, incapable of causing transitions from the discrete state to a neighbor state. Such a slow time dependence is called *adiabatic*. For an adiabatically time-dependent potential $\hat{V}^\eta(t)$, the discrete state $|\psi(t)\rangle$ is at any time t_0 a very good approximation to the solution of the time-independent Schrödinger equation that contains the time-independent potential $\hat{V}(t_0)$. The energy $E(t)$ of the discrete state $|\psi(t)\rangle$ is at any finite time equal to E . Only for very large times $|t| > \pm 1/\eta$ does the interaction become so weak that the state $|\psi(t)\rangle$ becomes an eigenstate of $\hat{H}_0$, and the energy $E(t)$ goes against the associated eigenvalue E_0 of the unperturbed Hamilton operator $\hat{H}_0$.

9.1.8 Gell-Mann-Low Formulas

The Møller operators relate the wave functions $|\psi\rangle$ of the interacting system, that satisfies the Schrödinger equation

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle, \quad (9.71)$$

to the corresponding unperturbed wave function $|\psi_0\rangle$, satisfying

$$\hat{H}_0|\psi_0\rangle = E_0|\psi_0\rangle. \quad (9.72)$$

Formally, this correspondence can be specified in a unique way by multiplying $\hat{V}$ by a coupling constant g , and by continuing g smoothly from $g = 0$, where the system is free, to the value $g = 1$, where it is fully interacting. The energy $E(g)$ and the associated discrete state $|\psi(g)\rangle$ are continuous functions of g interpolating between E_0 and E , and between $|\psi_0\rangle$ and $|\psi\rangle$, respectively.

The two Møller operators $\hat{\Omega}^{(\pm)}$ of Eq. (9.32) associated with the potential $\hat{V}_I^\eta$ carry the nondegenerate discrete state $|\psi_0\rangle$ into two different solutions of the interacting Schrödinger equation (9.71) as follows (*first Gell-Mann-Low formula*):³

$$|\psi^{(\pm)}\rangle = \lim_{\eta \rightarrow 0} \hat{U}_I^\eta(0, \mp\infty) |\psi_0\rangle \frac{1}{z_\eta^{(\pm)}}. \quad (9.73)$$

To have a finite limit, the transformed state has been divided by a normalization factor $z_\eta^{(\pm)}$ defined by the expectation value

$$z_\eta^{(\pm)} \equiv \langle \psi_0 | \hat{U}_I^\eta(0, \mp\infty) | \psi_0 \rangle. \quad (9.74)$$

The phase determines the energy shift via the *second Gell-Mann-Low formula*:

$$\Delta E = E - E_0 = \mp \lim_{\eta \rightarrow 0} g \frac{\partial}{\partial g} \varphi_\mp^\eta. \quad (9.75)$$

In order to prove the statements (9.73) and (9.75), let us denote the states on the right-hand side of (9.73) without the normalization factors by

$$|\eta^{(\pm)}\rangle \equiv \hat{U}_I^\eta(0, \mp\infty) |\psi_0\rangle. \quad (9.76)$$

For small but fixed η , these states satisfy the Schrödinger equation

$$[\hat{H}_0 + \hat{V}^\eta(0)] |\eta^{(\pm)}\rangle = E_\eta |\eta^{(\pm)}\rangle, \quad (9.77)$$

where E_η is some η -dependent energy. The proof is based on the observation that in front of the state $|\psi_0\rangle$, the η -dependent Møller operators

$$\hat{\Omega}_\eta^{(\pm)} \equiv \hat{U}_I^\eta(0, \mp\infty) \quad (9.78)$$

satisfy the obvious commutation rule

$$[\hat{H}_0, \hat{U}_I^\eta(0, \mp\infty)] |\psi_0\rangle = \hat{H}_0 |\eta^{(\pm)}\rangle - E_0 |\eta^{(\pm)}\rangle. \quad (9.79)$$

We now expand $\hat{U}_I^\eta(0, \mp\infty)$ according to (9.19) as

$$\begin{aligned} \hat{U}_I^\eta(0, -\infty) &= \hat{T} \left(e^{-ig \int_{-\infty}^0 dt e^{\eta t} \hat{V}_I(t)} \right) \\ &= \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} \int_{-\infty}^0 dt_1 \cdots \int_{-\infty}^0 dt_n e^{\eta \sum_{i=1}^n t_i} \hat{T} \left(\hat{V}_I(t_1) \cdots \hat{V}_I(t_n) \right). \end{aligned} \quad (9.80)$$

³M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951).

The operators $\hat{V}_I(t)$ in the interaction picture have the time dependence (9.11), which yields

$$\frac{d}{dt}\hat{V}_I(t) = i [\hat{H}_0, \hat{V}_I(t)]. \quad (9.81)$$

Using (9.80) and (9.81) we find

$$\begin{aligned} [\hat{H}_0, \hat{U}_I^\eta(0, -\infty)] &= -i \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} \int_{-\infty}^0 dt_1 \cdots \int_{-\infty}^0 dt_n e^{\eta \sum_{i=1}^n t_i} \\ &\quad \times \sum_{i=1}^n \frac{\partial}{\partial t_i} \hat{T}(\hat{V}_I(t_1) \cdots \hat{V}_I(t_i) \cdots \hat{V}_I(t_n)). \end{aligned} \quad (9.82)$$

Since the integrand is symmetric in the time variables, we may replace the sum $\sum_{i=1}^n \partial/\partial t_i$ by n -times the time derivative $\partial/\partial t_n$. Taking the derivative $\partial/\partial t_n$ to the left of the switching factors $e^{\eta t_i}$, the integral becomes

$$\begin{aligned} &-i \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} n \int_{-\infty}^0 dt_1 \cdots \int_{-\infty}^0 dt_{n-1} \int_{-\infty}^0 dt_n \times \frac{\partial}{\partial t_n} [e^{\eta \sum_{i=1}^n t_i} \hat{T}(\hat{V}_I(t_1) \cdots \hat{V}_I(t_n))] \\ &+ i\eta \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} n \int_{-\infty}^0 dt_1 \cdots \int_{-\infty}^0 dt_n e^{\eta \sum_{i=1}^n t_i} \hat{T}(\hat{V}_I(t_1) \cdots \hat{V}_I(t_n)). \end{aligned} \quad (9.83)$$

The second sum is equal to

$$i\eta g \frac{\partial}{\partial g} \hat{U}_I^\eta(0, -\infty). \quad (9.84)$$

The first sum contains integrals over pure time derivatives which amount to pure surface terms. Moreover, since the integrand vanishes at $t_n = -\infty$, only the $t_n = 0$ -term contributes. The time $t_n = 0$ is the latest of all time variables. Thus it can be moved to the left of the time-ordering symbol, and we arrive at the equation

$$[\hat{H}_0, \hat{U}_I^\eta(0, -\infty)] = -g \hat{V}_I(0) \hat{U}_I^\eta(0, -\infty) + i\eta g \frac{\partial}{\partial g} \hat{U}_I^\eta(0, -\infty). \quad (9.85)$$

In a similar way we derive

$$[\hat{H}_0, \hat{U}_I^\eta(0, +\infty)] = -g \hat{V}_I(0) \hat{U}_I^\eta(0, +\infty) - i\eta g \frac{\partial}{\partial g} \hat{U}_I^\eta(0, +\infty). \quad (9.86)$$

An important property of these formulas is that, in the presence of a level shift, the second term on the right-hand side proportional to η is nonzero in the limit $\eta \rightarrow 0$. To see this, take Eq. (9.85), and rewrite it in a slightly different way as

$$\begin{aligned} \hat{H} \hat{U}_I^\eta(0, \mp\infty) &= [\hat{H}_0 + g \hat{V}_I(0)] \hat{U}_I^\eta(0, \mp\infty) \\ &= \hat{U}_I^\eta(0, \mp\infty) \hat{H}_0 \pm i\eta g \frac{\partial}{\partial g} \hat{U}_I^\eta(0, \mp\infty). \end{aligned} \quad (9.87)$$

If this equation is applied to the state $|\psi_0\rangle$, it shows that the state $|\eta^{(\pm)}\rangle$ of (9.76) satisfies the modified Schrödinger equation

$$\hat{H}|\eta^{(\pm)}\rangle = \left(E_0 \pm i\eta g \frac{\partial}{\partial g}\right) |\eta^{(\pm)}\rangle. \quad (9.88)$$

If we had taken the limit $\eta \rightarrow 0$ carelessly, we would have arrived at the equation $\hat{H}|\eta^{(\pm)}\rangle = E_0|\eta^{(\pm)}\rangle$, and would have concluded erroneously that $|\eta\rangle_{\mp}$ are solutions of the fully interacting Schrödinger equation with energy E_0 . For the continuum states, this conclusion is indeed correct, and we have

$$\hat{H}\hat{U}_I(0, \mp\infty) = \hat{U}_I(0, \mp\infty) \hat{H}_0 \quad (9.89)$$

rather than (9.87). This agrees with Eq. (9.33). For the discrete states, the energy is in general shifted by the interaction. Hence the derivative $g(\partial/\partial g)|\eta^{(\pm)}\rangle$ must diverge like $1/\eta$, so that it gives a finite contribution in (9.88). The origin of the divergence is a diverging normalization of the state $|\eta^{(\pm)}\rangle$, and the divergence is eliminated by making use of the states on the right-hand side of (9.73):

$$|\psi_{\eta}^{(\pm)}\rangle \equiv |\eta^{(\pm)}\rangle \frac{1}{z_{\eta}^{(\pm)}}. \quad (9.90)$$

These have a definite limit for $\eta \rightarrow 0$. For these states, Eq. (9.88) implies

$$\hat{H}|\psi_{\eta}^{(\pm)}\rangle = \left(E_0 \pm i\eta g \frac{\partial}{\partial g} \log z_{\eta}^{(\pm)}\right) |\psi_{\eta}^{(\pm)}\rangle. \quad (9.91)$$

The level shifts caused by the interaction are given by the formula

$$\Delta E = \lim_{\eta \rightarrow 0} i\eta g \frac{\partial}{\partial g} \log z_{\eta}^{(\pm)}. \quad (9.92)$$

Note that, in the limit $\eta \rightarrow 0$, the two states $|\psi_{\eta}^{(\pm)}\rangle$ coincide. This is seen as follows. The state $|\eta^{(+)}\rangle$ evolves after an infinitely long time into $\hat{U}_I^{\eta}(\infty, -\infty)|\psi_0\rangle$. There it becomes again an eigenstate of $\hat{H}_0$ due to the commutation relation (9.70). Thus it must coincide with $|\psi_0\rangle$ up to some overall factor $e^{i\varphi_{\eta}^{(+)}}$ (recall that $|\psi_0\rangle$ is nondegenerate by assumption). Similarly, we may evolve the state $|\psi_0\rangle$ backwards in time via $|\eta^{(-)}\rangle$ into $\hat{U}_I^{\eta}(\infty, -\infty)|\psi_0\rangle$, i.e., into the initial state rather than $|\psi_0\rangle$.

Note that $|\eta\rangle_{-} \equiv |\eta\rangle_{+} e^{i\varphi_{\eta}^{\eta}}$. When forming $|\psi_{\eta}\rangle_{\mp}$ from $|\eta\rangle_{\pm}$, the pure phase between $|\psi_0\rangle$ and $\hat{U}_I^{\eta}(\infty, -\infty)|\psi_0\rangle$ cancels. Thus the two states $|\psi_{\eta}\rangle_{\mp}$ must indeed be identical. The phase φ^{η} associated with the total time evolution operator $\hat{U}_I^{\eta}(\infty, -\infty)$, defined by

$$e^{i\varphi^{\eta}} \equiv \langle\psi_0|\hat{U}_I^{\eta}(\infty, -\infty)|\psi_0\rangle, \quad (9.93)$$

is obviously related to the previously introduced phases $\varphi_{\mp}^{\eta}$ by the relations

$$\varphi^{\eta} = \varphi_{-}^{\eta} - \varphi_{+}^{\eta} = 2\varphi_{-}^{\eta} = -2\varphi_{+}^{\eta}. \quad (9.94)$$

This equation can also be written in terms of matrix elements as

$$\langle \psi_0 | \hat{U}_I^\eta(\infty, -\infty) | \psi_0 \rangle = \langle \psi_0 | \hat{U}_I^\eta(\infty, 0) | \psi_0 \rangle \langle \psi_0 | \hat{U}_I^\eta(0, -\infty) | \psi_0 \rangle, \quad (9.95)$$

which may come somewhat as a surprise. In general, there is certainly an identity containing a sum over a complete set of orthonormal eigenstates in the middle:

$$\langle \psi_0 | \hat{U}_I^\eta(\infty, -\infty) | \psi_0 \rangle = \sum_n \langle \psi_0 | \hat{U}_I^\eta(\infty, 0) | \psi_n \rangle \langle \psi_n | \hat{U}_I^\eta(0, -\infty) | \psi_0 \rangle. \quad (9.96)$$

It is the adiabatic slowness of the switching-on process of the interaction which does not permit a transition to an excited intermediate state, making (9.95) valid.

The level shift can also be expressed in terms of the η -dependent S -matrix:

$$S^\eta = \hat{U}_I^\eta(\infty, -\infty) = \hat{U}_I^\eta(\infty, 0) \hat{U}_I^\eta(0, -\infty). \quad (9.97)$$

Indeed, by multiplying Eq. (9.88) for $|\eta^{(+)}\rangle$ by $\langle \psi_\eta^{(+)}|$ from the left, we find

$$\langle \psi_\eta^{(\pm)} | \hat{H} - E_0 | \eta^{(\pm)} \rangle = \Delta E \langle \psi_\eta^{(\pm)} | \eta^{(\pm)} \rangle = \pm i\eta g \langle \psi_\eta^{(\pm)} | \partial_g | \eta^{(\pm)} \rangle, \quad (9.98)$$

such that we obtain, with the abbreviation $\partial_g \equiv \partial/\partial g$:

$$\Delta E = \pm i\eta g \frac{\langle \psi_\eta^{(\pm)} | \partial_g | \eta^{(\pm)} \rangle}{\langle \psi_\eta^{(\pm)} | \eta^{(\pm)} \rangle} \quad (9.99)$$

$$= \pm i\eta g \frac{\langle \psi_0 | \hat{U}_I^\eta(\pm\infty, 0) \partial_g \hat{U}_I^\eta(0, \mp\infty) | \psi_0 \rangle}{\langle \psi_0 | \hat{U}_I^\eta(\pm\infty, 0) \hat{U}_I^\eta(0, \mp\infty) | \psi_0 \rangle}. \quad (9.100)$$

Similarly, taking the equation for $\langle \eta^{(\pm)}|$ and multiplying it by $|\psi_\eta^{(\pm)}\rangle$ from the right, we find

$$\Delta E = \pm i\eta g \frac{\langle \psi_0 | [\partial_g \hat{U}_I^\eta(\pm\infty, 0)] \hat{U}_I^\eta(0, \mp\infty) | \psi_0 \rangle}{\langle \psi_0 | \hat{U}_I^\eta(\pm\infty, 0) \hat{U}_I^\eta(0, \mp\infty) | \psi_0 \rangle}. \quad (9.101)$$

Adding the two results with the upper sign gives

$$\Delta E = i\frac{\eta}{2} g \frac{\partial}{\partial g} \log \langle \psi_0 | S^\eta(\infty, -\infty) | \psi_0 \rangle. \quad (9.102)$$

Note that the matrix element $\langle \psi_0 | S^\eta(\infty, -\infty) | \psi_0 \rangle$ is a pure phase $e^{i\varphi^\eta}$. This is seen as follows. The state $|\eta^{(+)}\rangle$ develops after an infinitely long time into $\hat{U}_I^\eta(\infty, -\infty) | \psi_0 \rangle$. There it becomes again an eigenstate of $\hat{H}_0$ due to the commutation relation (9.70). Thus it must coincide with $|\psi_0\rangle$ up to some overall factor $e^{i\varphi^\eta}$ (recall that $|\psi_0\rangle$ is nondegenerate by assumption). Hence we arrive at the level shift formula

$$\Delta E = -\frac{\eta}{2} g \frac{\partial}{\partial g} \varphi^\eta. \quad (9.103)$$

One sometimes finds this result stated in the opposite direction:

$$\varphi^\eta = -2 \frac{1}{\eta} \int_0^g \frac{dg'}{g'} \Delta E(g'). \quad (9.104)$$

To lowest order in g , where $\Delta E \propto g$, the formula becomes

$$\varphi^\eta \approx -2 \frac{g}{\eta} \Delta E + O(g^2). \quad (9.105)$$

This formula may be used for a lowest-order estimate of the change of a particle mass due to interactions.

Actually, in applications, the exponential switching factor is somewhat difficult to handle. A much more direct way of cutting off the interaction uses a step function along the time axis, i.e., it assumes the total interaction time T to be finite. The connection between T and η is found from the correspondence between integrals

$$\int_{-\infty}^{\infty} dt e^{-\eta|t|} = \frac{2}{\eta} \rightarrow \int_{-T/2}^{T/2} dt = T. \quad (9.106)$$

With this, we may rewrite (9.104) as

$$\varphi^\eta = -T \int_0^g \frac{dg'}{g'} \Delta E(g'). \quad (9.107)$$

9.2 Scattering by External Potential

After this development, it is straightforward to derive scattering amplitudes for a particle in an external potential $V(\mathbf{x})$ of a finite range.

9.2.1 The T -Matrix

Imagine a scattering center with a region of nonzero potential concentrated around the origin. A wave packet of a given average momentum $\mathbf{p}$ and energy E approaches this region along the x -axis from negative infinity. As long as it is far from the scattering center, it follows the free-particle Schrödinger equation

$$\hat{H}_0 |\psi(t)\rangle = i \partial_t |\psi(t)\rangle, \quad (9.108)$$

with the unperturbed Hamiltonian $\hat{H}_0 = \mathbf{p}^2/2M$. As the particle approaches the potential, the state is driven by the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. In the interaction representation we study the time evolution of a state which diagonalizes the unperturbed Hamiltonian $\hat{H}_0$. An artificially modified Schrödinger equation shows best how the incoming states change due to an interaction $\hat{V}_I \exp(-\eta|t|)$. The modification by the artificial switching factor $\exp(-\eta|t|)$ enables us to remove the scattering potential long before the scattering process happens. This frees us from the necessity of assuming the incoming wave to be localized in a packet long before the scattering

process. Instead, we can take it to be a pure plane wave, a momentum eigenstate $|\mathbf{p}\rangle$ solving the time-independent Schrödinger equation

$$\hat{H}_0|\mathbf{p}\rangle = E_{\mathbf{p}}|\mathbf{p}\rangle, \quad (9.109)$$

with an energy $E_{\mathbf{p}} = \mathbf{p}^2/2M$. The incoming wave function is

$$\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{p}\mathbf{x}/\hbar}. \quad (9.110)$$

The particle has the same probability everywhere in space, also in the scattering region. The amplitude for the incoming state $|\mathbf{p}\rangle$ to be scattered into another eigenstate with momentum $|\mathbf{p}'\rangle$ is given by the matrix elements

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\hat{U}_I(\infty, -\infty)|\mathbf{p}\rangle. \quad (9.111)$$

Decomposing $\hat{U}_I(\infty, -\infty)$ into the product of Møller operators,

$$\hat{U}_I(\infty, -\infty) = \hat{U}_I(\infty, 0)\hat{U}_I(0, -\infty) = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}, \quad (9.112)$$

we can also write

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'^{(-)}|\mathbf{p}^{(+)}\rangle, \quad (9.113)$$

where $|\mathbf{p}^{(\pm)}\rangle$ are the states

$$|\mathbf{p}^{(\pm)}\rangle \equiv \hat{\Omega}^{(\pm)}|\mathbf{p}\rangle. \quad (9.114)$$

The time evolution does not change the energy under the assumption of an infinitesimally small η , such that these states satisfy the full Schrödinger equation with the same energy $E = E_{\mathbf{p}} = \mathbf{p}^2/2M$:

$$\hat{H}|\mathbf{p}^{(\pm)}\rangle = E_{\mathbf{p}}|\mathbf{p}^{(\pm)}\rangle. \quad (9.115)$$

It is useful to take advantage of this property of the scattering process by rewriting the matrix element (9.111) in another way, using the explicit operator (9.24):

$$\begin{aligned} \langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle &= \lim_{t_2 \rightarrow \infty} \langle \mathbf{p}'|\hat{U}_I(t_2, 0)|\mathbf{p}^{(+)}\rangle \\ &= \lim_{t_2 \rightarrow \infty} \langle \mathbf{p}'|e^{i\hat{H}_0 t_2} e^{-i\hat{H} t_2}|\mathbf{p}^{(+)}\rangle \\ &= \lim_{t_2 \rightarrow \infty} e^{i(E_{\mathbf{p}'} - E_{\mathbf{p}})t_2} \langle \mathbf{p}'|\mathbf{p}^{(+)}\rangle. \end{aligned} \quad (9.116)$$

Then we apply the Lippmann-Schwinger equation (9.54) for $|\mathbf{p}^{(+)}\rangle$, to arrive at

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \lim_{t_2 \rightarrow \infty} e^{i(E_{\mathbf{p}'} - E_{\mathbf{p}})t_2} \left[\langle \mathbf{p}'|\mathbf{p}\rangle + \frac{1}{E_{\mathbf{p}} - E_{\mathbf{p}'} + i\eta} \langle \mathbf{p}'|\hat{V}|\mathbf{p}^{(+)}\rangle \right]. \quad (9.117)$$

The first term in brackets is nonzero only if the momenta are equal, $\mathbf{p}' = \mathbf{p}$, in which case the energies are also equal, $E_{\mathbf{p}'} = E_{\mathbf{p}}$. The right-hand side is unaffected by the limit $t_2 \rightarrow -\infty$ in the prefactor.

We shall imagine the system to be enclosed in a box of a large volume V (not to be confused with the potential $\hat{V}$). Then the momenta are discrete and the first term is simply

$$\delta_{\mathbf{p}', \mathbf{p}}.$$

It describes the amplitude for the *direct beam* to appear behind the scattering region, containing all unscattered particles. The second term describes scattering. Here the limit $t_2 \rightarrow \infty$ in the prefactor is nontrivial. If $E' \neq E$, it oscillates so fast that it can be set equal to zero, by the Riemann-Lebesgue lemma (see Ref. [13] on p. 387).

For $E' = E$, it is identically equal to unity so that

$$\lim_{t_2 \rightarrow \infty} \frac{e^{i(E'-E)t_2}}{E - E' + i\eta} = \begin{cases} 0, & E' \neq E, \\ -i/\eta, & E' = E. \end{cases} \quad (9.118)$$

Such a property defines a δ -function in the energy. Only the normalization needs adjustment, which is done as follows:

$$\lim_{t_2 \rightarrow \infty} \frac{i}{2\pi} \frac{e^{i(E'-E)t_2}}{E - E' + i\eta} = \delta(E' - E). \quad (9.119)$$

Indeed, if we integrate the left-hand side over a smooth function $f(E')$ and set $E' \equiv E + \xi/t_2$, then the E' -integral can be rewritten as

$$-\frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{d\xi}{t_2} \frac{e^{i\xi}}{\xi/t_2 - i\eta} f(E + \xi/t_2). \quad (9.120)$$

In the limit of large t_2 , the function $f(E)$ can be taken out of the integral, and the contour of integration can then be closed in the upper half-plane giving $e^{-\eta t_2}$. Since η is an infinitesimal quantity, this is the same result as the one that would be obtained from the right-hand side of (9.119). The δ -function (9.28) ensures the conservation of energy in the scattering process.

Another way to verify formula (9.119) is to rewrite the left-hand side as

$$\frac{1}{2\pi} \int_{-\infty}^{t_2} dt e^{i(E'-E-i\eta)t}, \quad (9.121)$$

which obviously tends to $\delta(E' - E)$ in the limit $t_2 \rightarrow \infty$.

Let us also express the Lippmann-Schwinger equation in terms of wave functions. Multiplying (9.54) by the local states $\langle \mathbf{x} |$ from the left, and identifying the interacting states $|\psi^{(+)}\rangle$ with the states $|\mathbf{p}^{(+)}\rangle$ in Eq. (9.114) that arises from an incoming particle wave of momentum $\mathbf{p}$, the left-hand side is the full Schrödinger wave function

$$\psi^{(+)}(\mathbf{x}) \equiv \langle \mathbf{x} | \mathbf{p}^{(+)} \rangle, \quad (9.122)$$

which is an eigenstate of Eq. (9.37):

$$\hat{H}|\mathbf{p}^{(+)}\rangle = E|\mathbf{p}^{(+)}\rangle. \quad (9.123)$$

The first term on the right-hand side is the plane wave (9.110). The second term in (9.54),

$$\langle \mathbf{x}|\mathbf{p}\rangle^{\text{sc}} \equiv \langle \mathbf{x}|\frac{1}{E - \hat{H}_0 + i\eta}\hat{V}|\mathbf{p}^{(+)}\rangle, \quad (9.124)$$

is the scattering state. After inserting a completeness relation $\int d^3x' |\mathbf{x}'\rangle\langle \mathbf{x}'| = 1$, this takes the form of an integral equation

$$\langle \mathbf{x}|\mathbf{p}\rangle^{\text{sc}} = \int d^3x' \langle \mathbf{x}|\frac{1}{E - \hat{H}_0 + i\eta}|\mathbf{x}'\rangle V(\mathbf{x}') \langle \mathbf{x}'|\mathbf{p}^{(+)}\rangle. \quad (9.125)$$

Another way of stating this is

$$\langle \mathbf{x}|\mathbf{p}\rangle^{\text{sc}} = \int d^3x' \langle \mathbf{x}|\hat{G}_0(E)|\mathbf{x}'\rangle \hat{V}(\mathbf{x}') \langle \mathbf{x}'|\mathbf{p}^{(+)}\rangle, \quad (9.126)$$

where $\langle \mathbf{x}|\hat{G}_0(E)|\mathbf{x}'\rangle$ are the matrix elements of the free-particle resolvent defined in Eq. (9.57):

$$\langle \mathbf{x}|\hat{G}_0(E)|\mathbf{x}'\rangle = \langle \mathbf{x}|\frac{1}{E - \hat{H}_0 + i\eta}|\mathbf{x}'\rangle. \quad (9.127)$$

Thus the result of the full Lippmann-Schwinger equation is the wave function

$$\langle \mathbf{x}|\mathbf{p}^{(+)}\rangle = \langle \mathbf{x}|\mathbf{p}\rangle + \langle \mathbf{x}|\mathbf{p}\rangle^{\text{sc}}. \quad (9.128)$$

It solves the interacting Schrödinger equation (9.123) and shows explicitly the free incoming wave plus the scattered wave. Asymptotically, the scattered wave is usually an outgoing asymptotically spherical wave emerging from the scattering center.

We are now prepared to introduce the so-called T -matrix as the quantity

$$\langle \mathbf{p}'|\hat{T}(E)|\mathbf{p}\rangle \equiv \langle \mathbf{p}'|\hat{V}|\mathbf{p}^{(+)}\rangle = \langle \mathbf{p}'|\hat{V}\hat{\Omega}^{(+)}|\mathbf{p}\rangle, \quad (9.129)$$

so that the S -matrix decomposes into a direct-beam contribution plus an energy-conserving scattering contribution as follows:

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\mathbf{p}\rangle - 2\pi i\delta(E' - E)\langle \mathbf{p}'|\hat{T}(E)|\mathbf{p}\rangle. \quad (9.130)$$

In terms of $\hat{T}$, the Lippmann-Schwinger equation (9.54) reads

$$|\mathbf{p}^{(+)}\rangle = |\mathbf{p}\rangle + \frac{1}{E - \hat{H}_0 + i\eta}\hat{V}|\mathbf{p}^{(+)}\rangle = |\mathbf{p}\rangle + \frac{1}{E - \hat{H}_0 + i\eta}\hat{T}(E)|\mathbf{p}\rangle. \quad (9.131)$$

Equation (9.61) for the Møller operator implies that the T -matrix obeys the implicit equation

$$\hat{T}(E) = \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0 - i\eta} \hat{T}(E). \quad (9.132)$$

Its matrix elements satisfy an integral equation for the T -matrix. Note that $\hat{T}(E)$ can be expressed in terms of the Møller operator (9.53) as

$$\hat{T} = \hat{V} \hat{\Omega}^{(+)} \quad (9.133)$$

If we multiply the state vectors (9.131) by ket vectors $\langle \mathbf{x} |$ from the left, we obtain the position representation of the Lippmann-Schwinger equation:

$$\langle \mathbf{x} | \mathbf{p}^{(+)} \rangle = \langle \mathbf{x} | \mathbf{p} \rangle + \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} | \mathbf{p}^{(+)} \rangle = \langle \mathbf{x} | \mathbf{p} \rangle + \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\eta} \hat{T}(E) | \mathbf{p} \rangle. \quad (9.134)$$

The first term $\langle \mathbf{x} | \mathbf{p} \rangle$ is once more the incoming wave, and the second term is the T -matrix representation of the scattered wave (9.125):

$$\langle \mathbf{x} | \mathbf{p} \rangle^{\text{sc}} \equiv \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\eta} \hat{V} | \mathbf{p}^{(+)} \rangle = \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\eta} \hat{T} | \mathbf{p} \rangle. \quad (9.135)$$

9.2.2 Asymptotic Behavior

Let us calculate the asymptotic form of the scattered wave (9.135) in the form (9.126), where it is expressed in terms of the free-particle resolvent in Eq. (9.57):

$$\langle \mathbf{x} | \mathbf{p} \rangle^{\text{sc}} = -\frac{i}{\hbar} \int d^3x' \langle \mathbf{x} | \hat{G}_0(E) | \mathbf{x}' \rangle \hat{V}(\mathbf{x}') \langle \mathbf{x}' | \mathbf{p}^{(+)} \rangle. \quad (9.136)$$

The matrix elements of the resolvent have the Fourier decomposition

$$\begin{aligned} \langle \mathbf{x} | \hat{G}_0(E) | \mathbf{x}' \rangle &= i\hbar \int \frac{d^3p}{(2\pi\hbar)^3} \langle \mathbf{x} | \mathbf{p} \rangle \frac{i\hbar}{E - E_{\mathbf{p}} + i\eta} \langle \mathbf{p} | \mathbf{x}' \rangle \\ &= i\hbar \int \frac{d^3p}{(2\pi\hbar)^3} \frac{e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar}}{E - \mathbf{p}^2/2M + i\eta}. \end{aligned} \quad (9.137)$$

Introducing $p_E \equiv \sqrt{2M(E + i\eta)}$, the momentum integral yields

$$\langle \mathbf{x} | \hat{G}_0(E) | \mathbf{x}' \rangle = -2Mi\hbar \int \frac{d^3p}{(2\pi\hbar)^3} \frac{e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar}}{\mathbf{p}^2 - p_E^2} = -\frac{2Mi}{\hbar} \frac{1}{4\pi} \frac{e^{ip_E|\mathbf{x}-\mathbf{x}'|/\hbar}}{|\mathbf{x} - \mathbf{x}'|}. \quad (9.138)$$

For each $\mathbf{x}'$, this is a wave function whose time dependence is given by an exponential $e^{-iEt/\hbar}$. It represents an outgoing spherical wave emerging from $\mathbf{x}'$. Had we chosen the opposite sign of $i\eta$ in the denominator of (9.137), the exponential would have been $e^{-ip_E|\mathbf{x}-\mathbf{x}'|/\hbar}$ which, together with the time dependence $e^{-iEt/\hbar}$, would have

represented an incoming spherical wave. With the choice (9.138), the scattered wave (9.136) is a superposition of outgoing spherical waves emerging from all points $\mathbf{x}'$ in the potential $V(\mathbf{x}')$. As such it is an adaptation of the ancient Huygens principle of light waves to Schrödinger's material waves.

The outgoing spherical waves observed at some point $\mathbf{x}$ come from all points $\mathbf{x}'$ in the scattering potential $V(\mathbf{x}')$. They appear as a common outgoing spherical wave whose shape is found by going in (9.138) to the asymptotic regime of large $\mathbf{x}$. As long as $|\mathbf{x}'| \ll |\mathbf{x}| = r$, we can expand

$$|\mathbf{x} - \mathbf{x}'| \equiv r - \hat{\mathbf{x}} \cdot \mathbf{x}' + \dots, \quad (9.139)$$

so that (9.136) simplifies to

$$\langle \mathbf{x} | \mathbf{p} \rangle^{\text{sc}} \xrightarrow{r \rightarrow \infty} -\frac{e^{ip_E r/\hbar}}{4\pi r} \frac{2M}{\hbar^2} \int d^3x' e^{-ip_E \hat{\mathbf{x}} \cdot \mathbf{x}'/\hbar} V(\mathbf{x}') \langle \mathbf{x}' | \mathbf{p}^{(+)} \rangle. \quad (9.140)$$

Since the scattering is elastic the energy of the incoming particles $E_{\mathbf{p}}$ is equal to the energy of the outgoing particles $E_{\mathbf{p}'}$. Those arriving at the point $\mathbf{x}$ emerge with a momentum $\mathbf{p}'$ whose size is equal to that of $\mathbf{p}$ and whose direction is $\hat{\mathbf{x}}$. Thus we define the outgoing momentum in the spherical wave as

$$\mathbf{p}' = p_E \hat{\mathbf{x}}, \quad (9.141)$$

and rewrite the exponent in (9.140) as

$$e^{-ip_E \hat{\mathbf{x}} \cdot \mathbf{x}'/\hbar} \rightarrow e^{-i\mathbf{p}' \cdot \mathbf{x}'/\hbar}. \quad (9.142)$$

With the scattered wave (9.140), the total wave function (9.134) may be written as a sum of an incoming plane wave and an outgoing spherical wave

$$\langle \mathbf{x} | \mathbf{p}^{(+)} \rangle \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \left(e^{i\mathbf{p}\mathbf{x}/\hbar} + \frac{e^{ipr/\hbar}}{r} f_{\mathbf{p}'\mathbf{p}} \right). \quad (9.143)$$

The prefactor of the spherical wave $f_{\mathbf{p}'\mathbf{p}}$ is called the *scattering amplitude*. Explicitly, it is given by the integral⁴:

$$f_{\mathbf{p}'\mathbf{p}} = -\sqrt{V} \frac{1}{4\pi} \frac{2M}{\hbar^2} \int d^3x' e^{-i\mathbf{p}' \cdot \mathbf{x}'/\hbar} V(\mathbf{x}') \langle \mathbf{x}' | \mathbf{p}^{(+)} \rangle. \quad (9.144)$$

From the asymptotic behavior (9.143), where the wave function is decomposed into an incoming plane wave and an outgoing spherical wave, we deduce immediately that the square of $f_{\mathbf{p}'\mathbf{p}}$ determines the scattering cross section. The argument goes as follows: The incoming wave has the particle current density

$$\mathbf{j} = -(i/M)\psi^* \nabla \psi = \frac{\mathbf{v}}{V}. \quad (9.145)$$

⁴For the phase convention see, for example, the textbook by L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon Press, London, 1965.

The outgoing spherical wave has an amplitude $f_{\mathbf{p}'\mathbf{p}}e^{ipr}/r\sqrt{V}$, and describes radial particle flow with current density

$$\mathbf{j}' = |f_{\mathbf{p}'\mathbf{p}}|^2 \frac{\hat{\mathbf{x}}}{r^3} \frac{v}{V}. \quad (9.146)$$

The ratio between the two $|\mathbf{j}'|/|\mathbf{j}|$ is identified with $d\sigma/r^2d\Omega$, and defines the differential cross section:

$$\frac{d\sigma}{d\Omega} = |f_{\mathbf{p}'\mathbf{p}}|^2. \quad (9.147)$$

If the potential is weak, the full wave function $\langle \mathbf{x} | \mathbf{p}^{(+)} \rangle$ on the right-hand side can be approximated by the incoming plane wave $\langle \mathbf{x} | \mathbf{p} \rangle$, and one obtains the scattering amplitude in the *Born approximation*

$$f_{\mathbf{p}'\mathbf{p}} \approx -\frac{1}{4\pi} \frac{2M}{\hbar^2} \int d^3x' e^{-i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}'/\hbar} V(\mathbf{x}'). \quad (9.148)$$

The momentum difference $\mathbf{q} \equiv \mathbf{p}' - \mathbf{p}$ is equal to the *momentum transfer* of the scattering process. Thus the scattering amplitude in the Born approximation is, up to a factor $-2M/\hbar^2$, equal to the Fourier components of the potential at the momentum transfer $\mathbf{q}$:

$$\tilde{V}(\mathbf{q}) \equiv \int d^3x' e^{-i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}'/\hbar} V(\mathbf{x}'). \quad (9.149)$$

For a potential $V(\mathbf{x}) = g\delta(\mathbf{x})$, where $\tilde{V}(\mathbf{q}) = g$, the scattering amplitude in the Born approximation is

$$f_{\mathbf{p}'\mathbf{p}} = -\frac{M}{2\pi\hbar^2} g. \quad (9.150)$$

The Born formula (9.148) will be generalized to D dimensions further down in Eq. (9.249).

9.2.3 Partial Waves

The scattering amplitudes are often analyzed separately for each angular momentum of the scattered particles. For equal incoming and outgoing energies $E_{\mathbf{p}'} = E_{\mathbf{p}}$, which implies that also the momenta are equal $|\mathbf{p}'| = |\mathbf{p}| = p$, the T -matrix $\langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle$ in Eq. (9.129) has a partial-wave expansion

$$\langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle = \frac{(2\pi)^3}{V} \sum_{l=0}^{\infty} T_l(p) \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}(\hat{\mathbf{p}}). \quad (9.151)$$

Here $Y_{lm}(\hat{\mathbf{p}})$ are the spherical harmonics defined in (4F.1), which are now associated with the momentum direction $\hat{\mathbf{p}}$:

$$Y_{lm}(\hat{\mathbf{p}}) = Y_{lm}(\theta, \varphi) \equiv (-1)^m \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\varphi}. \quad (9.152)$$

They satisfy the orthogonality relation (4F.3), which we shall write in the form

$$\int d^2\hat{\mathbf{p}} Y_{l'm'}^*(\hat{\mathbf{p}}) Y_{lm}(\hat{\mathbf{p}}) = \delta_{l'l} \delta_{m'm}, \quad (9.153)$$

where $\int d^2\hat{\mathbf{p}}$ denotes the integral over the surface of a unit sphere:

$$\int d^2\hat{\mathbf{p}} \equiv \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\varphi. \quad (9.154)$$

It is useful to view the spherical harmonics as matrix elements of eigenstates $|lm\rangle$ of angular momentum [recall (4.846)] with localized states $\langle\hat{\mathbf{p}}|$ on the unit sphere:

$$\langle\hat{\mathbf{p}}|lm\rangle \equiv Y_{lm}(\hat{\mathbf{p}}). \quad (9.155)$$

The latter satisfy the orthogonality relation:

$$\langle\hat{\mathbf{p}}'|\hat{\mathbf{p}}\rangle = \delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}), \quad (9.156)$$

where $\delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}})$ is the δ -function on a unit sphere:

$$\delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) \equiv \delta(\cos\theta' - \cos\theta) \delta(\varphi' - \varphi). \quad (9.157)$$

With the help of the addition theorem for the spherical harmonics

$$\frac{2l+1}{4\pi} P_l(\cos\Delta\vartheta) = \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}^*(\hat{\mathbf{p}}), \quad \cos\Delta\vartheta \equiv \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}, \quad (9.158)$$

the *partial-wave expansion* (9.151) becomes

$$\langle\mathbf{p}'|\hat{T}|\mathbf{p}\rangle = \frac{(2\pi)^3}{V} \sum_{l=0}^{\infty} T_l(p) \frac{2l+1}{4\pi} P_l(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}), \quad (9.159)$$

where $P_l(\cos\theta) \equiv P_l^0(\cos\theta)$ are the Legendre polynomials (4F.7).

A similar expansion of the S -matrix (9.130) requires decomposing the scalar product $\langle\mathbf{p}'|\mathbf{p}\rangle = \delta_{\mathbf{p}',\mathbf{p}}$ into partial waves. In a large volume V , this is replaced by $(2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p})/V$, which is decomposed into a directional and a radial part as

$$\delta_{\mathbf{p}',\mathbf{p}} = \frac{(2\pi)^3}{V} \delta^{(3)}(\mathbf{p}' - \mathbf{p}) = \delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) \frac{(2\pi)^3}{V} \frac{1}{p^2} \delta(p' - p). \quad (9.160)$$

The directional δ -function on the right-hand side has a partial-wave expansion which is, in fact, the completeness relation (4E.1) for the states $|lm\rangle$,

$$\sum_{l=0}^{\infty} \sum_{m=-l}^l |lm\rangle \langle lm| = 1, \quad (9.161)$$

after being sandwiched between the localized states $|\hat{\mathbf{p}}\rangle$ on the unit sphere. Using the matrix elements (9.155) and the orthogonality relation (9.156), we find from (9.161):

$$\delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}^*(\hat{\mathbf{p}}). \quad (9.162)$$

The radial part of (9.160) can be rewritten as

$$\frac{(2\pi)^3}{V} \frac{1}{p^2} \delta(p' - p) = \frac{(2\pi)^3}{V} \frac{1}{p^2} \frac{dE}{dp} \delta(E' - E) = \frac{(2\pi)^3}{V} \frac{1}{\rho_E} \delta(E' - E), \quad (9.163)$$

where $E = E_{\mathbf{p}} = \mathbf{p}^2/2M$, $E' = E_{\mathbf{p}'} = \mathbf{p}'^2/2M$, $p \equiv |\mathbf{p}|$, with

$$\rho_E \equiv \frac{p^2}{dE/dp} = Mp \quad (9.164)$$

being proportional to the density of energy levels on the E -axis in a large volume V . The quantity $\rho_E \times V/(2\pi)^3$ is the density of states. With the help of ρ_E we can rewrite the sum over all momentum states as follows:

$$\sum_{\mathbf{p}} = \int \frac{d^3p V}{(2\pi)^3} = \int d^2\hat{\mathbf{p}} \frac{V}{(2\pi)^3} \int dE \rho_E. \quad (9.165)$$

Thus we find the expansion

$$\langle \mathbf{p}' | \mathbf{p} \rangle = \delta_{\mathbf{p}', \mathbf{p}} = \frac{(2\pi)^3}{V} \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}(\hat{\mathbf{p}}) \frac{1}{\rho_E} \delta(E' - E). \quad (9.166)$$

In a partial-wave expansion for the S -matrix (9.130), the overall δ -function for the energy conservation is conventionally factored out and one writes:

$$\langle \mathbf{p}' | \hat{S} | \mathbf{p} \rangle = \frac{(2\pi)^3}{V} \frac{1}{\rho_E} \delta(E' - E) \sum_{l=0}^{\infty} S_l(p) \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}(\hat{\mathbf{p}}). \quad (9.167)$$

Recalling (9.130), we find the relation between the *partial-wave scattering amplitudes* $S_l(p)$ and those of the T -matrix:

$$S_l(p) = 1 - 2\pi i \rho_E T_l(p). \quad (9.168)$$

The potential scattering under consideration is purely elastic. For such processes, the unitarity property (9.44) of the S -matrix implies

$$\int \frac{d^3p'' V}{(2\pi)^3} \langle \mathbf{p}' | \hat{S}^\dagger | \mathbf{p}'' \rangle \langle \mathbf{p}'' | \hat{S} | \mathbf{p} \rangle = \langle \mathbf{p}' | \mathbf{p} \rangle. \quad (9.169)$$

Inserting the partial-wave decomposition (9.167) and using (9.165) as well as the orthogonality relation (9.153), we derive from (9.169) the unitarity property of the partial waves of elastic scattering

$$S_l^*(p)S_l(p) = 1, \quad (9.170)$$

implying that $S_l(p)$ is a pure phase factor:

$$S_l(p) = e^{2i\delta_l(p)}. \quad (9.171)$$

For the amplitudes $T_l(p)$ in (9.168), this implies

$$T_l(p) = -\frac{1}{\pi\rho_E} e^{i\delta_l(p)} \sin \delta_l(p). \quad (9.172)$$

The quantities $\delta_l(p)$ are the *phase shifts* observed in the scattered waves of angular momentum l with respect to the incoming waves.

In order to show this we use the expansion formula

$$e^{iz \cos \vartheta} = \sqrt{\frac{\pi}{2z}} \sum_{l=0}^{\infty} i^l J_{l+1/2}(z) (2l+1) P_l(\cos \vartheta), \quad (9.173)$$

where the Bessel functions $J_{l+1/2}(z)$ can be expressed in terms of spherical Bessel functions $j_l(z)$ as

$$J_{l+1/2}(z) = \sqrt{\frac{2z}{\pi}} j_l(z). \quad (9.174)$$

The expansion (9.173) may be viewed as a special case of the Dirac bracket expansion

$$\langle \mathbf{x} | \mathbf{p} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{p}\mathbf{x}} = \sum_{l=0}^{\infty} \psi_l(pr) \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{x}}) Y_{lm}(\hat{\mathbf{p}}) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \psi_l(pr) P_l(\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}), \quad (9.175)$$

where $r \equiv |\mathbf{x}|$, and

$$\psi_l(pr) = \frac{1}{\sqrt{V}} i^l 4\pi j_l(pr) \quad (9.176)$$

are partial-wave amplitudes of the plane wave. Far from the scattering region, the spherical Bessel functions have the asymptotic behavior

$$j_l(z) \rightarrow \frac{\sin(z - \pi l/2)}{pr}, \quad (9.177)$$

implying for the partial waves

$$\psi_l(pr) = \frac{1}{\sqrt{V}} i^l 4\pi \frac{\sin(pr - \pi l/2)}{pr}. \quad (9.178)$$

We now turn to the partial-wave expansion of the scattered wave (9.135) in the Lippmann-Schwinger equation. Inserting a complete set of free momentum eigenstates into the right-hand side, we obtain

$$\langle \mathbf{x} | \mathbf{p} \rangle^{\text{sc}} = \int \frac{d^3 p' V}{(2\pi)^3} \langle \mathbf{x} | \mathbf{p}' \rangle \frac{1}{E - E' + i\eta} \langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle. \quad (9.179)$$

Inserting the partial-wave decompositions (9.159) and (9.175), the right-hand side becomes

$$\begin{aligned} & \int \frac{d^3 p' V}{(2\pi)^3} \langle \mathbf{x} | \mathbf{p}' \rangle \frac{1}{E - E' + i\eta} \langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle \\ &= \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{x}}') Y_{lm}(\hat{\mathbf{p}}) i^l 4\pi \int_0^{\infty} dp' p'^2 \frac{j_l(p'r) T_l(p)}{E - E' + i\eta}. \end{aligned} \quad (9.180)$$

Adding this to the incoming wave function, we find the total partial waves:

$$\psi_l^{\text{tot}}(pr) = \frac{1}{\sqrt{V}} 4\pi i^l \left[j_l(pr) + \int_0^{\infty} dp' p'^2 \frac{j_l(p'r) T_l(p)}{E - E' + i\eta} \right]. \quad (9.181)$$

For large r , we use the asymptotic form (9.177) to write the second term in the brackets as

$$\int_0^{\infty} dp' p'^2 \frac{T_l(p')}{E - E' + i\eta} \frac{e^{i(p'r - \pi l/2)} - e^{-i(p'r - \pi l/2)}}{2ip'r}. \quad (9.182)$$

Being at large r , the integral is oscillating very fast as a function of p' . It receives a sizable contribution only from a neighborhood of the pole term in the energy.⁵ There we can approximate

$$E - E' \approx \frac{dE}{dp}(p - p'), \quad (9.183)$$

and approximate $p' \approx p$ in all terms, except for the fast oscillating exponential. The ensuing integral

$$\frac{1}{dE/dp} p^2 \int dp' \frac{T_l(p')}{p - p' + i\eta} \frac{e^{i(p'r - \pi l/2)} - e^{-i(p'r - \pi l/2)}}{2ip'r} \quad (9.184)$$

can be extended to the entire p' -axis with a negligible error for large r . The part containing the second exponential is evaluated by closing the contour of integration in the lower half-plane. There the integrand is regular so that the contour can be contracted to a point yielding zero. In the part with the first exponential we close the contour in the upper half-plane and deform it to pick up the pole at $p' = p + i\eta$. Then Cauchy's theorem yields

$$\frac{1}{dE/dp} p^2 \int dp' \frac{T_l(p')}{p - p' + i\eta} \frac{e^{i(p'r - \pi l/2)} - e^{-i(p'r - \pi l/2)}}{2ip'r} = -\frac{2\pi p^2}{dE/dp} T_l(p) e^{-i\pi l/2} \frac{e^{ip'r}}{2p'r}, \quad (9.185)$$

⁵This is a consequence of the *Riemann-Lebesgue lemma* cited in Ref. [13] on p. 387.

so that the total wave function (9.181) becomes

$$\begin{aligned}\psi_l^{\text{tot}}(pr) &\xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} 4\pi \left[i^l j_l(pr) - 2\pi \rho_E T_l(p) \frac{e^{ipr}}{2pr} \right] \\ &\xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{4\pi i^l}{2ipr} \left[e^{ipr} - (-1)^l e^{-ipr} - 2\pi i \rho_E T_l(p) e^{ipr} \right].\end{aligned}\quad (9.186)$$

Using (9.168), this is equal to

$$\psi_l^{\text{tot}}(pr) \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{4\pi i^l}{2ipr} \left[S_l(p) e^{ipr} - (-1)^l e^{-ipr} \right]. \quad (9.187)$$

Inserting the unitary form (9.171) for elastic scattering, this becomes

$$\psi_l^{\text{tot}}(pr) \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{4\pi}{p} i^l e^{i\delta_l(p)} \frac{\sin(pr - \pi l/2 + \delta_l(p))}{r}. \quad (9.188)$$

This shows that $\delta_l(p)$ is indeed the phase shift of the scattered waves with respect to the incoming partial waves (9.178).

At small momenta, the $l = 0$ (s -wave) phase shift dominates the scattering process since the particles do not have enough energy to overcome the centrifugal barrier.

For short-range potentials, the s -wave phase shift diverges for $p \rightarrow 0$, and the leading two orders in p may be parametrized as follows

$$p \cot \delta_0 = -\frac{1}{a_s} + \frac{1}{2} r_{\text{eff}} p^2 + \dots \quad (9.189)$$

The parameter a_s is the s -wave *scattering length*, and r_{eff} is called the *effective range* of the scattering process.

The direct small- k expansion of δ_0 is

$$\delta_0(p) = -a_s p - \left(a_s^2 r_{\text{eff}} - \frac{a_s^3}{3} \right) p^3 + \dots \quad (9.190)$$

For small p , only the s -wave scattering length is relevant. There the s -wave scattering amplitude behaves like [recall (9.172)]

$$T_0(p) \approx -\frac{1}{\pi M p} \left[\delta_0(p) + i\delta_0^2(p) - \frac{2}{3}\delta_0^3(p) + \dots \right] \approx \frac{a_s}{\pi M} \left[1 - i a_s p + (a_s r_{\text{eff}} - a_s^2) k^2 + \dots \right]. \quad (9.191)$$

Inserting this into (9.159), we see that in the limit $p \rightarrow 0$:

$$\langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle \rightarrow (2\pi)^3 \frac{a_s}{4\pi^2 V M} = 2\pi \frac{a_s}{M} \frac{1}{V}, \quad (9.192)$$

which by (9.262) is also equal to g_R/M .

For a nonzero angular momentum l , the effective-range formula (9.189) leads to the small- p behavior

$$p^{2l+1} \cot \delta_l = -\frac{1}{a_l} + \frac{1}{2} r_{\text{eff}l} p^2 + \dots \quad (9.193)$$

Although (9.189) and (9.193) are small- p approximations, the range of validity may extend to quite large momenta if the potential is of short range. It may include a resonance in the scattering amplitude, in which case one may use the approximation

$$f_l(p) \equiv \frac{4\pi}{p \cot \delta_l(p) - ip}. \quad (9.194)$$

In general, one may parametrize the S -matrix element in the vicinity of a resonance by the unitary ansatz

$$S_l(p) = e^{2i\delta_l(p)} \equiv \frac{E - E_R - i\Gamma_R/2}{E - E_R + i\Gamma_R/2}, \quad (9.195)$$

where E_R is the energy of the resonance and Γ_R its decay rate. At every resonance or bound state, $\delta_l(p)$ passes through $\pi/2$ plus an integer multiple of π . This is guaranteed by *Levinson's theorem* [4], according to which the number of bound states in a potential is equal to the difference $[\delta_l(0) - \delta_l(\infty)]/\pi$.

We may also write

$$f_l(p) \equiv \frac{4\pi}{p} \frac{-\Gamma_R/2}{E - E_R + i\Gamma_R/2}, \quad (9.196)$$

and

$$S_l(p) = e^{-2ip a_{\text{eff}l}(p)}, \quad (9.197)$$

with

$$a_{\text{eff}l} \equiv a_l + \frac{1}{2p} \arctan \frac{\Gamma_R(E - E_R)}{(E - E_R)^2 + \Gamma_R^2/4}. \quad (9.198)$$

9.2.4 Off-Shell T -Matrix

In scattering experiments, only matrix elements are observables in which the energy E is equal to the energies $E_{\mathbf{p}} \equiv \mathbf{p}^2/2M = E_{\mathbf{p}'} \equiv \mathbf{p}'^2/2M$ of incoming and outgoing particles. For mathematical purposes, however, one also defines a T -matrix for unequal energies $E \neq E_{\mathbf{p}} \neq E_{\mathbf{p}'}$, as the matrix elements of the operator

$$\hat{T}(E) = \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0 + i\eta} \hat{T}(E). \quad (9.199)$$

This is called the *off-shell T -matrix*. It can be expressed in terms of the resolvent $\hat{G}_0(E)$ in (9.57) as

$$\hat{T}(E) = \hat{V} + \hat{V} \hat{G}_0(E) \hat{T}(E). \quad (9.200)$$

This is an implicit equation for $\hat{T}(E)$ that can be solved iteratively by the geometric series

$$\hat{T}(E) = \hat{V} + \hat{V}\hat{G}_0(E)\hat{V} + \hat{V}\hat{G}_0(E)\hat{V}\hat{G}_0(E)\hat{V} + \dots \quad (9.201)$$

Comparison with (9.60) shows that we may also write, instead of (9.200),

$$\hat{T}(E) = \hat{V} + \hat{V}\hat{G}(E)\hat{V}. \quad (9.202)$$

There are two further equivalent equations:

$$\hat{G}_0(E)\hat{T}(E) = \hat{G}(E)\hat{V}, \quad (9.203)$$

and

$$\hat{G}_0(E)\hat{T}(E)\hat{G}_0(E) = \hat{G}(E) - \hat{G}_0(E). \quad (9.204)$$

The latter can also be written as

$$\hat{T}(E) = (E - \hat{H}_0)\hat{G}(E)(E - \hat{H}_0) - (E - \hat{H}_0). \quad (9.205)$$

This equation gives a useful relation between the off-shell matrix elements of the T -matrix and those of the resolvents:

$$\begin{aligned} \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle &= (E - E_{\mathbf{p}})^2 [\langle \mathbf{p}' | \hat{G}(E) | \mathbf{p} \rangle - \langle \mathbf{p}' | \hat{G}_0(E) | \mathbf{p} \rangle] \\ &= (E - E_{\mathbf{p}})^2 \langle \mathbf{p}' | \hat{G}(E) | \mathbf{p} \rangle - (E - E_{\mathbf{p}}) \langle \mathbf{p}' | \mathbf{p} \rangle. \end{aligned} \quad (9.206)$$

Let us express the right-hand side in terms of the spectral representation of the resolvents. We take the completeness relation for the states (9.109):

$$\sum_{\mathbf{p}} |\mathbf{p}\rangle \langle \mathbf{p}| = 1, \quad (9.207)$$

and multiply this by the operator $1/(E - \hat{H}_0)$. Using the eigenvalue equation (9.109), we obtain the spectral representation of the free resolvent:

$$\hat{G}(E) = \sum_{\mathbf{p}} \frac{|\mathbf{p}\rangle \langle \mathbf{p}|}{E - E_{\mathbf{p}} + i\eta}. \quad (9.208)$$

The interacting resolvent $\hat{G}(E)$ has a similar representation. Let $|n\rangle$ be the complete set of eigenstates of the full Hamiltonian [consisting of the set of scattering states $|\psi_a^{(+)}\rangle$ plus the set of bound states $|\psi_\beta\rangle$ on the right-hand side of Eq. (9.62)]:

$$\hat{H}|n\rangle = E_n|n\rangle. \quad (9.209)$$

Then the completeness relation

$$\sum_n |n\rangle \langle n| = 1 \quad (9.210)$$

leads to the spectral representation

$$\hat{G}(E) = \sum_n \frac{|n\rangle \langle n|}{E - E_n}. \quad (9.211)$$

Rewriting $E - E_{\mathbf{p}} = (E - E_n) + (E_n - E_{\mathbf{p}})$, then Eq. (9.206) becomes

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle = \sum_n (E_n - E_{\mathbf{p}'}) (E - E_{\mathbf{p}}) \frac{\langle \mathbf{p}' | n \rangle \langle n | \mathbf{p} \rangle}{E - E_n + i\eta} + (E - E_{\mathbf{p}}) \left[\sum_n \langle \mathbf{p}' | n \rangle \langle n | \mathbf{p} \rangle - \langle \mathbf{p}' | \mathbf{p} \rangle \right]. \quad (9.212)$$

The second term vanishes due to the completeness relation (9.210), and can be dropped. This is true only if the potential has no hard core forbidding completely the presence of a particle inside some core volume V_{core} . In this case, the wave functions $\langle \mathbf{x} | n \rangle$ vanish identically inside V_{core} , and the wave functions are complete only outside V_{core} . Then the second term yields a correction to the first term

$$\langle \mathbf{p}' | \hat{T}_{\text{corr}}(E) | \mathbf{p} \rangle = -(E - E_{\mathbf{p}}) \int_{V_{\text{core}}} d^D x e^{i(\mathbf{p}' - \mathbf{p})\mathbf{x}}, \quad (9.213)$$

which is zero on shell. Using the identity $(E_n - E_{\mathbf{p}'}) \langle \mathbf{p}' | n \rangle = \langle \mathbf{p}' | \hat{H} - \hat{H}_0 | n \rangle = \langle \mathbf{p}' | \hat{V} | n \rangle$, the first term in (9.212) takes the form

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle = \sum_n (E - E_{\mathbf{p}}) \frac{\langle \mathbf{p}' | \hat{V} | n \rangle \langle n | \mathbf{p} \rangle}{E - E_n + i\eta}. \quad (9.214)$$

Replacing further $E - E_{\mathbf{p}}$ by $(E - E_n) + (E_n - E_{\mathbf{p}})$, this becomes

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle = \sum_n \langle \mathbf{p}' | \hat{V} | n \rangle \langle n | \mathbf{p} \rangle + \sum_n \frac{\langle \mathbf{p}' | \hat{V} | n \rangle \langle n | \hat{V} | \mathbf{p} \rangle}{E - E_n + i\eta}. \quad (9.215)$$

Let us now focus our attention upon a potential without bound states. Then we can use, instead of the discrete states $|n\rangle$ in the completeness relation (9.210), the continuous set of solutions $|\mathbf{p}^{(+)}\rangle$ of the Lippmann-Schwinger equation (9.131) with $E = E_{\mathbf{p}}$. Using Eq. (9.133), we find

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle = \sum_{\mathbf{p}''} \langle \mathbf{p}' | \hat{V} | \mathbf{p}''^{(+)} \rangle \langle \mathbf{p}''^{(+)} | \mathbf{p} \rangle + \sum_{\mathbf{p}''} \frac{\langle \mathbf{p}' | \hat{V} | \mathbf{p}''^{(+)} \rangle \langle \mathbf{p}''^{(+)} | \hat{V} | \mathbf{p} \rangle}{E - E_{\mathbf{p}''} + i\eta}. \quad (9.216)$$

Replacing the states in the first term $\langle \mathbf{p}''^{(+)} |$ by the result of the Lippmann-Schwinger equation (9.131), we obtain

$$\begin{aligned} \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle &= \langle \mathbf{p}' | \hat{V} | \mathbf{p}^{(+)} \rangle \\ &+ \sum_{\mathbf{p}''} \left[-\frac{\langle \mathbf{p}' | \hat{V} | \mathbf{p}''^{(+)} \rangle \langle \mathbf{p}''^{(+)} | \hat{V} | \mathbf{p} \rangle}{E_{\mathbf{p}} - E_{\mathbf{p}''} + i\eta} + \frac{\langle \mathbf{p}' | \hat{V} | \mathbf{p}''^{(+)} \rangle \langle \mathbf{p}''^{(+)} | \hat{V} | \mathbf{p} \rangle}{E - E_{\mathbf{p}''} + i\eta} \right]. \end{aligned} \quad (9.217)$$

Now we observe that the matrix elements $\langle \mathbf{p}' | \hat{V} | \mathbf{p}^{(+)} \rangle$ are the half-on-shell matrix elements of the T -matrix, whose energy E is equal to the energy $E_{\mathbf{p}}$ of the incoming state $|\mathbf{p}\rangle$:

$$\langle \mathbf{p}' | \hat{V} | \mathbf{p}^{(+)} \rangle = \langle \mathbf{p}' | \hat{T}(E_{\mathbf{p}}) | \mathbf{p} \rangle. \quad (9.218)$$

The left-hand momentum is arbitrary. Hence we can rewrite Eq. (9.217) as

$$\begin{aligned} \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle &= \langle \mathbf{p}' | \hat{T}(E_{\mathbf{p}}) | \mathbf{p} \rangle \\ &+ \sum_{\mathbf{p}''} \langle \mathbf{p}' | \hat{T}(E_{\mathbf{p}}) | \mathbf{p}'' \rangle \langle \mathbf{p} | \hat{T}(E_{\mathbf{p}}) | \mathbf{p}'' \rangle^* \left(-\frac{1}{E_{\mathbf{p}} - E_{\mathbf{p}''} + i\eta} + \frac{1}{E - E_{\mathbf{p}''} + i\eta} \right). \end{aligned} \quad (9.219)$$

After solving the Lippmann-Schwinger equation (9.131) to find $\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle$, this equation supplies us with the full off-shell T -matrix. For a hard-core potential, we must add the correction term (9.213). The off-shell T -matrix has a partial-wave expansion

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle = \frac{(2\pi)^3}{V} \sum_{l=0}^{\infty} T_l(p', p; E) \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}(\hat{\mathbf{p}}). \quad (9.220)$$

If we want to calculate the off-shell T -matrix, we usually must do this separately for each angular momentum. This has been done for various potentials. The result for a hard-core potential of radius a will be given in Eq. (9.287).

9.2.5 Cross Section

The square of the matrix elements of the T -matrix is experimentally observable as *differential cross section*. This quantity is defined by the probability rate $d\dot{P}(t)$ of scattering an incoming particle into a solid angle $d\hat{\Omega} = d\cos\theta d\varphi$ around the direction $\hat{\mathbf{p}} = (\sin\theta \cos\varphi, \sin\theta \sin\varphi, \cos\theta)$. Forming the ratio of this with the incoming particle current density j , i.e., with the rate of incoming particles per area, we obtain the *differential cross section*

$$\frac{d\sigma}{d\Omega} = \frac{d\dot{P}(t)}{d\Omega} \frac{1}{j}. \quad (9.221)$$

The total rate of scattered particles is given by the integral over this in all space directions

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}. \quad (9.222)$$

The two quantities, which have the dimension of an area, are determined by the matrix elements of the T -matrix, as we shall now demonstrate.

The time-dependent version of the incoming wave functions (9.175) is

$$\langle \mathbf{x} | \mathbf{p}, t \rangle = \psi_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} e^{-i(E_0 t - \mathbf{p}\mathbf{x})}. \quad (9.223)$$

The associated incoming current density is

$$\mathbf{j} = \frac{1}{2M_i} \psi^\dagger(\mathbf{x}, t) \overleftrightarrow{\nabla} \psi(\mathbf{x}, t) = \frac{1}{V} \frac{\mathbf{p}}{M} = \frac{1}{V} \mathbf{v}, \quad (9.224)$$

the factor $1/V$ reflecting the normalization $\langle \mathbf{p}' | \mathbf{p} \rangle = \delta_{\mathbf{p}', \mathbf{p}}$ of one particle per total volume. In order to find the rate of outgoing particles, we form the time derivative

$$\begin{aligned} \frac{dP(t)}{dt} &= \frac{d}{dt} |\langle \mathbf{p}' | \hat{U}_I(t, t_0) | \mathbf{p} \rangle|^2 = \frac{d}{dt} \langle \mathbf{p}' | \hat{U}_I(t, t_0) | \mathbf{p} \rangle \langle \mathbf{p}' | \hat{U}_I(t, t_0) | \mathbf{p} \rangle^* \\ &= 2 \operatorname{Im} \left[\langle \mathbf{p}' | \hat{V}_I(t) \hat{U}_I(t, t_0) | \mathbf{p} \rangle \langle \mathbf{p}' | \hat{U}_I(t, t_0) | \mathbf{p} \rangle^* \right] \\ &= 2 \operatorname{Im} \left[\langle \mathbf{p}' | \hat{V}_I(t) \hat{U}_I(t, 0) \hat{U}_I(0, t_0) | \mathbf{p} \rangle \langle \mathbf{p}' | \hat{U}_I(t, 0) \hat{U}_I(0, t_0) | \mathbf{p} \rangle^* \right], \end{aligned} \quad (9.225)$$

which yields, in the limit $t_0 \rightarrow -\infty$, the expression

$$\frac{dP(t)}{dt} = 2 \operatorname{Im} \left[\langle \mathbf{p}' | \hat{V}_I(t) \hat{U}_I(t, 0) | \mathbf{p}^{(+)} \rangle \langle \mathbf{p}' | \hat{U}_I(t, 0) | \mathbf{p}^{(+)} \rangle^* \right]. \quad (9.226)$$

Inserting the explicit time dependence of $\hat{V}_I(t)$ from Eq. (9.15), and of $\hat{U}_I(t, 0)$ from Eq. (9.24), and using the fact that $\hat{H}_0$ acting on $|\mathbf{p}\rangle$ and $\hat{H}$ on $|\mathbf{p}^{(+)}\rangle$ produce the same energy eigenvalues, this becomes

$$\begin{aligned} \frac{dP(t)}{dt} &= 2 \operatorname{Im} \left[\langle \mathbf{p}' | e^{i\hat{H}_0 t} \hat{V} e^{-i\hat{H}_0 t} e^{i\hat{H}_0 t} e^{-i\hat{H} t} | \mathbf{p}^{(+)} \rangle \langle \mathbf{p}' | e^{i\hat{H}_0 t} e^{-i\hat{H} t} | \mathbf{p}^{(+)} \rangle^* \right] \\ &= -i \left[\langle \mathbf{p}' | V | \mathbf{p}^{(+)} \rangle \langle \mathbf{p}' | \mathbf{p}^{(+)} \rangle^* - \langle \mathbf{p}' | V | \mathbf{p}^{(+)} \rangle^* \langle \mathbf{p}' | \mathbf{p}^{(+)} \rangle \right]. \end{aligned} \quad (9.227)$$

We now use the Lippmann-Schwinger equation (9.131) to rewrite this as

$$\begin{aligned} \frac{dP(t)}{dt} &= -i \left\{ \langle \mathbf{p}' | V | \mathbf{p}^{(+)} \rangle \left[\langle \mathbf{p}' | \mathbf{p} \rangle + \frac{1}{E - E' - i\eta} \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle^* \right] \right. \\ &\quad \left. - \langle \mathbf{p}' | V | \mathbf{p}^{(+)} \rangle^* \left[\langle \mathbf{p}' | \mathbf{p} \rangle + \frac{1}{E - E' + i\eta} \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle \right] \right\}. \end{aligned} \quad (9.228)$$

On behalf of Eq. (9.129) and Sochocki's formula (7.197), this becomes

$$\frac{dP(t)}{dt} = 2 \langle \mathbf{p}' | \mathbf{p} \rangle \operatorname{Im} \langle \mathbf{p} | \hat{T} | \mathbf{p} \rangle + 2\pi \delta(E - E') |\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2. \quad (9.229)$$

The first term gives the rate of the transmitted particles in the direct beam. The second term gives the rate of scattered particles. If we collect the scattered particles of all final momenta in a sum $\sum_{\mathbf{p}'} = \int d^3p V / (2\pi)^3$, we find the total probability rate

$$\frac{dP}{dt} = \int \frac{d^3p' V}{(2\pi)^3} 2\pi \delta(E' - E) |\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2. \quad (9.230)$$

There exists a simple mnemonic rule for deriving this formula. The probability for a particle to go from the initial to the final state is given by the absolute square of the scattering amplitude (9.130):

$$P_{\mathbf{p}'\mathbf{p}} = |\langle \mathbf{p}' | \hat{S} | \mathbf{p} \rangle|^2 = |\langle \mathbf{p}' | \mathbf{p} \rangle - 2\pi i \delta(E' - E) \langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2. \quad (9.231)$$

Excluding the direct beam, this is equal to

$$P_{\mathbf{p}'\mathbf{p}} = [2\pi\delta(E' - E)]^2 |\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2. \quad (9.232)$$

Imagining the world to exist only for a finite time Δt , the δ -function of the energy at zero argument is really finite:

$$\delta(E)|_{E=0} = \int_{-\Delta t/2}^{\Delta t/2} \frac{dt}{2\pi} e^{iEt} \Big|_{E=0} = \frac{\Delta t}{2\pi}. \quad (9.233)$$

Thus we can write (9.232) as

$$P_{\mathbf{p}'\mathbf{p}} = \Delta t 2\pi\delta(E' - E) |\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2. \quad (9.234)$$

Integrating (9.234) over the final phase-space volume, we find the probability rate for going to all final states:

$$\frac{dP}{dt} = \frac{P}{\Delta t} = \int \frac{d^3p'V}{(2\pi)^3} 2\pi\delta(E' - E) |\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle|^2, \quad (9.235)$$

leading directly to Eq. (9.230). This formula is written in natural units with $c = \hbar = 1$. In proper physical units, the right-hand side carries a factor $1/\hbar$. With this factor, Eq. (9.235) is known as Fermi's *golden rule*.

The alert reader will have noted that, in going from (9.232) to (9.234), we have done an operation that is forbidden in mathematics: we have calculated the square of a distribution with the heuristic formula

$$\delta(0)\delta(\Delta E). \quad (9.236)$$

In the theory of distributions, such operations are illegal. Distributions form a linear space, implying that they can only be combined linearly with each other.

In the present context, there are two ways of going properly from (9.232) to (9.234). One is to use wave packets for the incoming and outgoing particles. This was done in the textbook [1]. Another way proceeds via a more careful evaluation of the δ -functions on a large but finite interval Δt where one uses, instead of $\delta(E' - E)$, the would-be δ -function

$$\delta(E' - E) \approx \int_{-\Delta t/2}^{\Delta t/2} dt e^{i(E' - E)t} = \frac{\sin |\Delta t(E' - E)/2|}{|E' - E|/2}. \quad (9.237)$$

Squaring this expression yields

$$[\delta(E' - E)]^2 \approx \frac{\sin^2[\Delta t(E' - E)/2]}{(E' - E)^2/4}. \quad (9.238)$$

To get the rate we must divide this by the time interval Δt , so we obtain a factor

$$\frac{1}{\Delta t} [\delta(\Delta E)]^2 \approx \frac{\sin^2[\Delta t(E' - E)/2]}{\Delta t(E' - E)^2/4}. \quad (9.239)$$

This function has a sharp peak around $E' - E = 0$. The area under it is 2π . Hence we obtain in the limit $\Delta t \rightarrow \infty$:

$$\frac{1}{\Delta t} [\delta(\Delta E)]^2 \approx \frac{\sin^2[\Delta t(E' - E)/2]}{\Delta t(E' - E)^2/4} \xrightarrow{\Delta t \rightarrow \infty} 2\pi \delta(E' - E), \quad (9.240)$$

and thus once more the previous heuristic result (9.234).

There exists also a more satisfactory solution that is free of the restriction of distributions to linear combinations. This is possible by defining consistently *products of distributions* in a unique way. We simply require that path integrals, which are completely equivalent to quantum mechanics, must share with the Schrödinger equation the property of being independent of the coordinates in which they are formulated [2].

The momentum integral can be split into an integral over the final energy and the final solid angle $d\Omega$. For a nonrelativistic particle in D dimensions, this goes as follows

$$\begin{aligned} \int \frac{d^D p}{(2\pi)^D} &= \frac{1}{(2\pi)^D} \int d\Omega \int_0^\infty dp p^{D-1} = \frac{1}{(2\pi)^D} \int d\Omega \int_0^\infty dE \rho_E \\ &= \frac{M}{(2\pi)^D} \int d\Omega \int_0^\infty dE p^{D-2}. \end{aligned} \quad (9.241)$$

The energy integral removes the δ -function in (9.229) and, by comparison with (9.221), we can identify the differential cross section as

$$\frac{d\sigma}{d\Omega} = \frac{MV p^{D-2}}{(2\pi)^D} 2\pi |T_{\mathbf{p}'\mathbf{p}}|^2 \frac{1}{j}, \quad (9.242)$$

where we have set

$$\langle \mathbf{p}' | \hat{T}(E) | \mathbf{p} \rangle \equiv T_{\mathbf{p}'\mathbf{p}}, \quad (9.243)$$

for brevity. Inserting $j = p/MV$ from (9.224), this becomes

$$\frac{d\sigma}{d\Omega} = \frac{M^2 V^2 p^{D-3}}{(2\pi)^{D-1}} |T_{\mathbf{p}'\mathbf{p}}|^2. \quad (9.244)$$

If the scattered particle moves relativistically, we have to replace M in (9.241) with $E = \sqrt{p^2 + M^2}$ inside the momentum integral, so that

$$\begin{aligned} \int \frac{d^D p}{(2\pi)^D} &= \frac{1}{(2\pi)^D} \int d\Omega \int_0^\infty dp p^{D-1} = \frac{1}{(2\pi)^D} \int d\Omega \int_0^\infty dE \rho_E^{\text{rel}} \\ &= \frac{1}{(2\pi)^3} \int d\Omega \int_M^\infty dE E p^{D-2}. \end{aligned} \quad (9.245)$$

In the relativistic case, the initial current is not proportional to p/M , which is the nonrelativistic velocity of the incoming particle beam, but to the relativistic velocity $v^{\text{rel}} = p/E$, so that the incoming current is

$$j = \frac{1}{V} \frac{p}{E}. \quad (9.246)$$

Hence the cross section becomes, in the relativistic case,

$$\frac{d\sigma}{d\Omega} = \frac{E^2 V^2 p^{D-3}}{(2\pi)^{D-1}} |T_{\mathbf{p}'\mathbf{p}}|^2. \quad (9.247)$$

Let us compare this with the result in Eq. (9.147), where we introduced a scattering amplitude $f_{\mathbf{p}'\mathbf{p}}$ whose absolute square is equal to the differential cross section:

$$\frac{d\sigma}{d\Omega} = |f_{\mathbf{p}'\mathbf{p}}|^2. \quad (9.248)$$

Thus we can identify [compare (9.148)]

$$f_{\mathbf{p}'\mathbf{p}} \equiv -\frac{MV}{(2\pi)^{(D-1)/2}} T_{\mathbf{p}'\mathbf{p}}, \quad (9.249)$$

where we have chosen the sign to agree with the convention in Landau and Lifshitz' textbook.

Using the partial-wave expansion (9.151) and (9.159), we obtain for $f_{\mathbf{p}'\mathbf{p}}$, in the three-dimensional nonrelativistic case, the expansion

$$f_{\mathbf{p}'\mathbf{p}} = \sum_{l=0}^{\infty} f_l(p) \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{p}}') Y_{lm}^*(\hat{\mathbf{p}}) = \sum_{l=0}^{\infty} f_l(p) \frac{2l+1}{4\pi} P_l(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}), \quad (9.250)$$

where from (9.172)

$$f_l(p) = -\frac{4\pi^2}{p} \rho_E T_l(p) = \frac{2\pi}{ip} [S_l(p) - 1] = \frac{4\pi}{p} e^{i\delta_l(p)} \sin \delta_l(p). \quad (9.251)$$

This guarantees that the radial particle current which leaves the scattering zone differs, on the unit sphere, by a factor $|f_{\mathbf{p}'\mathbf{p}}|^2$ from the incoming current, leading directly to the differential cross section (9.248).⁶

9.2.6 Partial Wave Decomposition of Total Cross Section

The contribution of the various partial waves to the total cross section is obtained by forming the absolute square of (9.250). After this, one integrates over all directions of the outgoing beam and uses the orthogonality relation (9.153) and the addition theorem (23.12) to express the total cross section as a sum over partial waves:

$$\begin{aligned} \sigma &= \int d\hat{\mathbf{p}}' |f_{\mathbf{p}'\mathbf{p}}|^2 = \sum_{l=0}^{\infty} f_l(p) f_l^*(p) \sum_{lm} \sum_{l'm'} \int d\hat{\mathbf{p}}' Y_{lm}(\hat{\mathbf{p}}') Y_{lm}(\hat{\mathbf{p}}) Y_{l'm'}^*(\hat{\mathbf{p}}') Y_{l'm'}^*(\hat{\mathbf{p}}) \\ &= \sum_{l=0}^{\infty} |f_l(p)|^2 \sum_{lm} Y_{lm}(\hat{\mathbf{p}}) Y_{lm}^*(\hat{\mathbf{p}}) = \sum_{l=0}^{\infty} |f_l(p)|^2 \frac{2l+1}{4\pi} P_l(1). \end{aligned} \quad (9.252)$$

⁶In D dimensions, the partial-wave expansion (9.251) is given by (9B.41).

Since $P_l(1) = 1$, this is equal to

$$\sigma = \sum_{l=0}^{\infty} \sigma_l = \sum_{l=0}^{\infty} |f_l(p)|^2 \frac{2l+1}{4\pi} = \frac{4\pi}{p^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(p). \quad (9.253)$$

As mentioned at the end of Subsection 9.2.3, there can be a resonance at small p if the effective range is large enough and a is positive. In the s -wave, we can approximate $f_0(p)$ in (9.251) by the expression (9.194):

$$f_0(p) \equiv \frac{4\pi}{k \cot \delta_0(p) - ik}. \quad (9.254)$$

Inserting the approximation (9.189), this becomes

$$f_0(p) \approx \frac{4\pi}{-\frac{1}{a} + \frac{1}{2}r_{\text{eff}}k^2 - ik}, \quad (9.255)$$

corresponding to the general resonance formula (9.197) for the S -matrix. In nuclear scattering, this is called a *Feshbach resonance*. It leads to a contribution to the cross section in Eq. (9.253):

$$\sigma_0 \equiv \frac{4\pi a^2}{(1 - ar_{\text{eff}}k^2/2)^2 + a^2k^2}. \quad (9.256)$$

The different values of the parameter a for various depths of a typical potential are illustrated in Fig. 9.1.

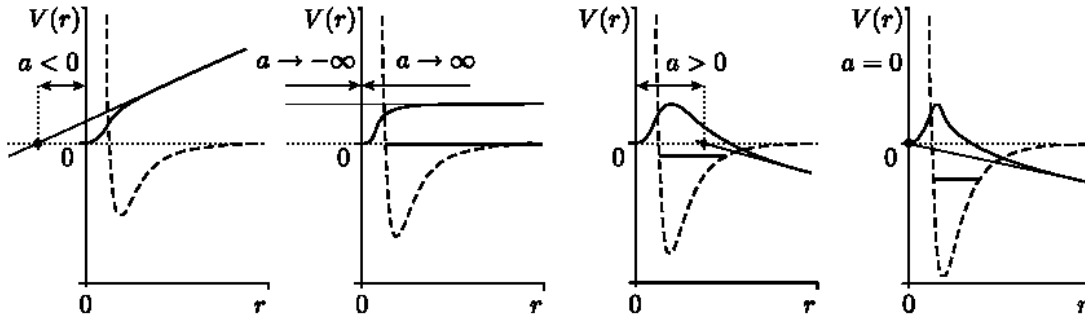


FIGURE 9.1 Behavior of wave function for different positions of a bound state near the continuum in a typical potential between atoms.

9.2.7 Dirac δ -Function Potential

As an example, consider a local interaction that may be approximated by a δ -function

$$V(\mathbf{x}) = g \delta^{(3)}(\mathbf{x}). \quad (9.257)$$

Between plane waves, this has the matrix elements

$$\langle \mathbf{p}' | V | \mathbf{p} \rangle = \frac{g}{V} \int d^3x e^{-i\mathbf{p}'\cdot\mathbf{x}} \delta^{(3)}(\mathbf{x}) e^{i\mathbf{p}\cdot\mathbf{x}} = \frac{g}{V}, \quad (9.258)$$

so that the Born approximation to the scattering amplitude is

$$f_{\mathbf{p}'\mathbf{p}} = -\frac{M}{2\pi\hbar^2} g. \quad (9.259)$$

Since g has the dimension energy times length³, or $\hbar^2/M$ times length, $f_{\mathbf{p}'\mathbf{p}}$ has the dimension length, making the cross section an area seen by the incoming beam.

For the δ -function potential, it is instructive to calculate also the next correction to the Born approximation. According to Eq. (9.132), it is given by

$$\begin{aligned} T_{\mathbf{p}'\mathbf{p}} &= V_{\mathbf{p}'\mathbf{p}} + \int \frac{d^3p'' V}{(2\pi)^3} V_{\mathbf{p}'\mathbf{p}''} \frac{1}{E - E(\mathbf{p}'') + i\eta} V_{\mathbf{p}''\mathbf{p}} + \dots \\ &= \frac{1}{V} \left[g + g^2 \int \frac{d^3p''}{(2\pi)^3} \frac{1}{E - E(\mathbf{p}'') + i\eta} + \dots \right]. \end{aligned} \quad (9.260)$$

Thus, for zero incoming momentum and energy E , the coupling constant g is effectively replaced by

$$g_R = g - g^2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta} + \dots, \quad (9.261)$$

and the T -matrix has the isotropic value

$$T_{\mathbf{p}'\mathbf{p}} \Big|_{|\mathbf{p}|=0, E=0} = \frac{1}{V} g_R. \quad (9.262)$$

The integral on the right-hand side diverges. A finite result can be obtained by assuming the initial g to be infinitesimally small such as to compensate for the divergence. This is the first place where one is confronted with a renormalization problem that is typical for all quantum field theories with a local interaction. A systematic treatment of this problem will be presented in Chapters 10 and 11.

Here this problem occurs for the first time, in the context of quantum mechanics. This is due to the fact that the Schrödinger equation for the δ -function potential does not have a proper solution. Nevertheless, it is possible to bypass the problem by renormalization and to solve the Lippmann-Schwinger equation (9.54) after all, yielding the full scattering amplitude (9.260). The zero-energy expression (9.261) is extended by repetition to a geometric series

$$g_R = g - g^2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta} + g^3 \left[\int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta} \right]^2 + \dots \quad (9.263)$$

The series for the inverse of this can be summed up to

$$\frac{1}{g_R} = \frac{1}{g} + \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta}. \quad (9.264)$$

Comparing (9.262) with (9.192), we see that the renormalized coupling determines the s -wave scattering length as being

$$a_s = \frac{M}{2\pi\hbar^2} g_R. \quad (9.265)$$

Together with (9.262) this agrees with (9.192).

The identification of the renormalized coupling constant g_R with the scattering length may be attributed to the use of a so-called pseudopotential for which the Schrödinger equation can be properly solved. Instead of the potential $g\delta^{(3)}(\mathbf{x})$ which in a Schrödinger equation picks out the value of a wave function at the origin when forming the product, one uses the condition $V(\mathbf{x})\psi(\mathbf{x}) = g\delta^{(3)}(\mathbf{x})\partial_r r\psi(\mathbf{x})$. This ensures that the s -wave scattering length is $a_s = Mg/2\pi\hbar^2$ as for a hard sphere of radius a_s .⁷

Note that (9.265) holds only for a particle of mass M in an external potential $g\delta^{(3)}(\mathbf{x})$. A two-body system involves the *relative Schrödinger equation* which contains the *reduced mass* $M_{\text{red}} = 1/(1/M_1 + 1/M_2)$ rather than M . Hence in a many-body system, g_R is related to the scattering length by

$$g_R = 4\pi\hbar^2/M. \quad (9.266)$$

A remark is useful in connection with the divergence of Eq. (9.267). It can be made finite by cutting off the momentum integral at some large value Λ to find

$$\frac{1}{g_R} = \frac{1}{g} + 2M \frac{4\pi}{(2\pi)^3} \int_0^\Lambda dp = \frac{1}{g} + 2M \frac{4\pi}{(2\pi)^3} \Lambda. \quad (9.267)$$

Since Λ is very large, one might be tempted to conclude that g_R must be positive for any g . However, as we shall see in Chapters 7 and 8, this conclusion is not allowed in renormalizable quantum field theories. According to the rules of renormalization, *any* divergence may be cancelled by a counterterm, and the sign of it is arbitrary. Only the renormalized quantity g_R is physical, and it must be fixed by experiment.

9.2.8 Spherical Square-Well Potential

For a square-well potential

$$V(\mathbf{x}) = \begin{cases} -V_0, & r < r_0, \\ 0, & r \geq 0, \end{cases} \quad (9.268)$$

the radial Schrödinger equation reads

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left[K^2 - \frac{l(l+1)}{r^2} \right] \right\} \psi_l(r) = 0, \quad (9.269)$$

⁷See K. Huang, *Statistical Mechanics*, Wiley, N.Y., 1963 (p.233). For higher partial waves see Z. Idziaszek and T. Calarco, (quant-ph/0507186).

where

$$K \equiv \sqrt{2M(E + V_0)}/\hbar. \quad (9.270)$$

There is only one solution which is regular at the origin:

$$\psi_l(r) = A j_l(Kr), \quad (9.271)$$

with an arbitrary normalization factor A .

For positive energy E , the solution in the outer region $r \geq a$ receives an admixture of the associated spherical Bessel function $n_l(kr)$:

$$\psi_l(r) = B [\cos \delta_l(k) j_l(kr) + \sin \delta_l(k) n_l(kr)], \quad (9.272)$$

where

$$k \equiv \sqrt{2ME}/\hbar, \quad (9.273)$$

and B , $\delta_l(k)$ must be determined from the boundary condition at $r = a$. The associated Bessel functions $n_l(z)$ have the asymptotic behavior orthogonal to (9.177):

$$n_l(z) \rightarrow -\frac{\cos(z - \pi l/2)}{pr}, \quad (9.274)$$

The continuity of the wave function fixes the ratio B/A . The continuity of the logarithmic derivative is independent of this ratio and fixes the phase shifts by the equation

$$K \frac{j'_l(Kr_0)}{j_l(Kr_0)} = k \frac{\cos \delta_l(k) j'_l(kr_0) - \sin \delta_l(k) n'_l(kr_0)}{\cos \delta_l(k) j_l(kr_0) - \sin \delta_l(k) n_l(kr_0)}. \quad (9.275)$$

For an s -wave, this reduces to

$$K \cot Kr_0 = k \cot(kr_0 + \delta_0). \quad (9.276)$$

Inserting (9.270) and (9.273), the resulting binding energy are plotted in Fig. 9.2. For small incoming energy, this equation becomes

$$K_0 \cot K_0 r_0 \approx k \cot(kr_0 + \delta_0), \quad (9.277)$$

where $K_0 \equiv \sqrt{2MV_0}/\hbar$, which is solved by

$$\delta_0(k) = -r_0 \left(1 - \frac{\tan K_0 r_0}{K_0 r_0} \right) k + \dots \quad (9.278)$$

This determines the phase shift to be

$$a_s = -r_0 \left(1 - \frac{\tan K_0 r_0}{K_0 r_0} \right). \quad (9.279)$$

The next term in the small- k expansion of (9.278) is

$$\frac{k^3}{6} \left(r_0^3 - 3a_s^2 r_0 - 2a_s^3 - \frac{3a_s}{K_0^2} \right), \quad (9.280)$$

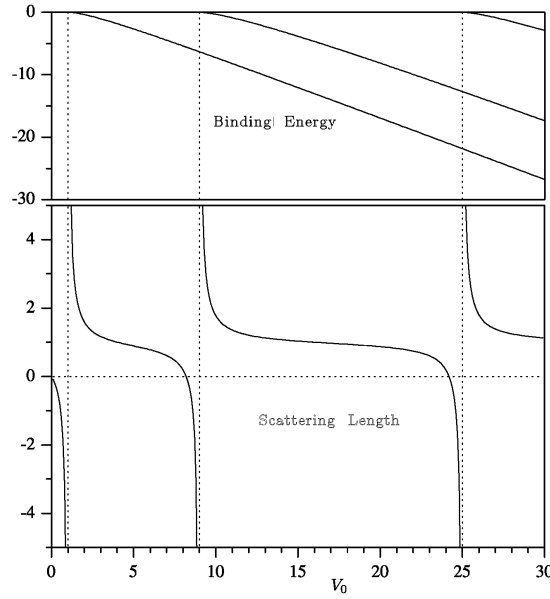


FIGURE 9.2 Behavior of binding energy (in units of $|V_0|$) and scattering length in an attractive square well potential of depth $|V_0|$ and radius R_0 for identical bosons of reduced mass M_{red} . The abscissa shows the potential depth in units of $\pi^2 \hbar^2 / 8M_{\text{red}} R_0^2$.

implying an effective radius defined in (9.190):

$$r_{\text{eff}} = \frac{r_0}{2} - \frac{r_0^3}{6a_s^2} + \frac{1}{2a_s K_0^2}. \quad (9.281)$$

At negative energies E , there are bound states which decrease for large r . The only solution of (9.269) with this property is the spherical Bessel function of the third kind (Hankel function of the first kind):⁸

$$\psi_l(k) = B h_l^{(2)}(kr) \equiv B [j_l(kr) - in_l(kr)], \quad (9.282)$$

which behaves like $e^{-(\kappa r - l\pi/2)}/kr$ for $E < 0$ where $k = i\sqrt{-2ME} \equiv i\kappa$. The energies of the bound states are found from the continuity of the logarithmic derivative at $r = r_0$:

$$i\kappa \frac{h_l^{(2)'}(i\kappa r_0)}{h_l^{(2)}(i\kappa r_0)} = K \frac{j_l'(Kr_0)}{j_l(Kr_0)}. \quad (9.283)$$

For the s -wave, this becomes

$$K \cot Kr_0 = -\kappa. \quad (9.284)$$

For a repulsive potential, Eq. (9.278) can be continued analytically to

$$\delta_0(k) = -r_0 \left(1 - \frac{\tanh |K_0| r_0}{|K_0| r_0} \right) k + \dots \quad (9.285)$$

⁸M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Subsection 10.1.1.

In the hard-core limit $V_0 \rightarrow \infty$, this yields an s -wave scattering length

$$a_s = -r_0, \quad (9.286)$$

and a vanishing effective range.

For the hard-core potential, equation (9.205) has been solved [3]. The l th partial wave amplitude is

$$T_l(k', k; E) = -(-1)^l \frac{2\pi\hbar^2 a}{(2\pi M)^3} \left\{ \frac{k_E^2 - k'^2}{k^2 - k'^2} k a j_l(k'a) j_{l+1}(ka) + (k \leftrightarrow k') \right. \\ \left. - k_E a \frac{h_{l+1}^{(2)}(ka)}{h_l^{(2)}(ka)} j_l(k') j_l(k) \right\}, \quad (9.287)$$

where $k_E \equiv \sqrt{2ME}/\hbar$.

9.3 Two-Particle Scattering

Usually, the final state has two or more particles leaving the interaction zone. The interaction energy is an integral over some local interaction density

$$\hat{V} = \int d^3x \hat{\mathcal{H}}_{\text{int}}(\mathbf{x}), \quad (9.288)$$

integrated over all space at a fixed time $x_0 = t = 0$. In this case, the matrix elements of the potential factorizes as

$$\langle \mathbf{p}' | \hat{V} | \mathbf{p} \rangle = \int d^3x \langle \mathbf{p}' | e^{i\hat{\mathbf{p}}\mathbf{x}} \hat{\mathcal{H}}_{\text{int}}(0) e^{-i\hat{\mathbf{p}}\mathbf{x}} | \mathbf{p} \rangle = V \delta_{\mathbf{p}'\mathbf{p}} \langle \mathbf{p}' | \hat{\mathcal{H}}_{\text{int}}(0) | \mathbf{p} \rangle, \quad (9.289)$$

where $\mathbf{p}$ and $\mathbf{p}'$ are the sum over all initial and final momenta, respectively. Thus the matrix elements of $\hat{V}$ always carry a $\delta_{\mathbf{p}'\mathbf{p}}$ -factor that ensures total momentum conservation. The same thing is true for the T -matrix $T_{\mathbf{p}'\mathbf{p}}$. This factor is customarily removed by defining the so-called t -matrix

$$T_{\mathbf{p}'\mathbf{p}} = V \delta_{\mathbf{p}'\mathbf{p}} t_{\mathbf{p}'\mathbf{p}}. \quad (9.290)$$

The Born approximation is now

$$t_{\mathbf{p}'\mathbf{p}} \approx \langle \mathbf{p}' | \hat{\mathcal{H}}_{\text{int}}(0) | \mathbf{p} \rangle. \quad (9.291)$$

Replacing the Kronecker δ for momentum conservation by its continuum limit,

$$\delta_{\mathbf{p}'\mathbf{p}} \rightarrow \frac{(2\pi)^3}{V} \delta^{(3)}(\mathbf{p}' - \mathbf{p}),$$

we can write (9.290) as

$$T_{\mathbf{p}'\mathbf{p}} = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p}) t_{\mathbf{p}'\mathbf{p}}, \quad (9.292)$$

i.e., the matrix elements (9.130) of the S -matrix become

$$\langle \mathbf{p}' | \hat{S} | \mathbf{p} \rangle = \langle \mathbf{p}' | \mathbf{p} \rangle - i(2\pi)^4 \delta^{(4)}(p' - p) t_{\mathbf{p}'\mathbf{p}}. \quad (9.293)$$

In a world of a finite volume V existing for a finite time T , the probability of going from an initial state $\mathbf{p}$ to a final state $\mathbf{p}'$ is given by the absolute square of (9.293). By analogy with (9.233), we have

$$\delta^{(4)}(p) \Big|_{p=0} = \int \frac{d^4 p}{(2\pi)^4} e^{ipx} \Big|_{p=0} = \frac{TV}{(2\pi)^4}, \quad (9.294)$$

so that we obtain the transition rate [compare (9.234)]. Thus we can write (9.232) as

$$P = TV(2\pi)^4 \delta^{(4)}(p' - p) |t_{\mathbf{p}'\mathbf{p}}|^2. \quad (9.295)$$

This has to be summed over all final particle states, and we obtain the rate

$$\frac{dP}{dt} = V \sum_{\text{final states}} (2\pi)^4 \delta^{(4)}(p' - p) |t_{\mathbf{f}\mathbf{i}}|^2. \quad (9.296)$$

We have changed the notation for the t -matrix $t_{\mathbf{p}'\mathbf{p}}$ and written it as $t_{\mathbf{f}\mathbf{i}}$ to emphasize the validity for a more general initial state $|\mathbf{i}\rangle$ and a larger variety of possible final states $|\mathbf{f}\rangle$.

If the particles $1', 2', \dots, n'$ leave the interaction zone, the sum over all final states in a volume V consists of an integral over the phase space

$$\sum_{\mathbf{p}'_1, \mathbf{p}'_2, \dots} = V^n \int \frac{d^3 p'_1}{(2\pi)^3} \int \frac{d^3 p'_2}{(2\pi)^3} \cdots \int \frac{d^3 p'_n}{(2\pi)^3}, \quad (9.297)$$

and (9.296) becomes

$$\frac{dP}{dt} = V^{n+1} \int \frac{d^3 p'_1}{(2\pi)^3} \int \frac{d^3 p'_2}{(2\pi)^3} \cdots \int \frac{d^3 p'_n}{(2\pi)^3} (2\pi)^4 \delta^{(4)}(p' - p) |t_{\mathbf{f}\mathbf{i}}|^2, \quad (9.298)$$

where $p = p_1 + p_2$ and $p' = p'_1 + p'_2 + \dots + p'_n$. By dividing out the current density of the incoming particles j , we find from this the cross section

$$\sigma = \frac{dP}{dt} \frac{1}{j}. \quad (9.299)$$

By omitting some of the final-state integrations, we may extract from this any desired differential cross section.

9.3.1 Center-of-Mass Scattering Cross Section

Let us assume the collision to take place in the center-of-mass frame with zero total momentum and $\mathbf{p} = \mathbf{p}_1 = -\mathbf{p}_2$ and a total energy E_{CM} . Then the δ -function fixes

$\mathbf{p}' = \mathbf{p}'_1 = -\mathbf{p}'_2$, and the equality of the total energies before and after the collision implies that

$$E'_1 + E'_2 = E_1 + E_2 = E_{\text{CM}}. \quad (9.300)$$

In order to be more explicit we have to distinguish the case of nonrelativistic and relativistic particles. It is useful to treat the relativistic case first and obtain the nonrelativistic result by going to the limit of small velocities. In the relativistic case with initial momenta $\mathbf{p}_{\text{CM}} = \mathbf{p}_1 = -\mathbf{p}_2$, final momenta $\mathbf{p}'_{\text{CM}} = \mathbf{p}'_1 = -\mathbf{p}'_2$, and energies

$$E_{1,2} = \sqrt{p_{\text{CM}}^2 + M_{1,2}^2}, \quad E'_{1,2} = \sqrt{p_{\text{CM}}'^2 + M_{1,2}'^2}, \quad (9.301)$$

the δ -function for the total energy reads, in the center-of-mass frame, with zero total momentum

$$\delta \left(\sqrt{p_{\text{CM}}'^2 + M_1'^2} + \sqrt{p_{\text{CM}}'^2 + M_2'^2} - E_{\text{CM}} \right). \quad (9.302)$$

This is zero unless p' makes the argument zero, which happens at

$$p'_{\text{CM}} = \frac{1}{2M} I(M, M'_1, M'_2), \quad (9.303)$$

where

$$I(M, M_1, M_2) \equiv \sqrt{M^2 - (M_1 + M_2)^2} \sqrt{M^2 - (M_1 - M_2)^2} \quad (9.304)$$

and

$$E_{\text{CM}} = M \equiv \sqrt{s}. \quad (9.305)$$

The energy E_{CM} is equal to the total mass, since the momentum in the center-of-mass frame is zero. Another notation for M is $\sqrt{s}$, where s is the so-called *Mandelstam variable*. The individual energies of the two particles are

$$\begin{aligned} E_{1,2} &= \sqrt{p_{\text{CM}}^2 - M_{1,2}^2} = \frac{1}{2M} \left[M^2 \pm (M_1^2 - M_2^2) \right], \\ E'_{1,2} &= \sqrt{p_{\text{CM}}'^2 - M_{1,2}'^2} = \frac{1}{2M} \left[M^2 \pm (M_1'^2 - M_2'^2) \right]. \end{aligned} \quad (9.306)$$

To evaluate the momentum integral over the δ -function (9.302), we use the formula

$$\delta(f(p') - f(p'_{\text{CM}})) = [f'(p')]^{-1} \delta(p' - p'_{\text{CM}}) \quad (9.307)$$

to write

$$\begin{aligned} &\delta \left(\sqrt{p'^2 + M_1'^2} + \sqrt{p'^2 + M_2'^2} - E_{\text{CM}} \right) \\ &= [(\partial/\partial p') (E'_1 + E'_2)]^{-1} \delta(p' - p'_{\text{CM}}) \\ &= \frac{E'_1 E'_2}{p'_{\text{CM}} (E'_1 + E'_2)} \delta(p' - p'_{\text{CM}}) = \frac{E'_1 E'_2}{p'_{\text{CM}} E_{\text{CM}}} \delta(p' - p'_{\text{CM}}). \end{aligned} \quad (9.308)$$

Then we obtain from (9.298) the total rate of scattered relativistic particles

$$\frac{dP(t)}{dt} = \frac{V^3}{(2\pi)^2} \frac{p'_{\text{CM}} E'_1 E'_2}{E_{\text{CM}}} \int d\Omega |t_{\text{fi}}|^2. \quad (9.309)$$

Since the t -matrix elements depend, in general, on more than just the initial and final total momenta $\mathbf{p}$ and $\mathbf{p}'$, they have been denoted generically by t_{fi} .

The initial current density is given by the relative velocity between two incoming particles in the center-of-mass frame:

$$j = \left(\frac{p_1}{E_1} - \frac{p_2}{E_2} \right) \frac{1}{V} = \frac{p_{\text{CM}} E_{\text{CM}}}{E_1 E_2} \frac{1}{V}. \quad (9.310)$$

Dividing $dP(t)/dt$ by j as demanded by (9.299) and omitting the integration over the solid angle in (9.309), we obtain the differential cross section in the center of mass:

$$\frac{d\sigma}{d\Omega_{\text{CM}}} = \frac{1}{(2\pi)^2} \frac{p'_{\text{CM}}}{p_{\text{CM}}} \frac{1}{E_{\text{CM}}} E'_1 E'_2 E_1 E_2 V^4 |t_{\text{fi}}|^2. \quad (9.311)$$

It is useful to realize that the combination of incoming currents and energies $j \times 2VE_1 E_2$ is a Lorentz-invariant quantity coinciding with $I(M, M_1, M_2)$ of Eq. (9.304). This follows immediately by inserting (9.303) into (9.310):

$$j = \frac{1}{2VE_1 E_2} I(M, M_1, M_2). \quad (9.312)$$

Thus we can write down an explicit formula for the cross section (9.299) in any frame of reference:

$$\sigma = \frac{2VE_1 E_2}{I(M, M_1, M_2)} V^n \int \frac{d^3 p'_1}{(2\pi)^3} \int \frac{d^3 p'_2}{(2\pi)^3} \cdots \int \frac{d^3 p'_n}{(2\pi)^3} \delta^{(4)}(p' - p) |t_{\text{fi}}|^2. \quad (9.313)$$

9.3.2 Laboratory Scattering Cross Section

In most experiments, the directly measured quantity is the laboratory cross section where an initial particle of momenta $|\mathbf{p}_1| = p_L$ and energy

$$E_L \equiv (E_1)_{\text{Lab}} = \sqrt{p_L^2 + M_1^2} \quad (9.314)$$

hits the particle 2 at rest. Then the incoming current is

$$j = \frac{p_L}{E_L V} = \frac{v_L}{V}, \quad (9.315)$$

rather than (9.310). The cross section of two particles going into two particles in the laboratory is from (9.298) and (9.299):

$$\sigma = \int \frac{d^3 p'_1 V}{(2\pi)^3} \frac{d^3 p'_2 V}{(2\pi)^3} (2\pi)^4 \delta^{(4)}(p' - p) |t_{\text{fi}}|^2 \frac{V}{j}. \quad (9.316)$$

The δ -function for the total energy depends on the final laboratory momenta $p_{1L} \equiv |\mathbf{p}_{1L}|$, $p_{2L} \equiv |\mathbf{p}_{2L}|$ as follows:

$$\delta \left(\sqrt{p_{1L}'^2 + M_1'^2} + \sqrt{p_{2L}'^2 + M_2'^2} - E_L - M_2 \right). \quad (9.317)$$

In contrast to the center-of-mass frame, the final momenta p_{1L}' and p_{2L}' are no longer equal, which complicates the further evaluation. We want to express them as functions of the initial energy and the scattering angle θ_L . For this, some kinematic considerations are necessary.

The total mass introduced in (9.305) is given by the Poincaré-invariant quantity

$$M^2 = s \equiv (p_1 + p_2)^2 = M_1^2 + M_2^2 + 2M_2 E_L. \quad (9.318)$$

Solving this we obtain the invariant expressions

$$E_L = (M^2 - M_1^2 - M_2^2) / 2M_2 \quad (9.319)$$

$$p_L = I(M, M_1, M_2) / 2M_2. \quad (9.320)$$

Observe that by inserting the last equation into the frame-independent expression (9.312), we find the correct current (9.315) in the laboratory frame. The relation between the laboratory and center-of-mass energies is

$$E_{1\text{CM}} = \frac{M_2 E_L + M_1^2}{\sqrt{M_1^2 + M_2^2 + 2E_L M_2}}, \quad (9.321)$$

$$E_{2\text{CM}} = \frac{M_2 E_L + M_2^2}{\sqrt{M_1^2 + M_2^2 + 2E_L M_2}}. \quad (9.322)$$

The relation between the laboratory and the center-of-mass momenta is

$$p_{\text{CM}} = p_L \frac{M_1}{\sqrt{M_1^2 + M_2^2 + 2E_L M_2}}. \quad (9.323)$$

The relation between the scattering angles in the two frames of reference is more involved. To find it, we consider a Lorentz invariant quantity that is formed from the momentum transfer, the so-called *Mandelstam variable* t :

$$t \equiv (p_1 - p_1')^2 = M_1^2 + M_1'^2 + 2(\mathbf{p}_1 \mathbf{p}_1' - E_1 E_1'). \quad (9.324)$$

In either frame, the scattering angles appear in the scalar product $\mathbf{p}_1 \mathbf{p}_1' = p_1 p_1' \cos \theta$. A calculation in the center-of-mass frame leads to the formula

$$\begin{aligned} \cos \theta_{\text{CM}} &= \frac{1}{2p_{\text{CM}} p_{\text{CM}}'} (t - M_1^2 - M_1'^2 + 2E_{1\text{CM}} E_{1\text{CM}}') \\ &= \frac{1}{I(M, M_1, M_2) I(M, M_1', M_2')} \\ &\times [M^4 + M^2(2t - M_1^2 - M_2^2 - M_1'^2 - M_2'^2) + (M_1^2 - M_2^2)(M_1'^2 - M_2'^2)]. \end{aligned} \quad (9.325)$$

In the laboratory frame, we take advantage of the fact that $p_2 = (M_2, \mathbf{0})$ and calculate t using energy-momentum conservation as

$$t = (p_1 - p'_1)^2 = (p'_2 - p_2)^2 = M_2'^2 + M_2^2 - 2M_2 E'_{2L}. \quad (9.326)$$

It is convenient to introduce another Lorentz-invariant *Mandelstam variable* u as

$$u \equiv (p_1 - p'_2)^2 = (p'_1 - p_2)^2 = M_2^2 - M_1'^2 - 2M_2 E'_{1L}. \quad (9.327)$$

The three *Mandelstam variables* s, t, u have the sum

$$s + t + u = M_1^2 + M_2^2 + M_1'^2 + M_2'. \quad (9.328)$$

This implies that all different kinematical configurations of a two-body scattering process can be represented in an invariant way by a point in an equilateral triangle of height $M_1^2 + M_2^2 + M_1'^2 + M_2'^2$, the so-called *Mandelstam triangle*. The heights over the three sides represent the quantities s, t, u .

Similar considerations can be made for the process of a particle decaying into three particles. Then a Poincaré-invariant way of picturing the distribution of the final products in a Mandelstam triangle is known as *Dalitz plot*.

The laboratory energy of all particles can be calculated from (9.319) and

$$E_{2L} = \frac{1}{M_2}(M_2^2 + M_2'^2 - t), \quad (9.329)$$

$$E'_{1L} = \frac{1}{M_2}(M_2^2 + M_1'^2 - u). \quad (9.330)$$

By evaluating the invariant (9.324) in the laboratory frame, we find the scattering angle in this frame:

$$\cos \theta_L = \frac{(M^4 - M_1^2 - M_2^2)(M_2^2 + M_1'^2 - u) + 2M_2^2(t - M_1^2 - M_1'^2)}{I(M, M_1, M_2)I(M, M_1', M_2)}. \quad (9.331)$$

The argument of the total energy δ -function (9.317) requires the knowledge of the momenta p'_1, p'_2 of the final particles as a function of the initial energy E_L and the scattering angle θ_L . These can now be calculated as follows. From (9.318) we find the invariant M as a function of E_L . This is inserted into (9.331) to obtain the invariant t as a function. Together with (9.328), this fixes the invariant u . Inserted into Eqs. (9.330), we find the final energy E'_{1L} , and from energy conservation also E'_{2L} . These determine the final momenta.

It is useful to generalize the definition of the scattering amplitude f that was introduced in (9.249) for the scattering of a nonrelativistic particle on an external potential. The generalization holds also in present case of two relativistic particles scattering on each other in the center-of-mass frame. As before, we define f so that its absolute square gives the differential cross section:

$$\frac{d\sigma}{d\Omega_{\text{CM}}} = |f|^2. \quad (9.332)$$

Then we see from (9.311) that f should be identified with

$$f = -\frac{1}{2\pi} \sqrt{\frac{p'_{\text{CM}}}{p_{\text{CM}}}} \frac{1}{E_{\text{CM}}} \sqrt{V^4 E'_1 E'_2 E_1 E_2} t_{\text{fi}}. \quad (9.333)$$

In the case of elastic scattering on a very heavy particle of mass M_2 (choosing the second particle to be the heavier one), this reduces back to the original definition.

In a more general scattering process in which two particles collide and produce a final state with n particles, the production cross section is given by

$$\sigma_{\text{fi}} = \frac{V}{j} \prod_{i=1}^n \left[\int \frac{d^3 p_i V}{(2\pi)} \right] (2\pi)^4 \delta^{(4)}(p' - p) |t_{\text{fi}}|^2, \quad (9.334)$$

with the prefactor $V/j = V^2 E_1 E_2 / p_{\text{CM}} E_{\text{CM}}$, as given by (9.310).

Scattering processes in a center-of-mass frame with zero total momentum can be observed directly in colliding beam experiments. There one has two beams impinging almost with opposite momenta (see Fig. 9.3). If $\hat{V}_{\text{int}}$ is the volume of the intersecting

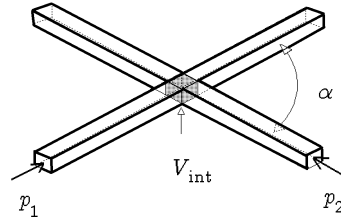


FIGURE 9.3 Geometry of particle beams in a collider. The angle of intersection α is greatly exaggerated. The intersection defines the interaction volume $\hat{V}_{\text{int}}$.

zone, the so-called *interaction volume*, and n_1 , n_2 are the particle densities in the two beams (particles per unit volume), the so-called *luminosity* of the colliding beam is obtained from the relative velocity v_{rel} by forming the product

$$L = v_{\text{rel}} \hat{V}_{\text{int}} n_1 n_2 = \frac{I(M, M_1, M_2)}{2E_1 E_2} \hat{V}_{\text{int}} n_1 n_2. \quad (9.335)$$

The rate of particle scattering is obtained by multiplying this with the differential cross section $d\sigma/d\Omega_{\text{CM}}$:

$$\frac{dN}{dt d\Omega_{\text{CM}}} = L \frac{d\sigma}{d\Omega_{\text{CM}}}. \quad (9.336)$$

Note that the luminosity increases linearly if the beams are focused upon a smaller area (since $n_1 n_2$ increases like $1/\text{area}^2$ while $\hat{V}_{\text{int}}$ increases like area).

9.4 Decay

The decay rate of an unstable particle into two particles is directly given by Eq. (9.298):

$$\frac{dP}{dt} = V^2 \int \frac{d^3 p'_1}{(2\pi)^3} \int \frac{d^3 p'_2}{(2\pi)^3} (2\pi)^4 \delta^{(4)}(p' - p) |t_{fi}|^2. \quad (9.337)$$

Evaluating this in the center-of-mass frame of the decaying particle yields

$$\Gamma = \frac{d}{dt} P(t) = \frac{V^3}{(2\pi)^2} \frac{p'_{\text{CM}} E'_1 E'_2}{M} \int d\Omega |t_{fi}|^2, \quad (9.338)$$

where M is the mass of the initial particle. If the particle has spin s and decays into final spins s'_1, s'_2 , an unpolarized initial state and all possible final spin orientations $m'_1 = -s'_1, \dots, s'_1$ and $m'_2 = -s'_2, \dots, s'_2$ lead to an isotropic distribution, and we can simplify (9.338) to

$$\Gamma = \frac{d}{dt} P(t) = \frac{V^3}{(2\pi)^2} \frac{p'_{\text{CM}} E'_1 E'_2}{M} \frac{4\pi}{2s+1} \sum_{m'_1, m'_2} |t_{fi}|^2. \quad (9.339)$$

9.5 Optical Theorem

The unitarity of the S -matrix (9.44),

$$\hat{S} \hat{S}^\dagger = \hat{S}^\dagger \hat{S} = 1, \quad (9.340)$$

implies an important theorem for the imaginary part of the diagonal elements of the T -matrix. Writing

$$S_{fi} = \delta_{fi} - i(2\pi)^4 \delta^{(4)}(p_f - p_i) t_{fi}, \quad (9.341)$$

we see that

$$-i(t_{ii} - t_{ii}^\dagger) = -\sum_f t_{if}^\dagger (2\pi)^4 \delta^{(4)}(p_f - p_i) t_{fi}, \quad (9.342)$$

where the sum runs over all possible many particle states. According to Eq. (9.333), the left-hand side is related to the imaginary part of the forward scattering amplitude f_{ii} as follows

$$\frac{2\pi E_{\text{CM}}}{V^2 E_1 E_2} \text{Im } f_{ii} = -\sum_n \prod_{i=1}^n \left[\int \frac{d^3 p_i V}{(2\pi)^3} \right] (2\pi)^4 \delta^{(4)}(p_f - p_i) |t_{fi}|^2. \quad (9.343)$$

Now, the right-hand side, if divided by the relative current density $j = p_{\text{CM}} E_{\text{CM}} / E_1 E_2 V$, is equal to $1/V$ times the sum over all cross sections σ_{fi} , i.e.,

it is equal to $-j/V$ times the total cross section $-(j/V)\sigma_{\text{tot}}$ [see (9.316)]. For the forward scattering amplitude f_{ii} this implies the simple relation

$$\frac{2\pi}{p_{\text{CM}}} f_{\text{ii}} = -\sigma_{\text{tot}}. \quad (9.344)$$

This relation is referred to as the *optical theorem* (in reference to a theorem relating the total absorption of light to the imaginary part of the forward-scattering amplitude).

9.6 Initial- and Final-State Interactions

Some inelastic scattering and decay processes are caused by a weak interaction Hamiltonian $\hat{H}_{\text{w}}$, which can be treated in Born approximation. This can happen while initial- and final states are still governed by strong interactions with a Hamiltonian $\hat{H}_{\text{s}}$. Suppose the total Hamiltonian contains these interactions additively, i.e.,

$$\hat{H} = \hat{H}_0 + \hat{V}_{\text{s}} + \hat{V}_{\text{w}}. \quad (9.345)$$

In specific applications, $\hat{H}_{\text{w}}$ may be *the* weak interaction of beta decay, say, and $\hat{H}_{\text{s}}$ a combination of electromagnetic and strong interactions. Alternatively, $\hat{H}_{\text{w}}$ may be an electromagnetic interaction, and $\hat{H}_{\text{s}}$ the strong interaction.

For time-independent interactions, the Møller operators are given by (9.32) and read explicitly

$$\Omega^{(\pm)} = \hat{U}_I(0, \mp\infty) = \lim_{t \rightarrow \mp\infty} e^{i(\hat{H}_0 + \hat{V}_{\text{w}} + \hat{V}_{\text{s}})t} e^{-i\hat{H}_0 t}. \quad (9.346)$$

The right-hand sides can obviously be decomposed into a product

$$\hat{U}_I(0, \mp\infty) = \hat{U}_{I\text{w}}(0, \mp\infty) \hat{U}_{I\text{s}}(0, \mp\infty), \quad (9.347)$$

where

$$\hat{U}_{I\text{w}}(0, \mp\infty) = \lim_{t \rightarrow \mp\infty} e^{i(\hat{H}_0 + \hat{V}_{\text{s}} + \hat{V}_{\text{w}})t} e^{-i(\hat{H}_0 + \hat{H}_{\text{s}})t}, \quad (9.348)$$

$$\hat{U}_{I\text{s}}(0, \mp\infty) = \lim_{t \rightarrow \mp\infty} e^{i(\hat{H}_0 + \hat{V}_{\text{s}})t} e^{-i\hat{H}_0 t}. \quad (9.349)$$

Thus we can write the Møller operators as

$$\Omega^{(\pm)} = \Omega_{\text{w}}^{(\pm)} \Omega_{\text{s}}^{(\pm)}, \quad (9.350)$$

with

$$\Omega_{\text{w}}^{(\pm)} = \hat{U}_{I\text{w}}(0, \mp\infty), \quad \Omega_{\text{s}}^{(\pm)} = \hat{U}_{I\text{s}}(0, \mp\infty). \quad (9.351)$$

Using this, we can express the scattering amplitude as follows:

$$S_{\text{fi}} = \langle f | \hat{U}_{I\text{s}}(\infty, 0) \hat{S}_{\text{w}} \hat{U}_{I\text{s}}(0, -\infty) | i \rangle, \quad (9.352)$$

where, by analogy with (9.42),

$$\hat{S}_w \equiv \hat{U}_{Iw}(\infty, -\infty) = \Omega_w^{(-)\dagger} \Omega_w^{(+)} \quad (9.353)$$

For a simple description of the effects of the initial- and the final-state interactions it is convenient to introduce, in a slight variation of (9.114), the notation

$$|i(\pm)\rangle \equiv \hat{U}_{Is}(0, \mp\infty)|i\rangle = \Omega_w^{(\pm)}|i\rangle, \quad (9.354)$$

where the symbols $(\pm)$ refer now to the activity of $\hat{H}_w$ in the time evolution. The scattering matrix elements become

$$\langle j|\hat{S}|i\rangle = \langle j(-)|\hat{S}_w|i(+)\rangle. \quad (9.355)$$

Under the assumption of a weak V_w , we replace $\hat{S}_w$ by its Born approximation and write

$$\hat{S}_w \approx -i \int_{-\infty}^{\infty} dt \hat{V}_{Iw}(t), \quad (9.356)$$

where

$$\hat{V}_{Iw}(t) \equiv e^{i(\hat{H}_0 + \hat{V}_s + \hat{V}_w)t} \hat{V}_w e^{-i(\hat{H}_0 + \hat{V}_s)t} \quad (9.357)$$

is the interaction representation of the weak interaction in the presence of the initial- and final-state interactions. The initial and final states are eigenstates of the operator $\hat{H}_0 + \hat{V}_s$ [see (9.15)]. The integration over t in (9.356) can now be done in (9.356), and leads to a δ -function of energy conservation [recall the derivation of (9.130)], so that

$$\langle j|\hat{S}|i\rangle = \langle j|i\rangle - 2\pi i \delta(E' - E) \langle j(-)|\hat{V}_w|i(+)\rangle. \quad (9.358)$$

For a local interaction which arises from an integral over an interaction density as in Eq. (9.288), we find that the initial- and final-state interactions are accounted for by the modified t -matrix

$$t_{\mathbf{p}'\mathbf{p}} \approx \langle \mathbf{p}'^{(-)}|\hat{\mathcal{H}}_{\text{int}}(0)|\mathbf{p}^{(+)}\rangle. \quad (9.359)$$

For the amplitude of multiparticle scattering (9.296), the corresponding expression is

$$t_{\text{fi}} \approx \langle f(-)|\hat{\mathcal{H}}_{\text{int}}(0)|i(+)\rangle. \quad (9.360)$$

9.7 Tests of Time-Reversal Violations

If the Hamiltonian is invariant under time-reversal, the time translation operator $U(t, t_0)$ fulfills the equation (7.123). This has the consequence that the scattering operator $\hat{S}$ of Eq. (9.42) satisfies

$$\mathcal{T}^\dagger \hat{S} \mathcal{T} = \hat{S}^\dagger. \quad (9.361)$$

To derive observable consequences from this, we first use the equations (7.118) and (7.119) to deduce trivially the equality for any matrix element between an initial state $|i\rangle$, obtained by applying one or more particle creation operators upon the vacuum, and a final state $|f\rangle$, obtained likewise:

$$\langle f|\hat{S}|i\rangle = \langle f|\mathbf{1}_A\hat{S}|i\rangle^*. \quad (9.362)$$

Invoking now time-reversal invariance by applying (9.361), we obtain

$$\langle f|\hat{S}|i\rangle = \langle f|\mathcal{T}^\dagger\hat{S}^\dagger\mathcal{T}|i\rangle^* = \langle f_T|\hat{S}^\dagger|i_T\rangle^* = \langle i_T|\hat{S}|f_T\rangle. \quad (9.363)$$

Here $|i_T\rangle$ denotes the time-reversed version of the state $|i\rangle$, in which all creation operators are replaced by the right-hand sides of (7.113), (7.322), etc. Thus momenta and spin directions are reversed, and there is a phase factor η_T for each particle.

9.7.1 Strong and Electromagnetic Interactions

Strong and electromagnetic interactions are time-reversal invariant. The matrix elements of the scattering operator $\hat{S}$, the scattering amplitudes, satisfy the identity

$$\langle \mathbf{p}_c, s_{3c}; \mathbf{p}_d, s_{3d} | \hat{S} | \mathbf{p}_a, s_{3a}; \mathbf{p}_b, s_{3b} \rangle = \eta \langle -\mathbf{p}_a, -s_{3a}; -\mathbf{p}_b, -s_{3b} | \hat{S} | -\mathbf{p}_c, -s_{3c}; -\mathbf{p}_d, -s_{3d} \rangle, \quad (9.364)$$

with some phase factor η of unit norm. When calculating the unpolarized cross section, we have to sum over the final states, and average over the initial states. In the center-of-mass frame, the cross section carries a phase-space factor p'_{CM}/p_{CM} , the ratio of final and initial center-of-mass momenta. It has to be removed to compare the squared amplitudes. Hence we obtain

$$\frac{\frac{d\sigma(ab \rightarrow cd)}{d\Omega}}{\frac{d\sigma(cd \rightarrow ab)}{d\Omega}} = \left(\frac{p_{CM}^{cd}}{p_{CM}^{ab}} \right)^2 \frac{(2s_c + 1)(2s_d + 1)}{(2s_a + 1)(2s_b + 1)}. \quad (9.365)$$

This is called the *principle of detailed balance*. It is important for the thermal equilibrium of chemical reactions. This equation was used in 1951 to determine the spin of the pion from a reaction in which two protons collide and produce a pion and a deuteron⁹:

$$p + p \rightleftharpoons d + \pi^+. \quad (9.366)$$

The principle of detailed balance says that

$$\frac{\frac{d\sigma(\rightarrow)}{d\Omega}}{\frac{d\sigma(\leftarrow)}{d\Omega}} = \frac{3}{4} \frac{q_\pi^2 (2s_\pi + 1)}{p_p^2}. \quad (9.367)$$

This relation was satisfied with $s_\pi = 0$.

⁹R.E. Marshak, Phys. Rev. **82**, 313 (1951); W.B. Cheston, Phys. Rev. **83**, 1118 (1951); R. Durbin, H. Loar, and J. Steinberger, Phys. Rev. **83**, 646 (1951); D.L. Clark, A. Roberts, and R. Wilson, Phys. Rev. **83**, 649 (1951).

9.7.2 Selection Rules in Weak Interactions

Consider a one-particle state $|i\rangle$ prepared by strong and electromagnetic interactions, which decays into a several-particle state $|b\rangle$ via weak interactions. Let $\hat{\mathcal{O}}$ be an observable which changes sign under time reversal:

$$\hat{\mathcal{O}}_T = -\hat{\mathcal{O}}. \quad (9.368)$$

Consider the expectation value of $\hat{\mathcal{O}}$ a long time after the decay. It is given by

$$\langle \hat{\mathcal{O}} \rangle = \langle i | \hat{U}(-\infty, \infty) \hat{\mathcal{O}} \hat{U}(\infty, -\infty) | i \rangle = \langle i | \hat{S}^\dagger \hat{\mathcal{O}} \hat{S} | i \rangle. \quad (9.369)$$

Using the antiunitarity of the time-reversal operator as expressed by Eqs. (7.118) and (7.119), the right-hand side can be rewritten as

$$\langle i | \hat{S}^\dagger \hat{\mathcal{O}} \hat{S} | i \rangle = \langle i | \mathbf{1}_A \hat{S}^\dagger \hat{\mathcal{O}} \hat{S} | i \rangle^* = \langle i | \mathcal{T}^\dagger \mathcal{T} \hat{S}^\dagger \hat{\mathcal{O}} \hat{S} | i \rangle^*. \quad (9.370)$$

Time-reversal invariance (9.361) brings this to

$$\langle i | \mathcal{T}^\dagger \hat{S} \hat{\mathcal{O}}_T \hat{S}^\dagger \mathcal{T} | i \rangle^* = \langle i_T | \hat{S} \hat{\mathcal{O}}_T \hat{S}^\dagger | i_T \rangle^*. \quad (9.371)$$

Since $\hat{\mathcal{O}}$ was assumed to be an observable, the expectation is real, and we can drop the complex conjugation at the end. This leaves us with the relation

$$\langle \hat{\mathcal{O}} \rangle = \langle i | \hat{S}^\dagger \hat{\mathcal{O}} \hat{S} | i \rangle = \langle i_T | \hat{S} \hat{\mathcal{O}}_T \hat{S}^\dagger | i_T \rangle. \quad (9.372)$$

If the decay is very slow, the scattering operator can be replaced by its Born approximation

$$\hat{S} \approx \hat{S}_B \equiv i \int_{-\infty}^{\infty} dt \hat{V}_{Iw}(t), \quad (9.373)$$

which is a Hermitian operator, up to a factor i (the direct term in (9.341) does not contribute to a decay process). But then (9.372) becomes

$$\langle \hat{\mathcal{O}} \rangle = \langle i | \hat{S}_B \hat{\mathcal{O}} \hat{S}_B | i \rangle = \langle i_T | \hat{S}_B \hat{\mathcal{O}}_T \hat{S}_B | i_T \rangle. \quad (9.374)$$

If the initial particle is spinless, then

$$|i_T\rangle = \eta_T |i\rangle, \quad |\eta_T| = 1. \quad (9.375)$$

Together with (9.368), this implies

$$\langle \hat{\mathcal{O}} \rangle = 0. \quad (9.376)$$

Thus, in a weak decay process, the expectation value of an observable that changes sign under time-reversal, is zero. Note that this result is independent of the phase η_T of the decaying particle.

Without the weakness assumption, the change to the Hermitian conjugates of the scattering operators in (9.372) would have prevented us from any conclusion.

Historically, the invariance under time reversal of weak interactions was apparently assured by the weak decays

$$K^+ \longrightarrow \pi^0 + \bar{\mu}^+ + \nu, \quad K^- \longrightarrow \pi^0 + \mu^- + \bar{\nu}. \quad (9.377)$$

The outgoing muon was initially found to have no average polarization orthogonal to the production plane formed by the momenta $\mathbf{p}_\mu$ and $\mathbf{p}_\pi$, i.e., the operator $\hat{O} = \boldsymbol{\sigma}_\mu \cdot (\hat{\mathbf{p}}_\mu \times \hat{\mathbf{p}}_\pi)$ had no measurable expectation value. Since this operator is odd under time reversal, the vanishing of $\langle \hat{O} \rangle$ seemed to confirm time-reversal invariance.¹⁰ However, as it turned out later, the breakdown of time-reversal invariance in weak interactions is much too small to be detected by a polarization experiment. There exists a much more sensitive experiment which shows the violation dramatically: the K^0 - $\bar{K}^0$ meson system. This will be discussed later.

9.7.3 Phase of Weak Amplitudes from Time-Reversal Invariance

If a particle decays weakly into two final particles, time-reversal invariance fixes the phase of the decay amplitude. Let us assume that the final-state interaction is purely elastic, i.e., that there are no other decay channels caused by the final-state interactions, then a weak decay can be treated in lowest-order perturbation theory. It has the amplitude

$$t_{ba} = \langle f(-) | \hat{H}_w | i(+) \rangle, \quad (9.378)$$

where the labels $(\pm)$ indicate the states defined in Section 9.6, containing the full effect of the initial- and final-state interactions. Under the assumption of time-reversal invariance of the weak interactions, we find

$$\langle f(-) | \hat{H}_w | i(+) \rangle = \langle i_T(-) | \hat{H}_w | f_T(+) \rangle = \langle f_T(+) | \hat{H}_w | i_T(-) \rangle^*. \quad (9.379)$$

If we choose the phase factors η_T of initial and final particles to be unity [see (4.226)], we obtain

$$\langle f(-) | \hat{H}_w | i(+) \rangle = \langle f_T(+) | \hat{H}_w | i_T(-) \rangle^*. \quad (9.380)$$

The initial state is a stationary single-particle state if the weak interactions are ignored. Hence

$$|i(+)\rangle \approx |i(-)\rangle. \quad (9.381)$$

We now rotate the matrix element on the right-hand side in space by 180 degrees, we reverse, in the center of mass frame, momentum and spin directions, and bring the time-reversed state back to the original form. Thus we obtain

$$\langle b(-) | \hat{H}_w | a(+) \rangle = \langle b(+) | \hat{H}_w | a(-) \rangle^*. \quad (9.382)$$

¹⁰This possibility of testing time-reversal invariance of weak interactions was pointed out by J.J. Sakurai, Phys. Rev. **109**, 980 (1958). See also M. Gell-Mann and A.H. Rosenfeld, Ann. Rev. Nucl. Sci. **7**, 407 (1957), Appendix A.

The amplitudes with $+$ and $-$ interchanged differ by a pure phase factor, that is precisely the scattering amplitude for the two-particle scattering in their final state:

$$\langle b(-)|\hat{H}_w|a(+)\rangle = e^{2i\delta} \langle b(+)|\hat{H}_w|a_T(-)\rangle. \quad (9.383)$$

The pure-phase nature is a consequence of the elasticity assumption of the two-particle scattering process. Together with (9.382), this fixes the phase:

$$\langle b(\mp)|\hat{H}_w|a(+)\rangle = \text{const.} \times e^{i\delta}. \quad (9.384)$$

This equation has many applications in phenomenological analyses [5].

Appendix 9A Green Function in Arbitrary Dimensions

In D dimensions, the Green function (9.138) in the scattered wave (9.136) of the Lippmann-Schwinger equation has the following form:

$$\langle \mathbf{x}|\hat{G}_0(E)|\mathbf{x}'\rangle = -2Mi\hbar \int \frac{d^D p}{(2\pi\hbar)^D} \frac{e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar}}{\mathbf{p}^2 - p_E^2}. \quad (9A.1)$$

The momentum integral has been calculated in Section 1.12 (also 9.1) of Ref. [2], for $E > 0$ yielding

$$\langle \mathbf{x}|\hat{G}_0(E)|\mathbf{x}'\rangle = \frac{M\pi}{\hbar} \frac{k_E^{D-2}}{(2\pi)^{D/2}} \frac{H_{D/2-1}^{(1)}(k_E|\mathbf{x}-\mathbf{x}'|)}{(k_E|\mathbf{x}-\mathbf{x}'|)^{D/2-1}}, \quad (9A.2)$$

where $k_E \equiv p_E/\hbar = \sqrt{2M(E+i\eta)}/\hbar$, and $H^{(1)}(z)$ is the Hankel function, whose leading large- z behavior is

$$H_\nu^{(1)} \approx \sqrt{\frac{2}{\pi z}} e^{i(z-\pi\nu/2-\pi/4)}, \quad (9A.3)$$

thus reproducing the previous result (9A.1) for $D = 3$.

In $D = 1$ dimension, the expression (9A.2) reduces to

$$\langle x|\hat{G}_0(E)|x'\rangle = \frac{M}{\hbar k_E} e^{ik_E|x-x'|}, \quad (9A.4)$$

so that the Lippmann-Schwinger equation (9.134) in one dimension reads

$$\langle x|\psi_k^{(+)}\rangle = \frac{1}{L^{1/2}} \left[e^{ikx} + i \frac{M}{\hbar^2 k_E} e^{ik_E|x-x'|} \int_{-\infty}^{\infty} dx V(x') \langle x'|\psi_k^{(+)}\rangle \right], \quad (9A.5)$$

where $k_E = \sqrt{2M(E+i\eta)}$ is equal to the wave number k of the incoming particles.

As a simple application, consider the case of a δ -function potential

$$V(x) = \frac{\hbar^2}{Ml} \delta(x), \quad (9A.6)$$

where (9A.5) becomes

$$\langle x|\psi_k^{(+)}\rangle = \frac{1}{L^{1/2}} \left[e^{ikx} + \frac{1}{ikl} e^{ik|x|} \int_{-\infty}^{\infty} \langle 0|\psi_k^{(+)}\rangle \right]. \quad (9A.7)$$

Setting $x = 0$ on the left-hand side determines

$$\langle 0|\psi_k^{(+)}\rangle = \frac{1}{L^{1/2}} \frac{ikl}{ikl-1}, \quad (9A.8)$$

and Eq. (9A.7) yields the fully interacting wave function

$$\langle x|\psi_k^{(+)}\rangle = \frac{1}{L^{1/2}} \left[e^{ikx} + \frac{1}{ikl-1} e^{ik|x|} \right]. \quad (9A.9)$$

The corresponding states $|\psi_k^{(-)}\rangle$ are

$$\langle x|\psi_k^{(-)}\rangle = \frac{1}{L^{1/2}} \left[e^{-ikx} + \frac{1}{-ikl-1} e^{-ik|x|} \right]. \quad (9A.10)$$

In the negative- x regime, the second wave runs to the left and its prefactor is the *reflection amplitude*

$$r = \frac{1}{ikl-1}. \quad (9A.11)$$

At positive x , the two exponentials run both to the right and the common prefactor

$$t = \frac{ikl}{ikl-1} \quad (9A.12)$$

is the transmission amplitude. The unitarity relation for this process is $|r|^2 + |t|^2 = 1$.

For an attractive δ -function, there is a bound-state pole at $k_B = 1/|l|$, corresponding to the energy

$$\varepsilon_B = -\frac{\hbar^2 k_B^2}{2M} = -\frac{\hbar^2}{2l^2 M} = -\frac{g^2 M}{2}. \quad (9A.13)$$

It is easy to verify that $\langle x|\psi_k^{(\pm)}\rangle$ satisfies the Schrödinger equation

$$\left[-\frac{\hbar^2 \partial_x^2}{2M} + \frac{\hbar^2}{Ml} \delta(x) - E \right] \langle x|\psi_k^{(\pm)}\rangle = 0, \quad (9A.14)$$

with the jump property of the solution at the position of the δ -function

$$\frac{\hbar^2 \partial_x}{2M} [\langle 0_+|\psi_k^{(\pm)}\rangle - \langle 0_-|\psi_k^{(\pm)}\rangle] = \frac{\hbar^2}{Ml} \langle 0|\psi_k^{(\pm)}\rangle. \quad (9A.15)$$

Let us also calculate the matrix elements of the resolvent operator (9.57), i.e., the Green function

$$\langle x|\hat{G}(E)|x'\rangle = \langle x|\frac{i\hbar}{E - \hat{H} + i\eta}|x'\rangle. \quad (9A.16)$$

It has the spectral representation

$$\langle x|\hat{G}(E)|x'\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{i\hbar}{E - E_{\mathbf{k}} + i\eta} \langle x|\psi_k^{(\pm)}\rangle \langle \psi_k^{(\pm)}|x'\rangle. \quad (9A.17)$$

Performing the integral over k we find, from the residue at k_E :

$$\langle x|\hat{G}(E)|x'\rangle = \frac{M}{\hbar k_E} \left[e^{ik_E|x-x'|} + \frac{1}{ik_E l - 1} e^{ik_E(|x|+|x'|)} \right]. \quad (9A.18)$$

This is related to the free Green function (9A.4) via Eq. (9.58).

The Green function (9A.18) can also be obtained with the help of the Wronski method¹¹ by combining the two independent solutions

$$f_1(x) = \sqrt{L} \langle x|\psi_{k_E}^{(+)}\rangle, \quad f_2(x) = f_1^*(x) \quad (9A.19)$$

¹¹See Subsection 3.2.1 in the textbook [2].

of the homogeneous Schrödinger equation $(\hat{H} - E)f(x) = 0$ in the form

$$\langle x|\hat{G}(E)|x\rangle = \langle x|\frac{i\hbar}{E - \hat{H}}|x'\rangle = \frac{2Mi}{\hbar} \frac{1}{W(x, x)} [\Theta(x - x')f_1(x)f_2(x') + \Theta(x' - x)f_1(x')f_2(x)], \quad (9A.20)$$

where $W(x, x)$ is the Wronski determinant

$$W(x, x) \equiv f_1'(x)f_2(x) - f_1(x)f_2'(x). \quad (9A.21)$$

Indeed, applying the operator $E - \hat{H} = E + \hbar^2 \partial_x^2 / 2M$ to (9A.20), we obtain $i\hbar \delta(x - x')$.

For the free system where $f_1(x) = e^{ik_E x}$, $f_2(x) = e^{-ik_E x}$, and $W(x, x) = 2ik_E$, this formula reproduces the above result (9A.4):

$$\langle x|\hat{G}_0(E)|x\rangle = \frac{2Mi}{\hbar} \frac{1}{W(x, x)} f_1(x_>)f_2(x_<) = \frac{M}{\hbar k_E} e^{ik_E |x - x'|}. \quad (9A.22)$$

In the presence of the δ -potential, where the Wronski determinant is calculated from the solutions (9A.19) as

$$W(x, x) = \frac{2ik_E^2 l}{k_E l + i}, \quad (9A.23)$$

the general formula (9A.20) yields

$$\langle x|\hat{G}(E)|x\rangle = \langle x|\frac{i\hbar}{E - \hat{H}}|x'\rangle = \frac{M}{\hbar k_E} \left[e^{ik_E |x - x'|} - \frac{1}{1 - ik_E l} e^{ik_E (|x| + |x'|)} \right]. \quad (9A.24)$$

From this, we find the bilocal density of states

$$\langle x|\hat{\rho}(E)|x'\rangle = \frac{1}{2\pi\hbar} \langle x|[\hat{G}(E + i\eta) - \hat{G}(E - i\eta)]|x\rangle = \frac{M}{2\pi\hbar^2 k_E} \left[\left(e^{ik_E (x - x')} + \frac{1}{ik_E l - 1} e^{ik_E (|x| + |x'|)} \right) + \text{c.c.} \right]. \quad (9A.25)$$

Integrating this over all energies in the continuum, i.e., by forming $\int_0^\infty dE = \hbar^2 \int_{-\infty}^\infty k_E dk_E / M$, we obtain

$$\int_0^\infty dE \langle x|\hat{\rho}(E)|x'\rangle = \delta(x - x') - \Theta(-l) \frac{1}{-l} e^{-(|x| + |x'|)l}. \quad (9A.26)$$

According to Eq. (9A.17), the same quantity is equal to

$$\int_0^\infty dE \int_{-\infty}^\infty \frac{dk}{2\pi} \langle x|\psi_k^{(+)}\rangle \delta(E - \hbar^2 k^2 / 2M) \langle \psi_k^{(+)}|x'\rangle = \int_{-\infty}^\infty \frac{dk}{2\pi} \langle x|\psi_k^{(+)}\rangle \langle \psi_k^{(+)}|x'\rangle. \quad (9A.27)$$

Hence Eq. (9A.26), together with the contribution of the single bound state wave function $\langle x|\psi_\beta\rangle = (1/\sqrt{-l})e^{-|x|l}$, yields

$$\int_{-\infty}^\infty \frac{dk}{2\pi} \langle x|\psi_k^{(+)}\rangle \langle \psi_k^{(+)}|x'\rangle + \delta(-l) \langle x|\psi_\beta\rangle \langle \psi_\beta|x'\rangle = \delta(x - x'), \quad (9A.28)$$

thus proving the completeness relation (9.62) of the states $\langle x|\psi_k^{(+)}\rangle$ and $\langle x|\psi_\beta\rangle = (1/\sqrt{-l})e^{-|x|l}$.

Appendix 9B Partial Waves in Arbitrary Dimensions

In D dimensions, the angular decomposition of the scattering amplitudes proceeds as follows. For equal incoming and outgoing energies $E_{\mathbf{p}'} = E_{\mathbf{p}}$, where $|\mathbf{p}'| = |\mathbf{p}| = p$, the T -matrix $\langle \mathbf{p}'|T|\mathbf{p}\rangle$ in Eq. (9.129) has an expansion

$$\langle \mathbf{p}'|T|\mathbf{p}\rangle = \frac{(2\pi)^D}{V} \sum_{l=0}^{\infty} T_l(p) \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}(\hat{\mathbf{p}}), \quad (9B.1)$$

where $Y_{l\mathbf{m}}(\hat{\mathbf{p}})$ are the hyperspherical harmonics associated with the momentum direction $\hat{\mathbf{p}}$. They generalize (4F.1), and their precise form is somewhat tedious to write down. Here we only recall that their magnetic quantum numbers form a $D - 2$ -dimensional vector of eigenvalues $(m_1, m_2, \dots, m_{D-2})$ running through the number

$$d_l = \frac{(2l + D - 2)(l + D - 3)!}{l!(D - 2)!} \quad (9B.2)$$

of different values for each l . The orthogonality (4F.3) becomes now:

$$\int d^2\hat{\mathbf{p}} Y_{l'\mathbf{m}'}^*(\hat{\mathbf{p}}) Y_{l\mathbf{m}}(\hat{\mathbf{p}}) = \delta_{l'l} \delta_{\mathbf{m}'\mathbf{m}}, \quad (9B.3)$$

where $\int d^{D-1}\hat{\mathbf{p}}$ denotes the integral over the surface of a unit sphere in D dimensions:

$$\int d^{D-1}\hat{\mathbf{p}} = S_D \equiv \frac{2\pi^{D/2}}{\Gamma(D/2)}. \quad (9B.4)$$

The spherical harmonics are matrix elements of eigenstates $|l\mathbf{m}\rangle$ of angular momentum [recall (4.846)] with localized states $|\hat{\mathbf{p}}\rangle$ on the unit sphere:

$$\langle \hat{\mathbf{p}} | l\mathbf{m} \rangle \equiv Y_{l\mathbf{m}}(\hat{\mathbf{p}}). \quad (9B.5)$$

The latter are orthogonal:

$$\langle \hat{\mathbf{p}}' | \hat{\mathbf{p}} \rangle = \delta^{(D-1)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}), \quad (9B.6)$$

where $\delta^{(D-1)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}})$ is the δ -function on a unit sphere.

The addition theorem (23.12) for the spherical harmonics is replaced by

$$\frac{2l + D - 2}{D - 2} \frac{1}{S_D} C_l^{(D/2-1)}(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}) = \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}^*(\hat{\mathbf{p}}), \quad (9B.7)$$

where the functions $C_l^{(\alpha)}(\cos \vartheta)$ are the hyperspherical Gegenbauer polynomials, the D -dimensional versions of the Legendre polynomials $P_l(\cos \theta)$ in Eq. (4F.7).

The Gegenbauer polynomials are related to Jacobi polynomials, which are defined in terms of hypergeometric functions by¹²

$$P_l^{(\alpha, \beta)}(z) \equiv \frac{1}{l!} \frac{\Gamma(l+1+\beta)}{\Gamma(1+\beta)} F_{2,1}(-l, l+1+\alpha+\beta; 1+\beta; (1+z)/2). \quad (9B.8)$$

The relation is¹³

$$C_l^{(\nu)}(z) = \frac{\Gamma(2\nu+l)\Gamma(\nu+1/2)}{\Gamma(2\nu)\Gamma(\nu+l+1/2)} P_l^{(\nu-1/2, \nu-1/2)}(z). \quad (9B.9)$$

Thus we can write

$$C_l^{(\nu)}(z) = \frac{1}{l!} \frac{\Gamma(l+2\nu)}{\Gamma(2\nu)} F_{2,1}(-l, l+2\nu; 1/2+\nu; (1+z)/2). \quad (9B.10)$$

For $D = 2$ and 3 , one has¹⁴

$$\lim_{\nu \rightarrow 0} \frac{1}{\nu} C_l^{(\nu)}(\cos \vartheta) = \frac{1}{2l} \cos l\vartheta, \quad (9B.11)$$

¹²M. Abramowitz and I. Stegun, op. cit., Formula 15.4.6.

¹³Ibid., Formula 15.4.5.

¹⁴I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.934.4.

$$C_l^{(1/2)}(\cos \vartheta) = P_l^{(0,0)}(\cos \vartheta) = P_l(\cos \vartheta). \quad (9B.12)$$

The *partial-wave expansion* (9B.1) becomes, in D dimensions:

$$\langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle = \sum_{l=0}^{\infty} T_l(p) \frac{2l+D-2}{D-2} \frac{1}{S_D} C_l^{(D/2-1)}(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}). \quad (9B.13)$$

A similar expansion for the S -matrix (9.130) requires expanding the scalar product $\langle \mathbf{p}' | \mathbf{p} \rangle = \delta_{\mathbf{p}', \mathbf{p}}$ into partial waves. In a large volume V , we replace this by $(2\pi)^D \delta^{(D)}(\mathbf{p}' - \mathbf{p})/V$. The δ -function is decomposed into a directional and a radial part

$$\delta_{\mathbf{p}', \mathbf{p}} = \frac{(2\pi)^D}{V} \delta^{(D)}(\mathbf{p}' - \mathbf{p}) = \delta^{(D-1)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) \frac{(2\pi)^D}{V} \frac{1}{p^{D-1}} \delta(p' - p). \quad (9B.14)$$

The directional δ -function on the right-hand side has a partial-wave expansion which is the completeness relation [compare (9.161) for the states $|l m\rangle$,

$$\sum_{l=0}^{\infty} \sum_{\mathbf{m}} |l \mathbf{m}\rangle \langle l \mathbf{m}| = 1, \quad (9B.15)$$

evaluated between the localized states $|\hat{\mathbf{p}}\rangle$ on the unit sphere. Using the matrix elements (9B.5) and the orthogonality relation (9B.6), we find from (9B.15):

$$\delta^{(D-1)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) = \sum_{l=0}^{\infty} \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}^*(\hat{\mathbf{p}}). \quad (9B.16)$$

The radial part of (9B.14) can be rewritten as

$$\frac{(2\pi)^D}{V} \frac{1}{p^{D-1}} \delta(p' - p) = \frac{(2\pi)^D}{V} \frac{1}{p^{D-1}} \frac{dE}{dp} \delta(E' - E) = \frac{(2\pi)^D}{V} \frac{1}{\rho_E} \delta(E' - E), \quad (9B.17)$$

where

$$\rho_E \equiv \frac{p^{D-1}}{dE/dp}. \quad (9B.18)$$

It allows us to rewrite the sum over all momentum states as follows:

$$\sum_{\mathbf{p}} = \int \frac{d^D p V}{(2\pi)^D} = \frac{V}{(2\pi)^D} \int d^{D-1} \hat{\mathbf{p}} \int dE \rho_E. \quad (9B.19)$$

Thus we find the expansion

$$\langle \mathbf{p}' | \mathbf{p} \rangle = \delta_{\mathbf{p}', \mathbf{p}} = \frac{(2\pi)^D}{V} \sum_{l=0}^{\infty} \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}(\hat{\mathbf{p}}) \frac{1}{\rho_E} \delta(E' - E). \quad (9B.20)$$

In a partial-wave expansion for the S -matrix (9.130), the overall δ -function for the energy conservation is conventionally factored out and one writes:

$$\langle \mathbf{p}' | \hat{S} | \mathbf{p} \rangle = \frac{(2\pi)^D}{V} \frac{1}{\rho_E} \delta(E' - E) \sum_{l=0}^{\infty} S_l(p) \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}(\hat{\mathbf{p}}). \quad (9B.21)$$

The relation between the partial-wave scattering amplitudes $S_l(p)$ and those of the T -matrix is again given by (9.168). The only change in D dimensions appears in ρ_E which acquires the form (9B.18).

In order to show this we use the expansion formula corresponding to (9.173),

$$e^{ih \cos \Delta \vartheta} = \sum_{l=0}^{\infty} a_l(h) \frac{l + D/2 - 1}{D/2 - 1} \frac{1}{S_D} C_l^{(D/2-1)}(\cos \Delta \vartheta), \quad (9B.22)$$

where

$$a_l(h) \equiv (2\pi)^{D/2} h^{1-D/2} i^l J_{l+D/2-1}(h). \quad (9B.23)$$

The expansion (9B.22) follows from the completeness of the polynomials $C_l^{(\nu)}(\cos \vartheta)$ at fixed ν , using the integration formulas¹⁵

$$\int_{-\pi/2}^{\pi/2} d\vartheta \sin^{\nu} \vartheta e^{h \cos \vartheta} C_l^{(\nu)}(\cos \vartheta) = \pi \frac{2^{1-\nu} \Gamma(2\nu + l)}{l! \Gamma(\nu)} h^{-\nu} I_{\nu+l}(h), \quad (9B.24)$$

$$\int_{-\pi/2}^{\pi/2} d\vartheta \sin^{\nu} \vartheta C_l^{(\nu)}(\cos \vartheta) C_{l'}^{(\nu)}(\cos \vartheta) = \pi \frac{2^{1-2\nu} \Gamma(2\nu + l)}{l! (l + \nu) \Gamma(\nu)^2} \delta_{ll'}. \quad (9B.25)$$

We now use (9B.22) to expand the incoming free-particle wave

$$\begin{aligned} \langle \mathbf{x} | \mathbf{p} \rangle &= \frac{1}{\sqrt{V}} e^{i\mathbf{p}\mathbf{x}} = \sum_{l=0}^{\infty} \psi_l(pr) \sum_{\mathbf{m}}^l Y_{l\mathbf{m}}(\hat{\mathbf{x}}) Y_{l\mathbf{m}}(\hat{\mathbf{p}}) \\ &= \sum_{l=0}^{\infty} \psi_l(pr) \frac{l + D/2 - 1}{D/2 - 1} \frac{1}{S_D} C_l^{(D/2-1)}(\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}), \end{aligned} \quad (9B.26)$$

where $r \equiv |\mathbf{x}|$, and

$$\psi_l(pr) = \frac{1}{\sqrt{V}} a_l(pr). \quad (9B.27)$$

Far from the scattering region, the spherical Bessel functions have the asymptotic behavior

$$J_{\nu}(z) \rightarrow \sqrt{\frac{2}{\pi z}} \sin(z - \nu\pi/2 + \pi/4), \quad (9B.28)$$

implying for the partial waves [compare (9.178)]

$$\psi_l(pr) = \frac{1}{\sqrt{V}} i^l 2 (2\pi)^{(D-1)/2} \frac{\sin\{pr - \pi[l/2 - (D-3)/4]\}}{(pr)^{(D-1)/2}}. \quad (9B.29)$$

We shall now calculate the asymptotic form of the outgoing waves. The second term of the Lippmann-Schwinger equation (9.131) yields the scattered wave, which reads in configuration space

$$\langle \mathbf{x} | \mathbf{p} \rangle^{\text{sc}} = \int \frac{d^D p' V}{(2\pi)^D} \langle \mathbf{x} | \mathbf{p}' \rangle \frac{1}{E - E' + i\eta} \langle \mathbf{p}' | T | \mathbf{p} \rangle. \quad (9B.30)$$

Inserting here the partial-wave decompositions (9B.1) and (9B.26), we find

$$\begin{aligned} &\int \frac{d^D p' V}{(2\pi)^D} \langle \mathbf{x} | \mathbf{p}' \rangle \frac{1}{E - E' + i\eta} \langle \mathbf{p}' | T | \mathbf{p} \rangle \\ &= \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{x}}') Y_{l\mathbf{m}}(\hat{\mathbf{p}}) \int_0^{\infty} dp' p'^{D-1} \frac{a_l(p'r) T_l(p)}{E - E' + i\eta}, \end{aligned} \quad (9B.31)$$

¹⁵I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formulas 7.321 and 7.313.

so that the total partial waves, including the scattered waves are

$$\psi_l^{\text{tot}}(pr) = \left[\psi_l(pr) + \int_0^\infty dp' p'^{D-1} \frac{\psi_l(p'r) T_l(p)}{E - E' + i\eta} \right]. \quad (9B.32)$$

In terms of the spherical Bessel functions of Eq. (9.174), this reads

$$\begin{aligned} \psi_l^{\text{tot}}(pr) &= \frac{1}{\sqrt{V}} 2(2\pi)^{(D-1)/2} \frac{1}{(pr)^{(D-3)/2}} i^l \\ &\times \left[j_{l+(D-3)/2}(pr) + p^{(D-3)/2} \int_0^\infty dp' p'^{(D+1)/2} j_{l+(D-3)/2}(p'r) \frac{T_l(p')}{E - E' + i\eta} \right]. \end{aligned} \quad (9B.33)$$

For large r , we use the asymptotic formula (9.177) to rewrite the integral as [compare (9.182)]

$$\int_0^\infty dp' p'^{(D+1)/2} \frac{T_l(p')}{E - E' + i\eta} \frac{e^{i\{p'r - \pi[l/2 - (D-3)/4]\}} - e^{-i\{p'r - \pi[l/2 - (D-3)/4]\}}}{2ip'r}. \quad (9B.34)$$

The integral can now be approximated as in (9.184):

$$\frac{1}{dE/dp} \int dp' p'^{(D+1)/2} \frac{T_l(p')}{p - p' + i\eta} \frac{1}{2ip'r} \left(e^{i\{pr - \pi[l/2 - (D-3)/4]\}} - e^{-i\{pr - \pi[l/2 - (D-3)/4]\}} \right). \quad (9B.35)$$

Together with the prefactor $p^{(D-3)/2}$ in (9B.33), this becomes

$$-\frac{2\pi p^{D-1}}{dE/dp} e^{-i\pi l/2} e^{i\pi(D-3)/4} \frac{e^{ipr}}{2pr}. \quad (9B.36)$$

In this way we find for the wave function (9B.33):

$$\begin{aligned} \psi_l^{\text{tot}}(pr) &\xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{2(2\pi)^{(D-2)/2}}{2i(pr)^{(D-1)/2}} \\ &\times \left[e^{i\{pr - \pi[l/2 - (D-3)/4]\}} - e^{-i\{pr - \pi[l/2 - (D-3)/4]\}} - 2\pi i \rho_E T_l(p) e^{i\pi(D-3)/4} e^{ipr} \right]. \end{aligned} \quad (9B.37)$$

Expressing $T_l(p)$ in terms of $S_l(p)$ using Eq. (9.168), we have

$$\psi_l^{\text{tot}}(pr) \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{2(2\pi)^{(D-1)/2}}{2i(pr)^{(D-1)/2}} \left[S_l(p) e^{i(pr - \pi(D-3)/4)} - (-1)^l e^{-ip(pr - \pi(D-3)/4)} \right]. \quad (9B.38)$$

Inserting the unitary form (9.171) for elastic scattering, this becomes

$$\psi_l^{\text{tot}}(pr) \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \frac{2(2\pi)^{(D-1)/2}}{p^{(D-1)/2}} i^l e^{i\delta_l(p)} \frac{\sin\{pr + \delta_l(p) - \pi[l/2 - (D-3)/4]\}}{r^{(D-1)/2}}. \quad (9B.39)$$

This shows again that $\delta_l(p)$ is the phase shift of the scattered waves with respect to the incoming partial waves (9B.29).

If we insert (9B.33) on the right-hand side of the partial wave expansion (9B.26), the first term gives again the incoming plane wave. The $T_l(p)$ -terms add to this a scattered wave, determined by Eq. (9B.33). The result is a total wave function for large r similar to (9.143):

$$\langle \mathbf{x} | \mathbf{p}^{(+)} \rangle \xrightarrow{r \rightarrow \infty} \frac{1}{\sqrt{V}} \left(e^{i\mathbf{p}\mathbf{x}} + \frac{e^{i(pr - \pi(D-3)/4)}}{r^{(D-1)/2}} f_{\mathbf{p}'\mathbf{p}} \right), \quad (9B.40)$$

where $f_{\mathbf{p}'\mathbf{p}}$ has the partial wave expansion generalizing (9.250):

$$f_{\mathbf{p}'\mathbf{p}} = \sum_{l=0}^{\infty} f_l(p) \sum_{\mathbf{m}} Y_{l\mathbf{m}}(\hat{\mathbf{p}}') Y_{l\mathbf{m}}(\hat{\mathbf{p}}) = \sum_{l=0}^{\infty} f_l(p) \frac{l + D/2 - 1}{D/2 - 1} \frac{1}{S_D} C_l^{(D/2-1)}(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}), \quad (9B.41)$$

with

$$f_l(p) = -\frac{(2\pi)^{(D+1)/2}}{p^{(D-1)/2}} \rho_E T_l(p) = \frac{(2\pi)^{(D-1)/2}}{ip^{(D-1)/2}} [S_l(p) - 1] = \frac{2(2\pi)^{(D-1)/2}}{p^{(D-1)/2}} e^{i\delta_l(p)} \sin \delta_l(p). \quad (9B.42)$$

Taking the absolute square of this, and integrating over all directions of the final momentum $\mathbf{p}'$, we find the partial wave decomposition of the total cross section:

$$\begin{aligned} \sigma &= \int d\hat{\mathbf{p}}' |f_{\mathbf{p}'\mathbf{p}}|^2 = \sum_{l=0}^{\infty} f_l(p) f_l(p)^* \sum_{\mathbf{l}\mathbf{m}} \sum_{\mathbf{l}'\mathbf{m}'} Y_{\mathbf{l}\mathbf{m}}(\hat{\mathbf{p}}') Y_{\mathbf{l}\mathbf{m}}(\hat{\mathbf{p}}) Y_{\mathbf{l}\mathbf{m}'}^*(\hat{\mathbf{p}}') Y_{\mathbf{l}\mathbf{m}'}^*(\hat{\mathbf{p}}) \\ &= \sum_{l=0}^{\infty} |f_l(p)|^2 \frac{l+D/2-1}{D/2-1} \frac{1}{S_D} C_l^{(D/2-1)}(1) = \sum_{l=0}^{\infty} |f_l(p)|^2 \frac{l+D/2-1}{D/2-1} \frac{1}{S_D} \frac{(l+D-3)!}{l!(D-2)!}, \end{aligned} \quad (9B.43)$$

where we have used the special value of the Gegenbauer function¹⁶

$$C_l^{(\nu)}(1) = \binom{l+2\nu-1}{l}. \quad (9B.44)$$

Inserting (9B.42), the cross section decomposes as

$$\sigma = \sum_{l=0}^{\infty} \sigma_l = \frac{4(2\pi)^{D-1}}{p^{D-1}} \sum_{l=0}^{\infty} \frac{l+D/2-1}{D/2-1} \frac{1}{S_D} \frac{(l+D-3)!}{l!(D-2)!} \sin^2 \delta_l(p). \quad (9B.45)$$

In three dimensions, this reduces to (9.253).

Appendix 9C Spherical Square-Well Potential in D Dimensions

For a square-well potential (9.268) in D dimensions, the radial Schrödinger equation (9.269) becomes

$$\left\{ \frac{d^2}{dr^2} + \frac{D-1}{r} \frac{d}{dr} + \left[k_E^2 - \frac{l(l+D-2)}{r^2} \right] \right\} \psi_l(r) = 0, \quad (9C.1)$$

where

$$K \equiv \sqrt{2M(E + V_0)}/\hbar. \quad (9C.2)$$

There is only one solution which is regular at the origin:

$$\psi_l(r) = \frac{A}{(Kr)^{D/2-1}} J_{D/2-1+l}(Kr), \quad (9C.3)$$

with an arbitrary normalization factor A .

For positive energy E , the solution in the outer region $r \geq a$ receives an admixture of the associated spherical Bessel function $n_l(kr)$:

$$\psi_l(r) = \frac{B}{(kr)^{D/2-1}} [\cos \delta_l(k) J_{D/2-1+l}(Kr) + \sin \delta_l(k) N_{D/2-1+l}(Kr)], \quad (9C.4)$$

where

$$k \equiv \sqrt{2ME}/\hbar, \quad (9C.5)$$

¹⁶M. Abramowitz and I. Stegun, op. cit., Formula 22.2.3.

and B , $\delta_l(k)$ must be determined from the boundary condition at $r = a$. The associated Bessel functions $N_{D/2-1+l}(z)$ have the asymptotic behavior orthogonal to (9B.28):

$$N_\nu(z) \rightarrow -\sqrt{\frac{2}{\pi z}} \cos(z - \nu\pi/2 + \pi/4). \quad (9C.6)$$

The continuity of the wave function fixes the ratio B/A . The continuity of the logarithmic derivative is independent of this ratio and fixes the phase shifts by the equation

$$\begin{aligned} & \frac{\partial_{r_0}[(Kr_0)^{1-D/2} J_{D/2-1+l}(Kr_0)]}{(Kr)^{1-D/2} J_{D/2-1+l}(Kr_0)} \\ &= \frac{\partial_{r_0}[\cos \delta_l(k)(Kr_0)^{1-D/2} J_{D/2-1+l}(Kr_0) - \sin \delta_l(k)(Kr_0)^{1-D/2} N_{D/2-1+l}(Kr_0)]}{\cos \delta_l(k)(Kr_0)^{1-D/2} J_{D/2-1+l}(Kr_0) - \sin \delta_l(k)(Kr_0)^{1-D/2} N_{D/2-1+l}(Kr_0)}. \end{aligned} \quad (9C.7)$$

This determines the phase shifts as follows:

$$\tan \delta_l(k) = \frac{k J_{D/2+l}(kr_0) J_{D/2-1+l}(K_0 r_0) - K_0 J_{D/2}(K_0 r_0) J_{D/2-1}(kr_0)}{k Y_{D/2+l}(kr_0) J_{D/2-1+l}(K_0 r_0) - K_0 J_{D/2+l}(K_0 r_0) Y_{D/2-1+l}(kr_0)}. \quad (9C.8)$$

For the s -wave in $D = 3$ dimensions, this reduces to

$$\tan \delta_0(k) = \frac{k \cos kr_0 \sin K_0 r_0 - K_0 \cos K_0 r_0 \sin kr_0}{k \sin kr_0 \sin K_0 r_0 - K_0 \cos K_0 r_0 \cos kr_0}, \quad (9C.9)$$

which is, of course, the same as (9.276). In $D = 2$ dimensions, we obtain

$$\tan \delta_0(k) = \frac{k J_1(kr_0) J_0(K_0 r_0) - K_0 J_1(K_0 r_0) J_0(kr_0)}{k Y_1(kr_0) J_0(K_0 r_0) - K_0 J_1(K_0 r_0) Y_0(kr_0)}, \quad (9C.10)$$

which is, for small k , equal to

$$\delta_0 \approx \frac{\pi}{2} \frac{K_0 r_0 J_1(K_0 r_0)}{J_0(K_0 r_0) + K_0 r_0 J_1(K_0 r_0) \log(kr_0 e^\gamma/2)}, \quad (9C.11)$$

where $\gamma \approx 0.577 216$ is the Euler-Mascheroni number.

The phase shifts for a repulsive potential are obtained by setting $K_0 = i\kappa_0 \equiv i\sqrt{2M|V_0|}/\hbar$ and by replacing

$$J_\nu(K_0 r_0) \rightarrow i^\nu I_\nu(\kappa_0 r_0), \quad Y_\nu(K_0 r_0) \rightarrow i^\nu \left[i I_\nu(\kappa_0 r_0) - \frac{2}{\pi} (-1)^\nu K_\nu(\kappa_0 r_0) \right]. \quad (9C.12)$$

In the limit of an infinitely high repulsive potential, the modified Bessel functions $I_\nu(z)$ diverge like $e^z/\sqrt{2\pi z}$, while $K_\nu(\kappa_0 r_0)$ go to zero exponentially fast like $\sqrt{\pi/2z} e^{-z}$. Hence

$$\tan \delta_0(k) \underset{V_0 \rightarrow \infty}{=} \frac{J_{D/2-1}(kr_0)}{Y_{D/2-1}(kr_0)}. \quad (9C.13)$$

In $D = 3$ dimensions, the right-hand side becomes $-\tan kr_0$, implying that $\delta_0(k) \equiv -kr_0$. In $D = 2$ dimensions, the right-hand side is $J_0(kr_0)/Y_0(kr_0)$ which has the small- k expansion

$$\tan \delta_0(k) = \frac{\pi}{2} \frac{1}{\log(kr_0 e^\gamma/2)}. \quad (9C.14)$$

For $D > 2$, the small- k expansion of (9C.13) is

$$\tan \delta_0(k) \underset{V_0 \rightarrow \infty}{=} -\pi \frac{(kr_0/2)^{D-2}}{\Gamma(D/2)\Gamma(D/2-1)}, \quad (9C.15)$$

which reduces correctly to $-kr_0$ for $D = 3$, but not to (9C.14) for $D = 2$, since the small z behavior of $Y_0(z) \approx (2/\pi) \log z$ cannot be obtained as $\nu \rightarrow 0$ -limit of the $\nu > 0$ behavior $Y_\nu(z) \rightarrow -(1/\pi)\Gamma(\nu)(z/2)^\nu$.¹⁷

¹⁷M. Abramowitz and I. Stegun, op. cit., Formulas 9.1.8 and 9.1.9.

Notes and References

For more details on scattering theory see

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*The only place outside of Heaven where you can be perfectly safe
from all the dangers and perturbations of love is Hell.*

C. S. LEWIS (1898–1963)

10

Quantum Field Theoretic Perturbation Theory

In this chapter we would like to develop a method for calculating the physical consequences of a small interaction in a nearly free quantum field theory. All results will be expressed as power series in the coupling strength. These power series will have many unpleasant mathematical properties to be discussed in later chapters. In this chapter, we shall ignore such problems and show only how the power series can be calculated in principle. More details can be found in standard textbooks [2, 3, 4].

10.1 The Interacting n -Point Function

We consider an interacting quantum field theory with a time-independent Hamiltonian. All physical information of the theory is carried by the n -point functions

$$G^{(n)}(x_1, \dots, x_n) = {}_H\langle 0 | T \phi_H(x_1) \phi_H(x_2) \cdots \phi_H(x_n) | 0 \rangle_H. \quad (10.1)$$

Here $|0\rangle_H$ is the Heisenberg ground state of the interaction system, i.e., the lowest steady eigenstate of the full Schrödinger Hamiltonian:

$$H|0\rangle_H = E|0\rangle_H. \quad (10.2)$$

The fields $\phi_H(x)$ are the fully interacting time-dependent Heisenberg fields, i.e., they satisfy

$$\phi_H(\mathbf{x}, t) = e^{-iHt} \phi_S(\mathbf{x}) e^{iHt}, \quad (10.3)$$

where

$$H = H_0 + V \quad (10.4)$$

is the full Hamiltonian of the scalar field. Note that the field on the right-hand side of Eq. (10.3) has the time argument $t = 0$ and is therefore the same in any picture $\phi_I(\mathbf{x}, 0) = \phi_H(\mathbf{x}, 0) = \phi_S(\mathbf{x}, 0)$ so that we shall also write

$$\phi_H(\mathbf{x}, t) = e^{-iHt} \phi(\mathbf{x}, 0) e^{iHt}. \quad (10.5)$$

We now express $\phi_H(x)$ in terms of the field $\phi_I(x)$ of the interaction picture and rewrite

$$G^{(n)}(x_1, \dots, x_n) = {}_H\langle 0|T[U_I(0, t_1)\phi_I(x_1)U_I(t_1, t_2)\phi_I(x_2)\cdots \\ \cdots U_I(t_{n-1}, t_n)\phi_I(x_n)U_I(t_n, 0)]|0\rangle_H, \quad (10.6)$$

where we have used the properties of the time displacement operator

$$U_I^{-1}(t, 0) = U_I^\dagger(t, 0) = U_I(0, t), \\ U_I(t_1, t_2) = U_I(t_1, 0)U_I^{-1}(0, t_2). \quad (10.7)$$

We shall now assume that the state $|0\rangle_H$ is a non-degenerate eigenstate of the full Hamiltonian. Then we can make use of the switching-on procedure of the interaction. Then, in the limit $t \rightarrow -\infty$, the vacuum state will develop towards the vacuum of the free field Hamiltonian H_0 . According to the Gell-Mann–Low formula we may write [5, 6]

$$|0\rangle_H = \frac{U_I(0, -\infty)|0\rangle}{\langle 0|U_I(0, \infty)|0\rangle}, \\ {}_H\langle 0| = \frac{\langle 0|U_I(\infty, 0)}{\langle 0|U_I(\infty, 0)|0\rangle}, \quad (10.8)$$

where $|0\rangle$ is the free-particle vacuum. The presence of a switching parameter η and its limit $\eta \rightarrow 0$ at the end are tacitly assumed. After this, formula (10.6) becomes

$$G^{(n)}(x_1, \dots, x_n) = \langle 0|U_I(\infty, 0)T\left(U_I(0, t_1)\phi_I(x_1)U_I(t_1, t_2)\phi_I(x_2)\cdots \right. \\ \left. \cdots U_I(t_{n-1}, t_n)\phi_I(x_n)U_I(t_n, 0)\right)U_I(0, -\infty)|0\rangle \\ \times 1/\langle 0|U_I(\infty, 0)|0\rangle\langle 0|U_I(0, -\infty)|0\rangle. \quad (10.9)$$

The product in the denominator can be combined to a single expression using the relation (9.95):

$$\langle 0|U_I(\infty, 0)|0\rangle\langle 0|U_I(0, -\infty)|0\rangle = \langle 0|U_I(\infty, -\infty)|0\rangle = \langle 0|S|0\rangle. \quad (10.10)$$

The numerator consists of the S -matrix operator $U_I(\infty, -\infty)$, time-sliced into $n+1$ pieces at $t_1, \dots, t_n$, with n fields $\phi(x_i)$, $i = 1, \dots, n$, inserted successively. It is gratifying to observe that due to the definition of the time-ordering operator, the expression can be written in the much more compact fashion

$$T\left(S\phi_I(x_1)\phi_I(x_2)\cdots\phi_I(x_n)\right), \quad (10.11)$$

so that we arrive at the simple formula

$$G^{(n)}(x_1, \dots, x_n) = \langle 0|T\left(S\phi_I(x_1)\cdots\phi_I(x_n)\right)|0\rangle/\langle 0|S|0\rangle \quad (10.12) \\ = \frac{\langle 0|Te^{-i\int_{-\infty}^{\infty} dt V_I(t)}\phi_I(x_1)\cdots\phi_I(x_n)|0\rangle}{\langle 0|e^{-i\int_{-\infty}^{\infty} dt V_I(t)}|0\rangle}.$$

The fields $\phi_I(x)$ are now expressed as

$$\begin{aligned}\phi_I(\mathbf{x}, t) &= e^{iH_0 t} \phi_S(\mathbf{x}) e^{-iH_0 t} \\ &= e^{iH_0 t} \phi(\mathbf{x}, 0) e^{-iH_0 t}.\end{aligned}\quad (10.13)$$

This implies that the field $\phi_I(\mathbf{x}, t)$ changes in time in the same way as the Heisenberg field $\phi_H(\mathbf{x}, t)$ would do if the Hamiltonian H were without interaction. This observation is the key to the upcoming evaluation of the n -point functions.

What is the interaction picture of the interaction V_I itself? We assumed V to be an arbitrary time-independent functional of $\phi_S(\mathbf{x})$,

$$V = V[\phi_S(\mathbf{x})]. \quad (10.14)$$

But then we may use (10.13) to calculate

$$V_I(t) = V[\phi_I(\mathbf{x}, t)]. \quad (10.15)$$

Thus the potential $V_I(t)$ in the interaction picture is simply the Schrödinger interaction V with the fields $\phi_S(\mathbf{x})$ replaced by $\phi_I(\mathbf{x}, t)$, which develop from the initial configuration $\phi(\mathbf{x}, 0)$ according to the free-field equations of motion.

The state $|0\rangle$ is the ground state of the free Hamiltonian H_0 , i.e., the vacuum state arising in the free-field quantization of Chapters 2 and 4. If we drop the indices I , we can state the interacting n -particle Green function as

$$G^{(n)}(x_1, \dots, x_n) = \frac{\langle 0 | T e^{-i \int_{-\infty}^{\infty} dt V[\phi(\mathbf{x}, t)]} \phi(x_1) \cdots \phi(x_n) | 0 \rangle}{\langle 0 | T e^{-i \int_{-\infty}^{\infty} dt V[\phi(\mathbf{x}, t)]} | 0 \rangle}, \quad (10.16)$$

where $\phi(\mathbf{x}, t)$ is the free field and $|0\rangle$ the vacuum associated with it.

Note that the functional brackets only hold for the spatial variable $\mathbf{x}$. All fields in $V[\phi(\mathbf{x}, t)]$ have the same time argument. In a local quantum field theory, the functional is a spatial integral over a density

$$e^{-i \int_{-\infty}^{\infty} dt V[\phi(\mathbf{x}, t)]} e^{-i \int_{-\infty}^{\infty} dt \int d^3x v(\phi(\mathbf{x}, t))}. \quad (10.17)$$

10.2 Perturbation Expansion for Green Functions

In general, it is very hard to evaluate expressions like (10.16). If the interaction term V_I is very small, however, it is suggestive to perform a power series expansion and write

$$\begin{aligned}e^{-i \int_{-\infty}^{\infty} dt V[\phi(\mathbf{x}, t)]} &= 1 - i \int_{-\infty}^{\infty} dt V[\phi(\mathbf{x}, t)] \\ &+ \frac{(-i)^2}{2!} \int_{-\infty}^{\infty} dt_1 dt_2 T(V[\phi(\mathbf{x}_1, t_1)] V[\phi(\mathbf{x}_2, t_2)]) + \dots\end{aligned}\quad (10.18)$$

In this way, we are confronted in (10.16) with the vacuum expectation value of many free fields $\phi(x)$, of which n are from the original product $\phi(x_1) \cdots \phi(x_n)$, the others

from the interaction terms. From Wick's theorem we know that we may reduce the expression to a sum over products of free-particle Green functions $G_0(x - x')$, with all possible pair contractions. The simplest formulation of this theorem was given in terms of the generating functional of all free-particle Green functions [recall (7.840)],

$$Z_0[j] = \langle 0 | T e^{i \int d^4x \phi(x) j(x)} | 0 \rangle, \quad (10.19)$$

where the subscript 0 emphasizes now the absence of interactions. This functional can also be used to compactly specify the perturbation expansion. Let us also introduce the generating functional for the interacting case, where the Green functions are expectation values of products of the Heisenberg fields $\phi_H(x)$ in the full Heisenberg vacuum state,

$$Z_H[j] \equiv {}_H \langle 0 | T e^{i \int d^4x \phi_H(x) j(x)} | 0 \rangle_H. \quad (10.20)$$

The functional derivatives of this yield the full n -point functions (10.1). The perturbation expansion derived above can now be phrased compactly in the formula

$$Z_H[j] \equiv Z_D[j]/Z[0], \quad (10.21)$$

where $Z[j]$ is the generating functional in the interaction or Dirac picture:

$$Z[j] \equiv \langle 0 | T e^{-i \int_{-\infty}^{\infty} dt V[\phi(x)] + i \int d^4x \phi(x) j(x)} | 0 \rangle. \quad (10.22)$$

The fields and the vacuum state in $Z[j]$ are those of the free field theory. Note that $Z_H[j]$ and $Z[j]$ differ only by an irrelevant constant $Z[0]$ which appears in the denominators of all Green functions (10.16), and which has an important physical meaning to be understood in Section 10.3.1. The main difference between them is the prescription of how they have to be evaluated.

As functionals of the sources j , the generating functional yields the perturbation expansion for all n -point functions. This can be verified by functional differentiations with respect to j and comparison of the results with (10.16) and (10.1).

Note that while the generating functional $Z_H[j]$ is normalized to unity for $j \equiv 0$, this is not the case for the auxiliary functional $Z[j]$. However, for generating n -point functions, $Z[j]$ is just as useful as the properly normalized $Z_H[j]$ if one only modifies the differentiation rule by the overall factor $Z[0]^{-1}$:

$$G^{(n)}(x_1, \dots, x_n) = \left[\frac{1}{Z[j]} \frac{\delta}{i \delta j(x_1)} \cdots \frac{\delta}{i \delta j(x_n)} Z[j] \right]_{j=0}. \quad (10.23)$$

This is what we shall do from now on so that we can refer to $Z[j]$ as a generating functional. This will also be of advantage when enumerating the different perturbative contributions to each Green function. Indeed, formula (10.23) enables us to write down an immediate, although formal and implicit, solution for the interacting generating functional: Since differentiation $\delta/\delta j(x)$ produces a field $\phi(x)$ we may

rewrite the interaction $V[\phi(x)]$ as $V[-i\delta/\delta j(x)]$. Then it is no longer a field operator. It may be removed from the vacuum expectation value by rewriting $Z[j]$ as

$$Z[j] = e^{-i \int_{-\infty}^{\infty} dt V[-i\delta/\delta j(x)]} Z_0[j]. \quad (10.24)$$

Recall that $Z_0[j]$ was calculated explicitly in (7.843) from Wick's theorem

$$Z_0[j] = \exp \left\{ -\frac{1}{2} \int d^4 y_1 d^4 y_2 j(y_1) G_0(y_1, y_2) j(y_2) \right\}. \quad (10.25)$$

The perturbation series of all n -point functions are now found by expanding the exponential in (10.24) in powers of V and performing the derivatives with respect to $\delta/\delta j(x)$. These produce precisely all Wick contractions involving the fields in the interaction.

The explicit evaluation is quite difficult for an arbitrary interaction. It is therefore advisable to learn dealing with such expressions by considering simple examples.

10.3 Feynman Rules for ϕ^4 -Theory

In order to understand the systematics of the perturbation expansion let us focus our attention on a very simple scalar field theory with the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 + \frac{g}{4!}\phi^4. \quad (10.26)$$

This is usually referred to as ϕ^4 -theory. Here m is the mass of the free particles, and g the interaction strength. We shall assume g to be small enough to be able to expand all interacting Green functions in a power series in g . It is well-known that the resulting series will be divergent since the coefficients of g^k at large order k will grow like $k!$. Fortunately, however, the limiting behavior of the coefficients is exactly known. This has made it possible to develop powerful resummation techniques for extracting reliable results from this series.

The interaction in the Schrödinger picture is

$$V[\phi_S(\mathbf{x})] = \frac{g}{4!} \int d^3 x \phi_S^4(\mathbf{x}). \quad (10.27)$$

In the interaction picture, after substituting $\phi_S(x)$ by the free field $\phi(x)$, the exponents in the formulas (10.16), (10.22) become

$$e^{-i \int_{-\infty}^{\infty} dt V[\phi_S(\mathbf{x}, t)]} = e^{-i \frac{g}{4!} \int d^4 x \phi^4(x)}. \quad (10.28)$$

In the functional formulation of the perturbation expansion, we have to calculate the series

$$Z[j] = e^{-i \frac{g}{4!} \int d^4 x (-i\delta/\delta j(x))^4} Z_0[j]$$

$$\begin{aligned}
&= \left[1 - i \frac{g}{4!} \int d^4x \left(-i \frac{\delta}{\delta j(x)} \right)^4 \right. \\
&\quad \left. + \frac{(-i)^2}{2!} \left(\frac{g}{4!} \right)^2 \int d^4x_1 d^4x_2 \left(-i \frac{\delta}{\delta j(x_1)} \right)^2 \left(-i \frac{\delta}{\delta j(x_2)} \right)^2 + \dots \right] \\
&\times e^{-\frac{1}{2} \int d^4y_1 d^4y_2 j(y_1) G_0(y_1, y_2) j(y_2)}. \quad (10.29)
\end{aligned}$$

The n -point functions are obtained according to (10.23) by expanding the exponential on the right-hand side in a power series, forming the n th functional derivatives with respect to j , and setting j to zero. The result has to be divided by $Z[0]$ which is also a power series in g . Certainly, n has to be even, otherwise the result vanishes. If we want to calculate $G^{(n)}$ up to a given power in g , say g^k , there are many different contributions. The denominator $Z[0]$ has to be expanded in powers of g , and its k th-order contributions come from the $\left(-\frac{1}{2} \int j G_0 j\right)^{2k} / (2k)!$ term in the expansion of the exponential. Here and in most of the following structural formulas we shall omit the integration variables, for brevity. The k th-order term has the form

$$Z_k[0] = \left(-i \frac{g}{4!}\right)^k \int \left(-i \frac{\delta}{\delta j_1}\right)^4 \cdots \left(-i \frac{\delta}{\delta j_k}\right)^4 \frac{1}{(2k)!} \left(-\frac{1}{2} \int j G_0 j\right)^{2k}. \quad (10.30)$$

In the numerator of (10.23), there are contributions of zeroth order in g to $G^{(n)}$ from the $(n/2)$ th terms which have the form $\left(-\frac{1}{2} \int j G_0 j\right)^{n/2}$. Then there are those of first order in g from the $(n/2 + 2)$ nd terms $\left(-\frac{1}{2} \int j G_0 j\right)^{n/2+2}$, of second order in g from the $(n/2 + 4)$ th term $\left(-\frac{1}{2} \int j G_0 j\right)^{n/2+4}$, etc. Forming the product of four derivatives $(\delta/\delta j)^4$ associated with every order in g , as well as the n derivatives for the Green function $G^{(n)}$, the expressions of k th order have the structure

$$\begin{aligned}
&\left(-i \frac{g}{4!}\right)^k \left(-i \frac{\delta}{\delta j_1}\right)^4 \cdots \left(-i \frac{\delta}{\delta j_n}\right)^4 \\
&\times \int \left(-i \frac{\delta}{\delta j}\right)^4 \cdots \left(-i \frac{\delta}{\delta j}\right)^4 \frac{1}{(n/2 + 2k)!} \left(-\frac{1}{2} \int j G_0 j\right)^{\frac{n}{2}+2k}. \quad (10.31)
\end{aligned}$$

The Green functions accurate to order g^k are then obtained by dividing the two power series (10.31) and (10.30) through each other and expanding the result again up to order g^k .

This all seems to be a horrendous task. It is, however, possible to devise a diagrammatic procedure for keeping track of the different contributions which will cause many simplifications. In particular, the division process is really quite trivial due to the fact that $Z[0]$ appears automatically as a factor in the calculation of the numerator of each n -point function.

Actually, formula (10.29), although it gives the most explicit answer to the problem, is quite cumbersome when it comes to actual calculations. The derivatives are an efficient analytic way of accounting for the set of all Wick contractions of pairs

of field operations. In the calculation of a specific n -point function, however, it is much more advantageous to insert the expansion (10.18) into formula (10.16), and to separate numerator and denominator by writing

$$G^{(n)}(x_1, \dots, x_n) \equiv \frac{1}{Z[0]} \bar{G}^{(n)}(x_1, \dots, x_n). \quad (10.32)$$

Here the unnormalized Green function $\bar{G}^{(n)}(x_1, \dots, x_n)$ is the unnormalized Green function. This has the expansion

$$\begin{aligned} \bar{G}^{(n)}(x_1, \dots, x_n) &\equiv \\ &= \langle 0|T \left\{ \left(1 - \frac{ig}{4!} \int d^4z \phi(z) + \frac{1}{2!} \left(\frac{-ig}{4!} \right)^2 \int d^4z_1 d^4z_2 \phi^4(z_1) \phi^4(z_2) + \dots \right) \right. \\ &\quad \left. \times \phi(x_1) \cdots \phi(x_n) \right\} |0\rangle, \end{aligned} \quad (10.33)$$

whereas the denominator $Z[0]$ in (10.32) has the series

$$Z[0] = \langle 0|T \left(1 - \frac{ig}{4!} \int d^4z \phi^4(z) + \frac{1}{2!} \left(\frac{-ig}{4!} \right)^2 \int d^4z_1 d^4z_2 \phi^4(z_1) \phi^4(z_2) + \dots \right) |0\rangle. \quad (10.34)$$

By performing the Wick contractions in the two expansions explicitly we obtain $\bar{G}_p^{(n)}$ and $Z_p[0]$, respectively, to be divided by one another.

10.3.1 The Vacuum Graphs

Because of its formal simplicity let us start a more explicit perturbation expansion with the calculation of $Z[0]$. To first-order in the coupling constant g we have to evaluate

$$Z_1[0] = -i \frac{g}{4!} \int d^4z \langle 0|T (\phi(z) \phi(z) \phi(z) \phi(z)) |0\rangle, \quad (10.35)$$

where we have written down the four powers of $\phi(z)$ separately in order to see better how to perform all pair contractions. The first field can be contracted with the three others. After this the second field has only one choice. Thus there are $3 \cdot 1$ contractions, all of the form

$$-i \frac{g}{4!} \int d^4z G_0(z, z) G_0(z, z), \quad (10.36)$$

so that

$$Z_1[0] = -i 3 \frac{g}{4!} \int d^4z G_0(z, z) G_0(z, z). \quad (10.37)$$

To order g^2 we have to evaluate

$$\frac{1}{2!} \left(-i \frac{g}{4!} \right)^2 \int d^4z_1 d^4z_2 \langle 0|T (\phi(z_1) \phi(z_1) \phi(z_1) \phi(z_1) \phi(z_2) \phi(z_2) \phi(z_2) \phi(z_2)) |0\rangle. \quad (10.38)$$

Expanding the expectation value of the product of eight fields into a sum over pair contractions, we obtain $7 \cdot 5 \cdot 3 \cdot 1 = 105$ contractions, 3^2 of them with $\phi(z_1)$'s and $\phi(z_2)$'s contracting among each other, for example,

$$\overbrace{\phi(z_1)\phi(z_1)}\overbrace{\phi(z_1)\phi(z_1)}|\overbrace{\phi(z_2)\phi(z_2)}\overbrace{\phi(z_2)\phi(z_2)}, \quad (10.39)$$

where we have explicitly separated the two interactions by a vertical line. There are further $4 \cdot 3 \cdot 2 = 24$ contractions, where each $\phi(z_1)$ connects with a $\phi(z_2)$, for example,

$$\overbrace{\phi(z_1)\phi(z_1)\phi(z_1)\phi(z_1)}\overbrace{\phi(z_2)\phi(z_2)\phi(z_2)\phi(z_2)}, \quad (10.40)$$

and $6 \cdot 6 \cdot 2 = 72$ of the mixed type, for example,

$$\overbrace{\phi(z_1)\phi(z_1)}\overbrace{\phi(z_1)\phi(z_1)}|\overbrace{\phi(z_2)\phi(z_2)}\overbrace{\phi(z_2)\phi(z_2)}. \quad (10.41)$$

The factors six counts the six choices of one contraction within each factor ϕ^4 after which there are only two possible interconnections.

The 105 terms obtained in this way correspond to the following integrals

$$\begin{aligned} \frac{1}{2!} \left(-i \frac{g}{4!} \right)^2 & \left[9 \left(\int d^4 z_1 G_0(z_1, z_1)^2 \right)^2 + 24 \int d^4 z_1 d^4 z_1 G_0(z_1, z_2)^4 \right. \\ & \left. + 72 \int d^4 z d^4 z G_0(z_1, z_1) G_0(z_1, z_2)^2 G_0(z_1, z_2)^2 G_0(z_2, z_2) \right]. \end{aligned} \quad (10.42)$$

It is useful to picture the different contributions by means of so-called *Feynman diagrams*: A line with x_1, x_2 at the ends

$$\overline{x_1} \longrightarrow x_2 = G_0(x_1, x_2) \quad (10.43)$$

represents a free-particle propagator. A vertex with four emerging lines

$$\begin{array}{c} \times \\ z \end{array} = -i \frac{g}{4!} \quad (10.44)$$

stands for the $\phi^4(z)$ interaction at the point z with the convention to carry a coupling constant $-ig/4!$. The spacetime variables of each vertex have to be integrated over. Then the only diagram to first order is

$$3 \bigcirc_{z_1} \bigcirc_{z_1}. \quad (10.45)$$

To second order there are three diagrams

$$9 \underbrace{\text{---}\bigcirc\bigcirc\text{---}}_{z_1} + 24 \underbrace{\text{---}\bigcirc\bigcirc\text{---}}_{z_2} + 24 \underbrace{\text{---}\bigcirc\bigcirc\text{---}}_{z_1 z_2} + 72 \underbrace{\text{---}\bigcirc\bigcirc\text{---}}_{z_1 z_2} . \quad (10.46)$$

To third order we find $11 \cdot 9 \cdot 7 \cdot 5 \cdot 3 \cdot 1 = 10\,395$ terms. The total number rapidly proliferates. Diagrams of this type consisting only of lines which close back into themselves are called *vacuum diagrams*.

When we discussed Eq. (7.140) we noticed an important statistical interpretation of the relativistic euclidean propagator $G(x, x')$. It describes the probability for a random walk of any length τ to go from x to x' , provided that its lengths are distributed with an exponential Boltzmann-like factor $e^{-\mu\tau}$. The loop expansion of the partition function in terms of vacuum diagrams may therefore be interpreted as a direct picture of the various topologies of random walks in a grand-canonical ensemble of walks of any length. For this reason, relativistic quantum field theories may be used to study random walk ensembles, in which case they are called *disorder field theories*. As mentioned in Chapter 7, such random walks appear in many physical systems in the form of vortex lines and defect lines.

This line interpretation of quantum fields has led to an entire quantum field theory of physical systems in which the statistical mechanics of line like excitations play an important role for understanding the observed behavior. Consider, for example, the phase transitions in liquid helium. Conventionally, they are understood by describing the liquid as an ensemble of a large number of atoms interacting by a van der Waals type of potential. At low temperatures, below the so-called λ -point $T_\lambda \approx 2.17\text{K}$, the atoms enter the superfluid phase in which all atoms behave in a coherent fashion [1]. At zero temperature the entire system lies in a ground state. As temperature rises, thermal fluctuations create small loops of vortex lines. Their average length grows, and at T_λ it diverges. The vortex lines proliferate and fill the entire sample. Since the inside of each vortex line contains a normal liquid, the superfluid becomes normal. This picture gives rise to a completely alternative quantum field theoretic description of superfluid He. At zero temperature, the superfluid is a vacuum for vortex lines, i.e., the disorder field describing them has a zero expectation value. As the temperature rises, more and more disorder excitations are generated, and the field acquires a finite expectation value.

The reader who wants to understand this interesting development is referred to the original literature¹. Some details will also be discussed in Chapter 19.2.

At this place it is also worth mentioning that the opposite direction of research has been pursued by a number of people, who are trying to understand as field theory as a system of an ensemble of lines. The formalism arising in this way is referred to as *string-inspired approach* to quantum field theory. It abandons the marvellous power of the field theoretic description of ensembles of lines in favor of some calculational advantages [10]. By construction, this approach conserves the

¹See Refs. [7, 8, 9].

number of lines, i.e., the number of particles. Thus it will not be efficient when particle condensation processes are important, since then vortex line numbers are certainly not conserved.

10.4 The Two-Point Function

Let us now turn to the numerator in the perturbation expansion for the n -point function (10.29). We shall first study the two-point function. Clearly, to zeroth order there is only the free-particle expression

$$\bar{G}^{(2)}(x_1, x_2) = \langle 0 | T \phi(x_1) \phi(x_2) | 0 \rangle = G_0(x_1, x_2) \quad (10.47)$$

corresponding to the Feynman diagram (10.43). To first order we have to find all contractions of the expression

$$\frac{-ig}{4!} \int d^4 z \langle 0 | T \phi(z) \phi(z) \phi(z) \phi(z) \phi(x_1) \phi(x_2) | 0 \rangle. \quad (10.48)$$

There are $5 \cdot 3 \cdot 1 = 15$ of them. They fall into two classes: 3 diagrams contain contractions only among the four fields $\phi(z)$ with the same z , multiplied by a contraction of $\phi(x_1)$ with $\phi(x_2)$. Analytically, they correspond to

$$3 \left(\frac{-ig}{4!} \right) \int d^4 z G_0^2(z, z) G_0(x_1, x_2), \quad (10.49)$$

i.e., this expression carries the same factor 3 that was found in the calculation (10.36) of the vacuum diagrams by themselves. The diagrammatic representation consists of a line and the vacuum diagram side by side

$$3 \text{ --- } x_1 \text{ --- } x_2 \quad \bigcirc \bigcirc. \quad (10.50)$$

Such a diagram is called *disconnected*. In general, the analytic expression represented by the disconnected diagram is the product of the expressions corresponding to the individual pieces.

The second class of first-order diagrams collects the contractions between the four $\phi(z)$ and $\phi(x_1)$ or $\phi(x_2)$. There are 12 of them with the analytic expression

$$12 \left(\frac{-ig}{4!} \right) \int d^4 z G_0(x_1, z) G_0(z, z) G_0(z, x_2). \quad (10.51)$$

They are pictured by the connected Feynman diagram

$$\text{--- } x_1 \text{ --- } x_2 \text{ --- } \bigcirc. \quad (10.52)$$

Thus the expansion to first order has the diagrammatic expansion

$$\bar{G}^{(2)}(x_1, x_2) = \text{--- } x_1 \text{ --- } x_2 + \left(3 \text{ --- } x_1 \text{ --- } x_2 \quad \bigcirc \bigcirc + 12 \text{ --- } x_1 \text{ --- } x_2 \text{ --- } \bigcirc \right). \quad (10.53)$$

Remembering the expansion of the denominator to this order

$$Z[0] = 1 + 3 \text{ (two circles joined at a point)} , \quad (10.54)$$

we see that the two-particle Green function is, to order g , given by the free diagram plus the diagram in Fig. 10.52:

$$G^{(2)}(x_1, x_2) = \text{free diagram} + 12 \text{ (two circles joined at a point)} . \quad (10.55)$$

The disconnected pieces involving the vacuum diagram have disappeared.

Consider now the second-order contributions. To obtain $\bar{G}$ we have to form all contractions of

$$\frac{1}{2!} \left(\frac{-ig}{4!} \right)^2 \int d^4 z_1 d^4 z_2 \langle 0 | T \phi(z_1) \phi(z_1) \phi(z_1) \phi(z_1) \phi(z_2) \phi(z_2) \phi(z_2) \phi(z_2) \times \phi(x_1) \phi(x_2) | 0 \rangle . \quad (10.56)$$

There are $9 \cdot 7 \cdot 5 \cdot 3 \cdot 1 = 945$ of them. These decompose into three classes. The first is disconnected and contains the 105 vacuum diagrams multiplied by $G_0(x_1, x_2)$,

$$\frac{1}{2!} \text{free diagram} \times \left(9 \text{ (two circles joined at a point)} + 24 \text{ (two circles joined at two points)} + 72 \text{ (three circles joined at a point)} \right) . \quad (10.57)$$

The second consists of mixed contributions in which the first order correction to $\bar{G}$ is combined with a first-order vacuum diagram to

$$\frac{1}{2!} \left(36 \cdot 2 \text{ (two circles joined at a point)} + 144 \text{ (two circles joined at two points)} \right) . \quad (10.58)$$

The third contains only the connected diagrams

$$\frac{1}{2!} \left(144 \cdot 2 \text{ (two circles joined at a point)} + 144 \cdot 2 \text{ (two circles joined at two points)} + 96 \cdot 2 \text{ (two circles joined at a point)} \right) . \quad (10.59)$$

In order to calculate the two-point function up to order g^2 we consider the expansion

$$\begin{aligned} \bar{G}(x_1, x_2) = & \left\{ \text{free diagram} + 12 \text{ (two circles joined at a point)} + 3 \text{free diagram} \text{ (two circles joined at a point)} \right. \\ & + \frac{1}{2!} \text{free diagram} \left(9 \text{ (two circles joined at a point)} + 24 \text{ (two circles joined at two points)} + 72 \text{ (three circles joined at a point)} \right) \\ & \left. + 36 \text{ (two circles joined at a point)} + 144 \text{ (two circles joined at two points)} + 144 \text{ (two circles joined at two points)} + 96 \text{ (two circles joined at a point)} \right\} \end{aligned} \quad (10.60)$$

and divide it by the expansion of $Z[0]$ calculated up to the same order. This consists of the diagrams

$$Z[0] = 1 + 3 \text{ (two circles joined at a point)} + \frac{1}{2!} \left(9 \text{ (two circles joined at a point)} + 24 \text{ (two circles joined at two points)} + 72 \text{ (three circles joined at a point)} \right) . \quad (10.61)$$

Dividing $\bar{G}(x_1, x_2)$ by $Z[0]$ gives the two-point function

$$G^{(2)}(x_1, x_2) = \text{diagram of a single line from } x_1 \text{ to } x_2 + 12 \text{diagram of a loop on a line from } x_1 \text{ to } x_2 + \frac{1}{2!} \left(144 \cdot 2 \text{diagram of two loops on a line from } x_1 \text{ to } x_2 + 144 \cdot 2 \text{diagram of two separate loops on lines from } x_1 \text{ to } x_2 + 96 \cdot 2 \text{diagram of a tadpole on a line from } x_1 \text{ to } x_2 \right) + \dots \quad (10.62)$$

10.5 The Four-Point Function

Let us now study the four-point function. To zeroth order, the numerator has the following trivial contributions in which all particles propagate freely

$$\bar{G}^{(4)}(x_1, x_2, x_3, x_4) = \text{diagram of two parallel lines } x_3 \text{ to } x_1, x_4 \text{ to } x_2 + \text{diagram of two crossing lines } x_3 \text{ to } x_2, x_4 \text{ to } x_1 + \text{diagram of two lines meeting at a vertex } x_3, x_4 \text{ to } x_1, x_2 \quad (10.63)$$

To first order we must form all contractions in

$$\frac{-ig}{4!} \int d^4 z_1 d^4 z_2 \langle 0 | T \phi(z_1) \phi(z_1) \phi(z_1) \phi(z_1) \times \phi(x_1) \phi(x_2) \phi(x_3) \phi(x_4) | 0 \rangle, \quad (10.64)$$

which yield the diagrams

$$\begin{aligned} & 4! \text{diagram of two crossing lines } x_3 \text{ to } x_2, x_4 \text{ to } x_1 \\ & + 12 \left(\begin{aligned} & \text{diagram of a loop on line } x_3 \text{ to } x_1 + \text{diagram of a loop on line } x_4 \text{ to } x_2 + \text{diagram of a loop on a crossing line } x_3 \text{ to } x_2, x_4 \text{ to } x_1 \\ & + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_1, x_2 + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_2, x_1 \\ & + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_1, x_2 + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_2, x_1 \end{aligned} \right) \\ & + \left(\begin{aligned} & \text{diagram of a loop on line } x_3 \text{ to } x_1 + \text{diagram of a loop on line } x_4 \text{ to } x_2 + \text{diagram of a loop on a crossing line } x_3 \text{ to } x_2, x_4 \text{ to } x_1 \\ & + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_1, x_2 + \text{diagram of a loop on a vertex } x_3, x_4 \text{ to } x_2, x_1 \end{aligned} \right) \times 3 \text{diagram of two separate loops} . \quad (10.65) \end{aligned}$$

We observe again the appearance of a factor $1 + 3 \text{diagram of two separate loops}$ containing the first-order vacuum diagram, which is canceled when forming the quotient (10.32). Thus $G^{(4)}$ can be written to this order as

$$\begin{aligned}
G^{(4)}(x_1, \dots, x_n) = & \left(\begin{array}{c} x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 2 \text{ perm} \right) \\
& + 4! \begin{array}{c} x_3 \text{---} x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \text{---} x_2 \end{array} + 12 \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 5 \text{ perm} \right) . \quad (10.66)
\end{aligned}$$

We now turn to the second-order diagrams for which we must form all contractions in (10.56) after exchanging its second line by $\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)|0\rangle$. Their total number is $11 \cdot 9 \cdot 7 \cdot 5 \cdot 3 \cdot 1 = 10395$ diagrams in $\bar{G}^{(4)}(x_1, x_2, x_3, x_4)$. These can be grouped into 105 vacuum diagrams of second order multiplied with the previously calculated zeroth-order diagram in $\bar{G}^{(4)}(x_1, x_2, x_3, x_4)$:

$$\frac{1}{2!} \left(\begin{array}{c} \text{---} \text{---} \\ \text{---} \text{---} \end{array} + \begin{array}{c} x_3 \text{---} x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \text{---} x_2 \end{array} + \begin{array}{c} \text{---} \text{---} \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ \text{---} \text{---} \end{array} \right) \left(9 \begin{array}{c} \text{---} \text{---} \text{---} \\ \bullet \quad \bullet \quad \bullet \end{array} + 24 \begin{array}{c} \text{---} \text{---} \\ \bullet \quad \bullet \end{array} + 72 \begin{array}{c} \text{---} \text{---} \text{---} \\ \bullet \quad \bullet \quad \bullet \end{array} \right). \quad (10.67)$$

Then there are those in which the vacuum diagrams appear in first order

$$\left[4! \begin{array}{c} x_3 \text{---} x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \text{---} x_2 \end{array} + 12 \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 5 \text{ perm} \right) \right] \times 3 \begin{array}{c} \text{---} \text{---} \\ \bullet \quad \bullet \end{array} . \quad (10.68)$$

Finally, there are 9504 terms without vacuum contributions

$$\begin{aligned}
& \frac{4!4!}{2!} \left\{ \left(\begin{array}{c} x_3 \text{---} x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \text{---} x_2 \end{array} + 2 \text{ perm} \right) + \left(\begin{array}{c} x_3 \text{---} x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \text{---} x_2 \end{array} + 3 \text{ perm} \right) \right. \\
& + \frac{1}{2} \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 2 \text{ perm} \right) \\
& \left. + \frac{1}{2} \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} \text{---} \text{---} \text{---} \\ x_3 \text{---} \text{---} x_1 \\ x_4 \text{---} \text{---} x_2 \end{array} + 5 \text{ perm} \right) \right\} . \quad (10.69)
\end{aligned}$$

$$\begin{aligned}
G^{(4)}(x_1, \dots, x_n) = & \left(\begin{array}{c} x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 2 \text{ perm} \right) \\
& + 4! \begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad / \\ \bullet \\ / \quad \diagdown \\ x_4 \quad x_2 \end{array} + 12 \left(\begin{array}{c} \text{---} \bigcirc \text{---} \\ x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 5 \text{ perm} \right) \\
& + \frac{4!4!}{2!} \left\{ \left(\begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad / \\ \bullet \quad \bullet \\ / \quad \diagdown \\ x_4 \quad x_2 \end{array} + 2 \text{ perm} \right) + \left(\begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad / \\ \bullet \quad \bullet \\ / \quad \diagdown \\ x_4 \quad x_2 \end{array} + 3 \text{ perm} \right) \right. \\
& + \frac{1}{2} \left(\begin{array}{c} \text{---} \bigcirc \text{---} \quad \text{---} \bigcirc \text{---} \\ x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} \text{---} \bigcirc \text{---} \\ x_3 \text{---} x_1 \\ x_4 \text{---} \bigcirc \text{---} x_2 \end{array} + 2 \text{ perm} \right) \\
& \left. + \frac{1}{3} \left(\begin{array}{c} \text{---} \bigcirc \text{---} \\ x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} \bigcirc \text{---} \bigcirc \text{---} \\ x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 5 \text{ perm} \right) \right\} + \mathcal{O}(g^3).
\end{aligned} \tag{10.70}$$

Faced with the rapid proliferation of diagrams for increasing order in the coupling constant, there is need to economize the calculation procedure. The cancellation of all disconnected pieces involving vacuum diagrams was a great simplification. But the remaining diagrams are still many, even at low order in perturbation theory. Fortunately, not all of these diagrams really require a separate calculation. First of all, there are many diagrams which consist of disconnected pieces, each of which already occurs in the expansion (10.62) of the two-point function. The total amplitude factorizes into the product of expressions, of which each is known from the calculation of $G^{(2)}$. Thus, we can save a great deal of labor if we separate the connected diagrams in $G^{(4)}$ and consider them separately. They are called the connected four-point functions with the notation $G_c^{(4)}(x_1, x_2, x_3, x_4)$. Their low-order expansion is simply

$$\begin{aligned}
G^{(4)}(x_1, \dots, x_4) = & \quad 4! \quad \begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ x_4 \quad x_2 \end{array} \quad (10.71) \\
& + \frac{4!4!}{2!} \left\{ \left(\begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ x_4 \quad x_2 \end{array} + 2 \text{ perm} \right) + \left(\begin{array}{c} x_3 \quad x_1 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ x_4 \quad x_2 \end{array} + 3 \text{ perm} \right) \right\}.
\end{aligned}$$

We only have to learn how to recover the full Green function from the connected one and the omitted diagrams which are all known from $G^{(2)}$. In our example it can easily be verified that these omitted parts are simply the product of two propagators $G^{(2)}$ together with the three perturbative corrections on the external legs

$$\begin{aligned}
G_c^{(2)} G_c^{(2)} + 2 \text{ perm} &= \left\{ \begin{array}{c} \text{diagram: } x_1 \text{---} x_2 \\ \text{diagram: } x_1 \text{---} \text{loop} \text{---} x_2 \end{array} + 12 \begin{array}{c} \text{diagram: } x_1 \text{---} \text{loop} \text{---} x_2 \end{array} \right. \\
&\quad \left. + \frac{1}{2!} \left(144 \cdot 2 \begin{array}{c} \text{diagram: } x_1 \text{---} \text{loop} \text{---} x_2 \end{array} + 144 \cdot 2 \begin{array}{c} \text{diagram: } x_1 \text{---} \text{loop} \text{---} x_2 \end{array} + 96 \cdot 2 \begin{array}{c} \text{diagram: } x_1 \text{---} \text{loop} \text{---} x_2 \end{array} \right) + \dots \right\}^2 + 2 \text{ perm} \\
&= \left(\begin{array}{c} x_3 \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 2 \text{ perm} \right) + 12 \left(\begin{array}{c} x_3 \text{---} \text{loop} \text{---} x_1 \\ x_4 \text{---} x_2 \end{array} + 5 \text{ perm} \right) \\
&\quad + \frac{4!4!}{2!} \left\{ \frac{1}{2} \left(\begin{array}{c} x_3 \text{---} \text{loop} \text{---} x_1 \\ x_4 \text{---} \text{loop} \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} x_3 \text{---} \text{loop} \text{---} x_1 \\ x_4 \text{---} \text{loop} \text{---} x_2 \end{array} + 2 \text{ perm} \right) \right. \\
&\quad \left. + \frac{1}{3} \left(\begin{array}{c} x_3 \text{---} \text{loop} \text{---} x_1 \\ x_4 \text{---} \text{loop} \text{---} x_2 \end{array} + 5 \text{ perm} \right) + \frac{1}{2} \left(\begin{array}{c} x_3 \text{---} \text{loop} \text{---} x_1 \\ x_4 \text{---} \text{loop} \text{---} x_2 \end{array} + 5 \text{ perm} \right) \right\}. \quad (10.72)
\end{aligned}$$

We shall see later that this is a completely general law if the field theory is in the so-called *normal phase*. In that phase, the general connectedness structure is

$$G^{(4)}(x_1, \dots, x_n) = G_c^{(4)}(x_1, \dots, x_n) + [G_c^{(2)}(x_1, x_2) G_c^{(2)}(x_3, x_n) + 2 \text{ perm}]. \quad (10.73)$$

Note that the expansion (10.62) of $G^{(2)}$ is connected. This is a general feature for a system that is in the normal phase, which will be contrasted with the *condensed phase* in a separated study in Chapters 16, 17, and 18.

For the higher Green functions we expect more elaborate connectedness relations than (10.73) and an even more drastic reduction of labor using these relations when calculating all diagrams. The question arises as to the general composition law of n -point functions from connected subunits.

To gain a first idea what this law could be, consider the free theory. Its generating functional is [see (5.438)]

$$Z_0[j] = \exp \left\{ -\frac{1}{2} \int d^4x d^4y j(x) G_0(x, y) j(y) \right\}. \quad (10.74)$$

If expanded in powers of j , it gives the sum of all n -point functions of the free theory. In accordance with Wick's theorem all these free n -point functions are disconnected and consist of sums of products of free Green functions G_0 , which themselves are the only connected two-point diagrams of the theory. The important point is that the exponential tells us in which way the connected diagrams G_0 can be combined such as to form all diagrams.

This may best be visualized diagrammatically by expanding the exponential in (10.74) in a power series

$$\begin{aligned} \exp\left(-\frac{1}{2} \text{---}\bullet\text{---}\bullet\right) &= 1 - \frac{1}{2} \text{---}\bullet\text{---}\bullet + \frac{1}{4!} 3 \text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet \\ &\quad - \frac{1}{6!} 15 \text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet + \dots + \frac{1}{n!} (n-1)!! \text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet\text{---}\bullet. \end{aligned} \quad (10.75)$$

The numbers behind the factors $1/n!$ in the second line show how many combinations of $n/2$ powers of G_0 occur in Wick's expansion. To obtain these numbers we have rewritten the $(n/2)$ th coefficient $\frac{1}{(n/2)!}(1/2)^{n/2}$ as $\frac{1}{n!}(n-1)!!$. This establishes contact with the previous counting rules: The denominator $n!$ is factorized out since it is canceled when going to the n -point function (which involves n differentiations $\delta/\delta j$). This leaves $(n-1)!!$ diagrams in agreement with the result found earlier when counting the diagrams directly. Thus we have verified, in the free-field case, the simple rule for the reconstruction and proper counting of *all* n -point functions, given only the connected ones (of which in this case there is only one). By expanding the exponential of the connected diagrams, which is here $\exp\{-\frac{1}{2} \text{---}\bullet\text{---}\bullet\}$, we can read off *all* connected plus disconnected diagrams behind the factors $1/n!$. In this way, the exponential of the connected diagram yields all diagrams.

Does this simple statement also hold in the interacting case? Here the generating functional is given by

$$Z_0[j] = \exp\left\{i \int d^4x \mathcal{L}_{\text{int}}\left(\frac{\delta}{i\delta j}\right)\right\} \exp\left\{-\frac{1}{2} \int d^4x d^4y j(x) G_0(x, y) j(y)\right\}. \quad (10.76)$$

The interactions also enter exponentially. It is then suggestive that also here the sum of all Green functions can be obtained by exponentiating all connected ones. The proof will be given later after having developed more powerful formal techniques. Let us here state only the result which may be written as a relation

$$1 + \sum_{n=0, k=0}^{\infty} \frac{1}{n!k!} G_k^{(n)} = \exp\left\{\sum_{n=0, k=1}^{\infty} \frac{1}{n!k!} G_{ck}^{(n)}\right\}, \quad (10.77)$$

where $G_k^{(n)}$ are all diagrams and $G_{ck}^{(n)}$ all connected diagrams in k th-order perturbation theory. A similar relation holds separately for each number of external lines. This will be of great help when it comes to calculating physical scattering amplitudes and cross sections.

We may illustrate the relation (10.77) for the previously calculated diagrams with $n = 2$ and $n = 4$. The left-hand side of relation (10.77) looks as follows

$$\begin{aligned}
& 1 + \text{---} + 12 \text{---} \bigcirc \text{---} + \frac{1}{2} \left(144 \text{---} \bigcirc \bigcirc \text{---} + 144 \text{---} \bigcirc \bigcirc \text{---} + 96 \text{---} \bigcirc \text{---} \right) \\
& + \left(\text{---} \text{---} + 2 \text{perm} \right) + \left\{ \text{---} \times \text{---} + 12 \left(\text{---} \bigcirc \text{---} + 5 \text{perm} \right) \right\} \\
& + \frac{1}{4!} \left\{ 9612 \left(\text{---} \bigcirc \text{---} + 2 \text{perm} \right) + 9612 \left(\text{---} \bigcirc \times \text{---} + 2 \text{perm} \right) \right. \\
& + 3496 \left(\text{---} \bigcirc \bigcirc \text{---} + 2 \text{perm} \right) + 3496 \left(\text{---} \bigcirc \bigcirc \text{---} + 2 \text{perm} \right) \\
& \left. + 2304 \left(\text{---} \bigcirc \text{---} + 2 \text{perm} \right) + 3496 \left(\text{---} \bigcirc \bigcirc \text{---} + 5 \text{perm} \right) \right\}. \quad (10.78)
\end{aligned}$$

The right-hand side has the form

$$\begin{aligned}
& \exp \left\{ \text{---} + 12 \text{---} \bigcirc \text{---} + \text{---} \times \text{---} \right. \\
& + \frac{1}{2!} \left(144 \text{---} \bigcirc \bigcirc \text{---} + 144 \text{---} \bigcirc \bigcirc \text{---} + 96 \text{---} \bigcirc \text{---} \right) \\
& \left. + \frac{1}{4!} \left[9612 \left(\text{---} \bigcirc \text{---} + 2 \text{perm} \right) + 9612 \left(\text{---} \bigcirc \times \text{---} + 3 \text{perm} \right) + \dots \right] \right\}. \quad (10.79)
\end{aligned}$$

Indeed, by multiplying out the square in the last line we recover the correct sum of disconnected diagrams of the four-point function.

Also the vacuum diagrams satisfy the law of exponentiation: Up to the second order we have for all disconnected pieces

$$Z[0] = 1 + 3 \bigcirc \bigcirc + \frac{1}{2!} \left(9 \bigcirc \bigcirc \bigcirc \bigcirc + 24 \bigcirc \bigcirc + 72 \bigcirc \bigcirc \bigcirc \right) + \dots, \quad (10.80)$$

and see that this can be obtained as an exponential of the connected vacuum diagrams

$$Z[0] = \exp \left\{ 3 \bigcirc \bigcirc + \frac{1}{2!} \left(24 \bigcirc \bigcirc + 72 \bigcirc \bigcirc \bigcirc \right) + \dots \right\} \equiv e^{W[0]}. \quad (10.81)$$

This corresponds to equation (10.77) for $n = 0$:

$$1 + \sum_{k=0}^{\infty} \frac{1}{k!} G_k^{(0)} = \exp \left[\sum_{k=1}^{\infty} \frac{1}{k!} G_{ck}^{(0)} \right], \quad (10.82)$$

where $G_k^{(0)}$ collect all vacuum diagrams and $G_{ck}^{(0)}$ all connected ones in k th-order perturbation theory.

10.6.1 One-Particle Irreducible Graphs

The decomposition into connected diagrams does not yet exhaust the possibilities of reducing calculational labor. If we inspect the connected diagrams for two and four-point functions

$$\begin{aligned} G^{(2)}(x_1, x_2) = & \text{diagram of a line from } x_1 \text{ to } x_2 + 12 \text{diagram of a loop on a line from } x_1 \text{ to } x_2 + \\ & + \frac{1}{2!} \left(144 \cdot 2 \text{diagram of two loops on a line from } x_1 \text{ to } x_2 + 144 \cdot 2 \text{diagram of two loops on a line from } x_1 \text{ to } x_2 + 96 \cdot 2 \text{diagram of a bubble on a line from } x_1 \text{ to } x_2 \right) + \dots \end{aligned} \quad (10.83)$$

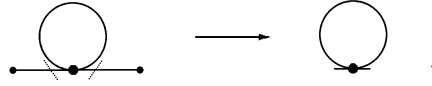
and

$$\begin{aligned} G^{(4)}(x_1, \dots, x_4) = & 4! \text{diagram of a central vertex connected to four external vertices } x_1, x_2, x_3, x_4 + \\ & + \frac{4!4!}{2!} \left\{ \left(\text{diagram of two vertices connected by two lines, each with two external legs} + 2 \text{ perm} \right) + \left(\text{diagram of a vertex with a loop and three external legs} + 3 \text{ perm} \right) \right\}, \end{aligned} \quad (10.84)$$

we discover that some of the diagrams contain a portion of others calculated at a lower order of perturbation theory in the same connected two-point functions $G_c^{(2)}$ or $G_c^{(4)}$. An example is the fourth diagram in $G_c^{(2)}$, which is a simple repetition of the second one. Similarly, the second diagram in $G_c^{(4)}$ is the composition of the first in $G_c^{(4)}$ with the second in $G_c^{(2)}$. It would be useful to find the rule according to which lower subdiagrams of $G_c^{(2)}$, $G_c^{(4)}$ reappear in higher ones of $G_c^{(2)}$ and $G_c^{(4)}$.

As far as $G_c^{(2)}$ is concerned, this rule turns out to be really simple: Let us characterize the repetition of a former subdiagram of $G_c^{(2)}$ topologically by noting that the diagram falls into two pieces by cutting one internal line. Such diagrams are called *one-particle reducible* (OPR); otherwise irreducible (OPI). Then the full connected two-point function $G_c^{(2)}$ may be composed from all OPI subdiagrams as follows: Consider the set of all OPI diagrams to the two-point function. They all carry a free Green function $G_0^{(2)}$ at the end of each leg which describes propagation of the particle up to the first interaction vertex. Cutting off these last Green functions

amounts diagrammatically to amputating the two legs of the diagram. The lowest order correction to the two-point function is amputated as follows:



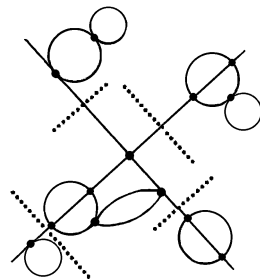
The two short little trunks indicate the places of amputation. Let $-i\Sigma$ be the sum of all these *amputated* OPI two-point functions. Then the geometric series

$$G_c^{(2)} = \frac{1}{G_0^{-1} + \Sigma} = G_0 + G_0(-i\Sigma)G_0 + G_0(-i\Sigma)G_0 + \dots \quad (10.85)$$

gives precisely the connected two-point function $G_c^{(2)}$. Thus the one-particle reducibility in the two-point function exhausts itself in a simple geometric series type of repetition of the irreducible pieces, each term in the string having the same factor. Also this result will be proved later in Chapter 13 when studying the general formal properties of perturbation theory.

The sum of all OPI connected two-point functions $-i\Sigma$ is usually referred to as self-energy.

Consider now the four-point function $G_c^{(4)}$. Here we recognize that any ornamentation of external legs can be taken care of by replacing the legs by the interacting two-point function. Thus we decide to introduce the concept of an arbitrary one-particle irreducible amputated Green function, shortly called the *vertex function* $\Gamma^{(n)}(x_1, \dots, x_n)$. For any connected n -point function, cut all simple lines such that the diagrams decompose. What remains are parts with two, four, or more trunks sticking out. The first set consists of the OPI self-energy diagrams discussed before. The others are called three-, four-, n -point vertex parts $\Gamma^{(n)}$, $n = 3, 4, \dots$. For example,



can be cut into four proper self-energy diagrams and one four-point vertex part. The sum of all composite diagrams obtained in this way composes the n -point vertex function denoted by a fat dot. The important reconstruction principle for all diagrams can now be stated as follows: The set of all connected diagrams in a four-point function is obtained by connecting all vertex functions in the four-point vertex function $G_c^{(4)}$ with the full connected Green function $G_c^{(2)}$ at each truncated leg. Analytically, this amounts to the formula (valid in normal systems)

There is an overall $(2\pi)^4 \delta^{(4)}$ -function which ensures the conservation of four-momenta. This is a consequence of the translational invariance of $G_0(x_1, x_2) = G_0(x_1 - x_2)$. The same factor appears in the Fourier transform of all interacting n -point functions since $G^{(n)}(x_1, \dots, x_n)$ depends only on the differences between the coordinates

$$G^{(n)}(x_1, \dots, x_n) = G^{(n)}(x_1 - x_n, x_2 - x_n, \dots, x_{n-1} - x_n, 0) \quad (10.91)$$

such that we can write

$$\begin{aligned} & \int d^4x_1 \dots d^4x_n e^{i\sum_{i=1}^n q_i x_i} G^{(n)}(x_1, \dots, x_n) \\ &= \int d^4(x_1 - x_n) \dots d^4(x_{n-1} - x_n) e^{i\sum_{i=1}^{n-1} q_i (x_i - x_n)} \left(\int d^4x_n e^{i\sum_{i=1}^n q_i x_n} \right) \\ & \quad \times G^{(n)}(x_1 - x_n, x_2 - x_n, \dots, x_{n-1} - x_n, 0). \end{aligned} \quad (10.92)$$

Thus we may define the Fourier transform of an n -point function directly without the factor of momentum conservation as

$$(2\pi)^4 \delta^{(4)}(q_1 + \dots + q_n) G^{(n)}(q_1, \dots, q_n) \equiv \int d^4x_1 \dots d^4x_n e^{i\sum_{i=1}^n q_i x_i} G^{(n)}(x_1, \dots, x_n). \quad (10.93)$$

Consider now the vacuum diagrams evaluated via the Fourier transforms. To first order we have

$$3 \text{ (two circles connected at two points)} = -3i \frac{g}{4!} \int d^4z G^2(z, z) = -3i \frac{g}{4!} \int d^4z \left[\int \frac{d^4q}{(2\pi)^4} \frac{i}{q^2 - m^2} \right]^2. \quad (10.94)$$

The integral over z can be defined meaningfully only if the system is enclosed in a finite box of volume V and studied in a finite time interval T . Then the integral $\int d^4z$ gives a factor VT . This would become infinite for large VT which is called the *thermodynamic limit*.

Even if VT is finite, there is still a divergence coming from the integral over the momenta p at large p . This is called an *ultraviolet divergence*. It reflects the singularity of $G_0(x_1, x_2)$ for $x_1 \rightarrow x_2$ (a so-called *short-distance singularity*). It will be the subject of the next chapter to show how to deal with this type of divergence. For $\bar{G}^{(2)}(x_1, x_2)$, the diagram of first order in g is

$$12 \text{ (circle with two external lines)} = -12i \frac{g}{4!} \int dz G(x_1, z) G(z, z) G(z, x_2). \quad (10.95)$$

Going to the Fourier transform this gives

$$\int \frac{d^4q}{(2\pi)^4} e^{-iq(x_1 - x_2)} \frac{i}{q^2 - m^2} \left(\int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2 - m^2} \right) \frac{i}{q^2 - m^2}, \quad (10.96)$$

which amounts to a contribution to the Fourier-transformed Green function:

$$\bar{G}^{(2)}(q) = -i \frac{g}{4!} 12 \frac{i}{q^2 - m^2} \int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2 - m^2} \frac{i}{q^2 - m^2}. \quad (10.97)$$

As another example take

$$\begin{array}{c} k+q_1+q_2 \\ q_4 \quad q_2 \\ \diagdown \quad \diagup \\ \text{---} \text{---} \text{---} \\ \diagup \quad \diagdown \\ q_3 \quad q_1 \\ k_2 \end{array} = \left(-\frac{ig}{4!}\right)^2 \int \bar{d}^4 k \frac{i}{k^2 - m^2 + i\eta} \frac{i}{(k+q_1+q_2)^2 - m^2 + i\eta} . \quad (10.98)$$

It is easy to see that the following rules hold for the translation of the spacetime diagrams to the analytic expression for the Fourier transformed Green function:

1. With each line associate a momentum label q and specify its direction of flow. Such a line represents a Fourier-transformed two-point function $G_0(q)$ pictured by

$$\text{---} = G_0(q) = \frac{i}{q^2 - m^2} . \quad (10.99)$$

The arrow has been omitted since its direction is irrelevant on account of the symmetry of $G_0(q)$ under $q \rightarrow -q$.

2. Each vertex



is associated with an amplitude

$$-i \frac{g}{4!} (2\pi)^4 \delta^{(4)}(q_1 + q_2 + q_3 + q_4) \frac{i}{q_4^2 - m^2} \frac{i}{q_3^2 - m^2} \frac{i}{q_2^2 - m^2} \frac{i}{q_1^2 - m^2}$$

containing a four-momentum conserving $(2\pi)^4 \delta^{(4)}$ -function for the incoming momenta. This is a consequence of the integration over z in the interaction.

3. We now distinguish external and internal lines, the latter connecting pairs of vertices with each other. We also call the corresponding momenta q_i external and internal, respectively. Then for every internal line, we integrate over all internal four momenta with the invariant measure $\int d^4 q_i / (2\pi)^4$. At the end we remove the associated overall δ -function of energy-momentum conservation.

Obviously, each $(2\pi)^4 \delta^{(4)}$ -function on the vertices cancels one internal momentum integral $\int d^4 p / (2\pi)^4$. Thus in a diagram of n th order with I internal lines, only $I - n$ internal integrations remain. These are referred to as *loop integrals*.

In general, loop integrations diverge at large loop momenta, the so-called *ultra-violet regime*. We shall learn in the next chapter how to deal with such divergent momentum space integrals.

10.7 Green Functions and Scattering Amplitudes

The Green functions carry all informations contained in the theory. In particular they can be used to extract scattering amplitudes. For definiteness, let us discuss

here the simplest and most important case of the elastic scattering among two particles. The free initial state that exists long before the interaction takes place is

$$|\psi_{\text{in}}\rangle = a_{\mathbf{q}_2}^\dagger a_{\mathbf{q}_1}^\dagger |0\rangle. \quad (10.100)$$

Long after the interaction, the state is given by

$$U_I^\eta(\infty, -\infty) a_{\mathbf{q}_2}^\dagger a_{\mathbf{q}_1}^\dagger |0\rangle. \quad (10.101)$$

If we analyze this state with respect to its free-particle content we find the amplitude

$$\langle 0 | a_{\mathbf{q}_4} a_{\mathbf{q}_3} U_I^\eta(\infty, -\infty) a_{\mathbf{q}_2}^\dagger a_{\mathbf{q}_1}^\dagger | 0 \rangle = \langle 0 | a_{\mathbf{q}_4} a_{\mathbf{q}_3} S^\eta a_{\mathbf{q}_2} a_{\mathbf{q}_1} | 0 \rangle. \quad (10.102)$$

We shall soon observe that this amplitude has a divergent phase arising in the limit of the switching parameter η tending to zero. It is caused by the same vacuum diagrams as before in the corresponding Green function. In order to obtain a well-defined $\eta \rightarrow 0$ -limit we define the 2×2 scattering amplitude as the ratio

$$S(\mathbf{q}_4, \mathbf{q}_3 | \mathbf{q}_1, \mathbf{q}_2) \equiv \frac{S_N(\mathbf{q}_4, \mathbf{q}_3 | \mathbf{q}_1, \mathbf{q}_2)}{Z[0]}, \quad (10.103)$$

with the numerator

$$S_N(\mathbf{q}_4, \mathbf{q}_3 | \mathbf{q}_1, \mathbf{q}_2) \equiv \langle 0 | a_{\mathbf{q}_4} a_{\mathbf{q}_3} T e^{-i \int_{-\infty}^{\infty} dt V_I(t)} a_{\mathbf{q}_2}^\dagger a_{\mathbf{q}_1}^\dagger | 0 \rangle, \quad (10.104)$$

and the denominator

$$Z[0] \equiv \langle 0 | e^{-i \int_{-\infty}^{\infty} dt V_I(t)} | 0 \rangle. \quad (10.105)$$

We shall often use the four-momentum notation $S(q_4, q_3 | q_1, q_2)$ for $S(\mathbf{q}_4, \mathbf{q}_3 | \mathbf{q}_1, \mathbf{q}_2)$ with the tacit understanding that, in the S -matrix, the energies are always on the mass shells $q^0 = \sqrt{\mathbf{q}^2 + m^2}$.

It is now easy to see how these amplitudes can be extracted from the Green functions calculated in the last section. There exists a mathematical framework to do this known as the *Lehmann-Symanzik-Zimmermann formalism* (LSZ-reduction formulas) [11]. Rather than presenting this we sketch here a simple pedestrian approach to obtain the same results.

We begin with the observation that if the energies q^0 on the mass shells of the particles, i.e., if $q^0 = \omega_{\mathbf{q}} = \sqrt{\mathbf{p}^2 + M^2}$, the particle operators $a_{\mathbf{q}}, a_{\mathbf{q}}^\dagger$ can be written as the large-time limits

$$a_{\mathbf{q}} = \lim_{x^0 \rightarrow -\infty} \sqrt{\frac{2q^0}{V}} \int d^3x e^{i(q^0 x^0 - \mathbf{q}\mathbf{x})} \phi(x), \quad (10.106)$$

$$a_{\mathbf{q}}^\dagger = \lim_{x^0 \rightarrow \infty} \sqrt{\frac{2q^0}{V}} \int d^3x e^{-i(q^0 x^0 - \mathbf{q}\mathbf{x})} \phi(x). \quad (10.107)$$

The limits have the important effect of eliminating undesired frequency contents in $\phi(x)$. Indeed, if we expand the field into creation and annihilation operators, we see that the right-hand side of Eq. (10.106) becomes

$$\begin{aligned} \lim_{x^0 \rightarrow -\infty} \sqrt{\frac{2q_0}{V}} \int d^3x e^{i(q^0 x^0 - \mathbf{q}\mathbf{x})} \sum_{\mathbf{q}} \frac{1}{\sqrt{2p^0 V}} (e^{-ipx} a_{\mathbf{p}} + \text{c.c.}) \\ = \lim_{x^0 \rightarrow -\infty} \sum_{\mathbf{p}} \delta_{\mathbf{p}, \mathbf{q}} [e^{i(q^0 - p^0)x^0} a_{\mathbf{p}} + e^{i(q^0 + p^0)x^0} a_{\mathbf{p}}^\dagger]. \end{aligned} \quad (10.108)$$

The spatial δ -function enforces $\mathbf{q} = \mathbf{p}$ and thus $q^0 = p^0$, so that the right-hand side becomes

$$a_{\mathbf{q}} + \lim_{x^0 \rightarrow -\infty} e^{i2q^0 x^0} a_{\mathbf{q}}^\dagger. \quad (10.109)$$

In the limit $x^0 \rightarrow -\infty$, the second exponential function oscillates rapidly with diverging frequency. Such an oscillating expression can be set equal to zero. The reason why this makes sense uses the fact that no physical state is completely sharp in momentum space but contains some, possibly very narrow, distribution function $f(\mathbf{q} - \mathbf{q}')$ in the momenta. Thus, instead of $a_{\mathbf{q}}$, we really deal with a packet state

$$\int \frac{d^3q'}{(2\pi)^3} f(\mathbf{q} - \mathbf{q}') a_{\mathbf{q}'},$$

with $f(\mathbf{q} - \mathbf{q}')$ sharply peaked around $\mathbf{q}$. Then Eq. (10.114) has to be smeared out with such a would-be δ -function, and the second term in (10.109) becomes

$$\lim_{x^0 \rightarrow -\infty} \int \frac{d^3q'}{(2\pi)^3} e^{i2q'^0 x^0} f(\mathbf{q} - \mathbf{q}') a_{\mathbf{q}'}^\dagger \rightarrow 0. \quad (10.110)$$

The vanishing of this in the limit $x^0 \rightarrow -\infty$ is a well-known consequence of the Riemann-Lebesgue Lemma (recall the remarks on p. 262). The other equation (10.107) is proved similarly.

We can now make use of formula (10.107), replace the operators $a_{\mathbf{q}}, a_{\mathbf{q}}^\dagger$ by time-ordered fields $\phi(x)$ and obtain, for the numerator part of the S matrix elements in Eq. (10.104), the following expression:

$$\begin{aligned} S_N(\mathbf{q}_4 \mathbf{q}_3 | \mathbf{q}_2 \mathbf{q}_1) = \frac{\sqrt{2^4 q_1^0 q_2^0 q_3^0 q_4^0}}{V^2} \lim_{\substack{x_1^0 > x_2^0 \rightarrow \infty \\ x_4^0 < x_3^0 \rightarrow -\infty}} e^{i[q_4^0 x_4^0 - \mathbf{q}_4 \mathbf{x}_4 + q_3^0 x_3^0 - \mathbf{q}_3 \mathbf{x}_3 - q_2^0 x_2^0 + \mathbf{q}_2 \mathbf{x}_2 - q_1^0 x_1^0 + \mathbf{q}_1 \mathbf{x}_1]} \\ \times \langle 0 | T \phi(x_4) \phi(x_3) S \phi(x_2) \phi(x_1) | 0 \rangle. \end{aligned} \quad (10.111)$$

The last factor is precisely the four-point function $G^{(4)}(x_4, x_3, x_2, x_1)$.

This formula looks somewhat cumbersome to implement in an actual calculation of the scattering amplitudes and it is useful to simplify it by evaluating the infinite-time limits more explicitly. We observe that the perturbation series for

$G^{(n)}(x_n, \dots, x_1)$ consists of sums of products of free two-point functions G_0 which contain, for each spacetime argument $x_1, x_2, \dots, x_n$ in $G^{(n)}$, a two-point function G_0 whose line ends at that point. Consider, for example, the point x_1 , and an associated Green function $G_0(z_1, x_1)$. The operation (10.108) at this point corresponds to taking the limit

$$\sqrt{\frac{2q_1^0}{V}} \lim_{x_1^0 \rightarrow -\infty} \int d^3x_1 e^{-i(q_1^0 x_1^0 - \mathbf{q}_1 \mathbf{x}_1)} \int \frac{d^4q}{(2\pi)^4} e^{-iq(z-x_1)} \frac{i}{q^2 - m^2 + i\eta}. \quad (10.112)$$

The spatial integral over $\mathbf{x}_1$ enforces $\mathbf{q} = \mathbf{q}_1$. The remaining integral over dq^0 can be done via Cauchy's residue theorem. Since $x_1^0 \rightarrow -\infty$, the contour of integration may be closed in the lower half of the complex q^0 -plane, where it contains only a pole at $q^0 = \omega_{\mathbf{q}_1} = \sqrt{\mathbf{q}_1^2 + m^2} - i\eta$. Thus the integral over q^0 can be done trivially, and we find, that the limit (10.111) has the effect of replacing, in the Green function $G(z, x_1)$ of the external leg, the amplitude by

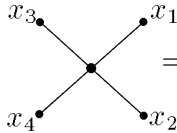
$$G(z, x_1) \longrightarrow \frac{1}{\sqrt{2q_1^0 V}} e^{-iq_1 z}, \quad (10.113)$$

with q_1^0 on the mass shell $q_1^0 = \sqrt{\mathbf{q}_1^2 + m^2}$. The right-hand side is simply the wave function $e^{-iq_1 z} / \sqrt{2q_1^0 V}$ of the incoming particle with the argument z of the nearest vertex in the Feynman diagram.

Similarly, we obtain for an outgoing particle of momentum q_3 the replacement

$$G(x_3, z) \longrightarrow \frac{1}{\sqrt{2q_3^0 V}} e^{iq_3 z}. \quad (10.114)$$

As a specific example, consider the simple vertex diagram in (10.84):



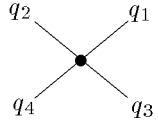
$$= -ig \int d^4z \ G(x_4, z) G(x_3, z) G(z, x_2) G(z, x_1). \quad (10.115)$$

Taking the limits in (10.111) this becomes

$$\begin{aligned} & \prod_{i=1}^4 \left(\frac{1}{\sqrt{2Vq_i^0}} \right) (-ig) \int d^4z \ e^{i(q_4 z + q_3 z - q_1 z - q_2 z)} \\ &= -ig \prod_{i=1}^4 \left(\frac{1}{\sqrt{2Vq_i^0}} \right) (2\pi)^4 \delta^{(4)}(q_4 + q_3 - q_2 - q_1). \end{aligned} \quad (10.116)$$

Thus, up to a factor $1/\sqrt{2Vq_i^0}$ for each particle, we remain precisely with the vertex contribution in momentum space, including the total four-momentum conservation factor.

In momentum space, the Feynman diagram (10.115) reads



$$= -ig \frac{i}{q_4^2 - m^2} \frac{i}{q_3^2 - m^2} \frac{i}{q_2^2 - m^2} \frac{i}{q_1^2 - m^2} .$$

Thus, the replacement of the four external lines by external physical states of momenta q_i corresponds to dropping the factors

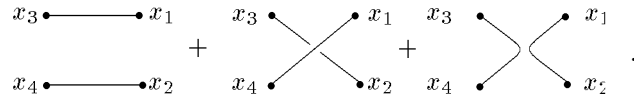
$$\frac{i}{q_i^2 - m^2}, \quad (10.117)$$

and replacing them by

$$\frac{1}{\sqrt{2Vq_i^0}}. \quad (10.118)$$

This corresponds to the amputation of the Feynman diagram for the four-point function introduced earlier when defining the vertex functions.

How about the disconnected diagrams in (10.70)? Consider first the three diagrams containing two disconnected lines



$$+ \quad + \quad +$$

In each of the diagrams we have to do the operations of the type (10.100). Take the first diagram and consider $G_0(x_3, x_1)$. It contributes a factor

$$\sqrt{\frac{2q_3^0}{V}} \sqrt{\frac{2q_1^0}{V}} \lim_{\substack{x_3^0 \rightarrow \infty \\ x_1^0 \rightarrow -\infty}} \int d^3x_3 d^3x_1 e^{i(q_3^0 x_3^0 - \mathbf{q}_3 \cdot \mathbf{x}_3 - q_1^0 x_1^0 + \mathbf{q}_1 \cdot \mathbf{x}_1)} G(x_3, x_1). \quad (10.119)$$

Performing the first limit $x_1 \rightarrow -\infty$ we get

$$\sqrt{\frac{2q_3^0}{V}} \lim_{x_3^0 \rightarrow \infty} \int d^3x_3 e^{iq_3 x_3} e^{-iq_1 x_3} \frac{1}{\sqrt{2q_1^0 V}} = \lim_{x_3^0 \rightarrow \infty} e^{i(q_3^0 - q_1^0)x_3^0} \delta_{\mathbf{q}_3 \mathbf{q}_1} = \delta_{\mathbf{q}_3 \mathbf{q}_1}. \quad (10.120)$$

This is just the amplitude for the particle 1 running to the final state 2 without interaction:

$$\langle \mathbf{q}_3 | \mathbf{q}_1 \rangle = \langle 0 | a_{\mathbf{q}_3} a_{\mathbf{q}_1}^\dagger | 0 \rangle = \delta_{\mathbf{q}_3, \mathbf{q}_1} \quad (10.121)$$

The same factor appears for the lower line of the diagram

$$\langle \mathbf{q}_4 | \mathbf{q}_2 \rangle. \quad (10.122)$$

Thus the first of the above three diagrams corresponds to the S -matrix element

$$\delta_{\mathbf{q}_3 \mathbf{q}_1} \delta_{\mathbf{q}_2 \mathbf{q}_4}. \quad (10.123)$$

The second diagram results in the same product of δ -functions, except that $\mathbf{q}_3$ and $\mathbf{q}_4$ are interchanged. The third diagram is different. Here the Fourier limit to be done is

$$\sqrt{\frac{2q_1^0}{V}} \sqrt{\frac{2q_2^0}{V}} \lim_{t_1 < t_2 \rightarrow -\infty} \int d^3x_1 d^4x_2^3 e^{-i(q_2^0 x_2^0 - \mathbf{q}_2 \mathbf{x}_2 - q_1^0 x_1^0 + \mathbf{q}_1 \mathbf{x}_1)} G(x_2, x_1). \quad (10.124)$$

The first limit on x_1 leads to

$$\sqrt{\frac{2q_2^0}{V}} \lim_{t_2 \rightarrow -\infty} \int d^3x_2 e^{-iq_2 x_2 - iq_1 x_2} \frac{1}{\sqrt{2q_1^0 V}}, \quad (10.125)$$

and the integration gives

$$\lim_{x_2 \rightarrow -\infty} e^{-i(q_2^0 + q_1^0)x_2^0} \delta_{\mathbf{q}_2, -\mathbf{q}_1}. \quad (10.126)$$

The limit $x_0 \rightarrow -\infty$ of the exponential oscillates infinitely rapid, so that the result vanishes for the same reasons as before.

Let us now look at the diagrams

$$12 \left(\begin{array}{c} \text{diagram with loop} \\ x_3 \text{---} \bullet \text{---} x_1 \\ x_4 \text{---} \bullet \text{---} x_2 \end{array} + 5 \text{ perm} \right) \quad (10.127)$$

contained in the set (10.70). From the lowest line, this obviously contains a factor

$$\langle \mathbf{q}_4 | \mathbf{q}_2 \rangle = \delta_{\mathbf{q}_4 \mathbf{q}_2}, \quad (10.128)$$

just as in (10.120). The upper line corresponds to the integral

$$12 \left(-\frac{ig}{4!} \right) \int d^4z \ G(x_3, z) G(z, z) G(z, x_1). \quad (10.129)$$

Adding this to the line without the loop correction leads to the one-loop corrected Green function

$$G_R(x_3, x_1) = 12 \left(-\frac{ig}{4!} \right) \int d^4z \ G(x_3, z) G(z, z) G(z, x_1). \quad (10.130)$$

The Fourier representation of the free Green function $i/(q^2 - m^2)$ is replaced by

$$\frac{i}{q^2 - m^2} \rightarrow \frac{i}{q^2 - m^2} - i \frac{g}{2} \int \frac{d^4q'}{(2\pi)^4} \frac{i}{q'^2 - m^2} \left[\frac{i}{q^2 - m^2} \right]^2. \quad (10.131)$$

This may be viewed as the first-order corrected Fourier transform of the renormalized propagator

$$G_R(x_2, x_1) = \int \frac{d^4q}{(2\pi)^4} e^{-iq(x_2 - x_1)} \frac{i}{q^2 - m^2 - \delta m^2} \quad (10.132)$$

with a mass shift

$$\delta m^2 = \frac{g}{2} \int \frac{d^4 q}{(2\pi)^4} \frac{i}{q^2 - m^2}. \quad (10.133)$$

The scattering amplitude is extracted from the amplitude with the renormalized Green function as before, the only difference being that the factor (10.118) contains now q_i^0 with the renormalized masses.

A similar mass shift occurs in the diagrams

$$\frac{4! 4!}{2!} \left(\begin{array}{c} x_3 \quad \bullet \quad x_1 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ x_4 \quad \bullet \quad x_2 \end{array} + 3 \text{ perm} \right) \quad (10.134)$$

contained in the set (10.70). The remaining diagrams of (10.70) account for the second-order mass shifts.

To study such mass shifts in general we make use of the Gell-Mann–Low formula for the energy shift [5, 6]. For the vacuum, the energy shifts by ΔE_0 can be taken from the matrix element

$$e^{-i\Delta E_0(t_2-t_1)} = \langle 0 | U_I^\eta(t_2, t_1) | 0 \rangle \quad (10.135)$$

by going to the limit $t_2 \rightarrow \infty$, $t_1 \rightarrow -\infty$. Consider now the single-particle state $a_{\mathbf{q}}^\dagger | 0 \rangle$. If the interaction is applied for $t_1 \rightarrow -\infty$ and $t_2 \rightarrow \infty$, the state

$$U_I^\eta(t_2, t_1) a_{\mathbf{q}}^\dagger | 0 \rangle \quad (10.136)$$

will be again a solution of the free Hamiltonian. Because of energy and momentum conservation, it must be equal to $a_{\mathbf{q}}^\dagger | 0 \rangle$ up to a phase which, due to (10.135), contains the information on the energy shift of this state. It consists of ΔE_0 for the vacuum plus $\Delta E_{\mathbf{q}}$ for the particle. Collecting both together, we may write

$$e^{-\Delta E(t_1-t_0)} \underset{t_1 \rightarrow \infty, t_2 \rightarrow -\infty}{=} \frac{\langle 0 | a_{\mathbf{q}} U_I^\eta(t_2, t_1) a_{\mathbf{q}}^\dagger | 0 \rangle}{\langle 0 | U_I^\eta(t_2, t_1) | 0 \rangle}. \quad (10.137)$$

Expanding U_I^η in powers of g , the lowest diagrams on the right-hand side are precisely the diagrams that appeared before:

$$G^{(2)}(x_1, x_2) = \overline{x_1 x_2} + 12 \overline{x_1 \bigcirc x_2} + \dots$$

Indeed, we find from (10.137) with $t_1 - t_0 = T$:

$$\begin{aligned} 1 - i\Delta E T &= 1 + 12 \left(\frac{-ig}{4!} \right) \frac{1}{2q^0 V} \int d^4 z \ G(z, z) \\ &= 1 - \frac{i}{2} g \frac{T}{2q^0} \int \frac{d^4 q}{(2\pi)^4} \frac{i}{q^2 - m^2}. \end{aligned} \quad (10.138)$$

Similarly, we may use formulas (10.106), (10.107), and the energy shifts $q^0 \rightarrow q^0 + \Delta E = q_R^0$, to write

$$a_{\mathbf{q}}^\dagger = \lim_{x^0 \rightarrow -\infty} \sqrt{\frac{2q_R^0}{V}} \int d^3x e^{i(q_R^0 x^0 - \mathbf{q}\mathbf{x})} \phi(x), \quad (10.139)$$

$$a_{\mathbf{q}} = \lim_{x^0 \rightarrow \infty} \sqrt{\frac{2q_R^0}{V}} \int d^3x e^{-i(q_R^0 x^0 - \mathbf{q}\mathbf{x})} \phi(x). \quad (10.140)$$

Now every particle line automatically receives a factor $e^{i\Delta E_q T}$, which removes precisely the phase factor (10.135).

To higher orders in g , it is somewhat hard to proceed in this fashion. The problem will be solved in the next section with more elegance.

Note that formula (10.137) allows us to evaluate the shift in the particle mass in another way. If $q^0 = \sqrt{\mathbf{q}^2 + m^2}$ is the energy before turning on the interaction, then

$$q^0 + \Delta E = \sqrt{\mathbf{q}^2 + m^2 + \delta m^2} = q^0 + \frac{\delta m^2}{2q^0} \quad (10.141)$$

is the energy afterwards, and we find once more the mass shift (10.133).

10.8 Wick Rules for Scattering Amplitudes

The possibility of obtaining external particle states from fields with the help of temporal limiting procedures of the type (10.107) allows us to incorporate the creation and annihilation operators of these particles into the general framework of Wick's contraction rules. Confronted with the numerator of the perturbative scattering amplitude in (10.103),

$$S_N(\mathbf{q}_4 \mathbf{q}_3 | \mathbf{q}_1 \mathbf{q}_2) \equiv \langle 0 | a_{\mathbf{q}_4} a_{\mathbf{q}_3} T e^{-i \int_{-\infty}^{\infty} dt V_I(t)} a_{\mathbf{q}_2}^\dagger a_{\mathbf{q}_1}^\dagger | 0 \rangle, \quad (10.142)$$

we may imagine the incoming particle operators on the one side to carry negative infinite time arguments, and the outgoing ones on the other side to carry positive infinite times. Then they can be brought inside the parentheses of the time-ordering operator. This, in turn, can be evaluated as usual via Wick contractions.

The results of the last section show that the Wick contractions leading to an external particles are

$$\overline{\phi(x)} a_{\mathbf{p}}^\dagger = [\overline{\phi(x)}, a_{\mathbf{p}}^\dagger] = \frac{1}{\sqrt{2V\omega_{\mathbf{p}}}} e^{-iqx}, \quad (10.143)$$

$$a_{\mathbf{p}} \overline{\phi(x)} = [a_{\mathbf{p}}, \overline{\phi(x)}] = \frac{1}{\sqrt{2V\omega_{\mathbf{p}}}} e^{-iqx}, \quad (10.144)$$

where $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$.

For Dirac particles, there are the corresponding contraction rules

$$\overline{\psi(x)a_{\mathbf{p},s_3}^\dagger} = \{\overline{\phi(x)}, a_{\mathbf{p}}^\dagger\} = \frac{1}{\sqrt{V E_{\mathbf{p}}}} u(\mathbf{p}, \mathbf{s}_3) e^{-ipx}, \quad (10.145)$$

$$\overline{a_{\mathbf{p},s_3}\psi(x)} = \{\overline{a_{\mathbf{p},s_3}}, \psi(x)\} = \frac{1}{\sqrt{V E_{\mathbf{p}}}} e^{ipx} \bar{u}(\mathbf{p}, \mathbf{s}_3), \quad (10.146)$$

and for antiparticles:

$$\overline{\psi(x)b_{\mathbf{p},s_3}^\dagger} = \{\overline{\phi(x)}, b_{\mathbf{p}}^\dagger\} = \frac{1}{\sqrt{V E_{\mathbf{p}}}} e^{-ipx} \bar{v}(\mathbf{p}, \mathbf{s}_3), \quad (10.147)$$

$$\overline{b_{\mathbf{p},s_3}\psi(x)} = \{\overline{a_{\mathbf{p},s_3}}, \psi(x)\} = \frac{1}{\sqrt{V E_{\mathbf{p}}}} v(\mathbf{p}, \mathbf{s}_3) e^{ipx}, \quad (10.148)$$

where $E_{\mathbf{p}} \equiv \sqrt{\mathbf{p}^2 + M^2}$.

10.9 Thermal Perturbation Theory

Since Wick's theorem was valid for thermal Green functions, we expect all perturbation expansions to have a simple generalization to the thermal case. Let us define a thermal Heisenberg picture for operators by

$$O_H(\tau) = e^{H\tau/\hbar} O_S e^{-H\tau/\hbar}, \quad (10.149)$$

and an interaction picture which moves according to the free equations of motion,

$$O_I(\tau) = e^{H_0 G \tau/\hbar} O_S e^{-H_0 G \tau/\hbar}. \quad (10.150)$$

Thus, a Heisenberg operator can be transformed to the free operator via

$$O_H(\tau) = U_I(0, \tau) O_I(\tau) U_I(\tau, 0) \quad (10.151)$$

where

$$U_I(\tau_2, \tau_1) = e^{H_0 G \tau_2/\hbar} e^{-H_G(\tau_2 - \tau_1)} e^{-H_0 G \tau_1/\hbar} \quad (10.152)$$

is the time displacement operator along the euclidean time axis τ . Therefore it has the same factorization property as the quantum mechanical operator $U_I(t_2, t_1)$ in Eq. (9.17):

$$U_I(\tau_3, \tau_2) U_I(\tau_2, \tau_1) = U_I(\tau_3, \tau_1). \quad (10.153)$$

Certainly

$$U_I(\tau_1, \tau_1) = 1. \quad (10.154)$$

However, in contrast to $U_I(t_2, t_1)$, this operator does *not* satisfy the unitarity relation (9.26), but instead:

$$U_I(\tau_2, \tau_1)^\dagger = U_I(-\tau_1, -\tau_2). \quad (10.155)$$

It obeys the following equation of motion

$$\begin{aligned} \hbar \partial_\tau U_I(\tau, \tau') &= e^{H_0 \tau / \hbar} (H_{0G} - H_G) e^{-H_G(\tau - \tau') / \hbar} e^{-H_0 G \tau' / \hbar} \\ &= -V_I(\tau) U_I(\tau, \tau'), \end{aligned} \quad (10.156)$$

where $V_I(\tau)$ is the time-dependent thermal interaction picture of the time independent Schrödinger perturbation $V = V_S$

$$V_I(\tau) = e^{H_0 G \tau / \hbar} V e^{-H_0 G \tau / \hbar}. \quad (10.157)$$

Therefore we can solve (10.156) for $U_I(\tau, \tau')$ using the standard exponential Neumann-Liouville expansion (9.19), now time-ordered with respect to the euclidean time τ :

$$\begin{aligned} U_I(\tau, \tau') &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \dots \int_{\tau'}^{\tau} d\tau_n T_T [V_I(\tau_1) \dots V_I(\tau_n)] \\ &= T_\tau e^{-\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau'' V_I(\tau'')}. \end{aligned} \quad (10.158)$$

By construction, $U_I(\tau, 0)$ satisfies the relation

$$e^{-H_G \tau / \hbar} = e^{-H_0 \tau / \hbar} U_I(\tau, 0). \quad (10.159)$$

Thus, using the thermal value for the imaginary time $\tau / \hbar = 1/k_B T \equiv \beta$, we obtain directly a perturbation expansion of the partition function

$$\begin{aligned} Z &= \text{Tr} (e^{-\beta H_G}) = \text{Tr} [e^{-\beta H_0 G} U_I(\beta, 0)] \\ &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n \text{Tr} [e^{-\beta H_0 G} T_\tau (V_I(\tau_1) \dots V_I(\tau_n))]. \end{aligned} \quad (10.160)$$

Consider now a thermal two-body Green function in the presence of interaction, defined for $\tau > \tau'$ as follows:

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &\equiv \text{Tr} [e^{-\beta H_G} \psi(\mathbf{x}, \tau) \psi^\dagger(\mathbf{x}', \tau')] / \text{Tr} (e^{-\beta H_G}) \\ &= \text{Tr} [e^{-\beta H_0 G} U_I(\beta, 0) U_I(0, \tau) \psi_I(\mathbf{x}, \tau) U_I(\tau, 0) \\ &\quad \times U_I(0, \tau') \psi_I^\dagger(\mathbf{x}', \tau') U_I(\tau', 0)] / \text{Tr} [e^{-\beta H_0 G} U_I(\beta, 0)]. \end{aligned} \quad (10.161)$$

For $\tau < \tau'$, on the other hand, we have

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &\equiv \pm \text{Tr} \left[e^{-\beta H_G} \psi^\dagger(\mathbf{x}', \tau') \psi(\mathbf{x}, \tau) \right] / \text{Tr} \left(e^{-\beta H_G} \right) \\ &= \text{Tr} \left[e^{-\beta H_0 G} U_I(0, \tau') \psi_I^\dagger(\mathbf{x}', \tau') U_I(\tau', 0) \right. \\ &\quad \left. \times U_I(0, \tau) \psi_I(\mathbf{x}, \tau) U_I(\tau, 0) \right] / \text{Tr} \left[e^{-\beta H_0 G} U_I(\beta, 0) \right]. \end{aligned} \quad (10.162)$$

Both equations may be combined in the single formula

$$G(\mathbf{x}, \tau; \mathbf{x}', \tau') = \text{Tr} \left[e^{-\beta H_0 G} T_\tau U_I(\beta, 0) \psi(\mathbf{x}, \tau) \psi^\dagger(\mathbf{x}', \tau') \right] / \text{Tr} \left[e^{-\beta H_0 G} U_I(\beta, 0) \right]. \quad (10.163)$$

In comparison with the field theoretic formulas (10.9) and (10.12), the vacuum expectation values are replaced by the Boltzmann-weighted thermal traces, and the vacuum expectation value of the S matrix operator $U_I(\infty, -\infty)$ in the denominators is replaced by the Boltzmann-weighted trace of the interaction operator $U_I(\hbar/k_B T, 0)$ along the euclidean time axis τ .

Note that the denominator ensures the existence of the zero temperature limit in just the same way as the phase factor did in the switching-on limit $\eta \rightarrow 0$. In fact, the grand canonical partition function in the denominator may be written as

$$Z_G = e^{\beta \Omega} = \sum_n e^{-(\beta E_n - \mu N_n)}, \quad (10.164)$$

such that the limit $T \rightarrow 0$ renders a pure exponential with the ground state energy

$$Z_G \xrightarrow{T \rightarrow 0} e^{-\beta(E_0 - \mu N_0)} \rightarrow e^{\pm \infty}. \quad (10.165)$$

This is the analogue of the infinite phase factor for the field theoretic denominator in Eq. (10.9).

Let us now expand the interaction operator $U_I(\hbar/k_B T, 0)$ in powers of the interaction, just as before in real time. This leads to a series of thermally averaged products of many fields $\psi_I(\mathbf{x}, \tau)$ which move according to the free field equations. Therefore Wick's theorem can be applied and we obtain an expansion of $G(\mathbf{x}, \tau; \mathbf{x}', \tau')$ completely analogous to the field theoretic one. The only difference is the finite-time interaction. When going to Fourier transformed space, the finite euclidean time interval is fully taken into account by the sum over the discrete imaginary Matsubara frequencies.

We have seen before that the evaluation of field-theoretic Green functions proceeds best via a Wick rotation of the energy in the perturbative digrams to an imaginary axis. This is precisely the axis along which the Matsubara frequencies are situated. Thus, as far as perturbation theory in Fourier transformed space is concerned, the diagrammatic rules are exactly the same, except that the Wick rotated integrals over the imaginary energy have to be replaced by the Matsubara frequency sums [recall Eq. (2.415)]:

$$\int \frac{dp^0}{2\pi} \rightarrow i \int_{-\infty}^{\infty} \frac{dp_E}{2\pi} \rightarrow \frac{k_B T}{\hbar} \sum_{\omega_m} = \frac{1}{\beta} \sum_{\omega_m}, \quad \omega_m = \frac{2\pi}{\hbar\beta} \begin{cases} m & \text{for bosons,} \\ m + \frac{1}{2} & \text{for fermions.} \end{cases} \quad (10.166)$$

In the limit of small temperatures, the Matsubara frequencies move closer and closer to each other, and sums over them tend to frequency integrals.

The two descriptions coincide, apart from the trivial presence of the chemical potential in the grand canonical energy. We conclude that the Wick-rotated calculation of field theoretic Green functions really amounts to thermal equilibrium physics in the limit of zero temperature.

Let us point out that the result (10.163) implies the same periodicity in $\hbar/k_B T = \beta$ of the full Green function $G(\mathbf{x}, \tau; \mathbf{x}', \tau')$ as in the free case (2.413). First, we observe that due to the time independence of the Hamiltonian, there is now translational invariance in euclidean time T such that $G(\mathbf{x}, \tau; \mathbf{x}', \tau')$ depends only on the difference $\tau - \tau'$:

$$\begin{aligned} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= \text{Tr} \left[e^{-H_G(\beta - \frac{\tau}{\hbar})} \psi(\mathbf{x}, 0) e^{-H_G \frac{\tau - \tau'}{\hbar}} \psi^\dagger(\mathbf{x}', 0) e^{-H_G \tau' / \hbar} \right] / \text{Tr}(e^{-\beta H_G}) \\ &= \text{Tr} \left[e^{-H_G(\beta - \frac{\tau}{\hbar})} \psi(\mathbf{x}, 0) e^{-H_G \tau - \tau' / \hbar} \psi^\dagger(\mathbf{x}', 0) \right] / \text{Tr}(e^{-\beta H_G}). \end{aligned} \quad (10.167)$$

Similarly, we conclude the dependence only on $\mathbf{x} - \mathbf{x}'$ by translational invariance in space, using $\psi(\mathbf{x}, \tau) = e^{i\mathbf{P}\mathbf{x}/\hbar} \psi(\mathbf{0}, \tau) e^{-i\mathbf{P}\mathbf{x}/\hbar}$ with the momentum operator $\mathbf{P}$. Thus we may write

$$G(\mathbf{x}, \tau; \mathbf{x}', \tau') = G(\mathbf{x} - \mathbf{x}', \tau - \tau'), \quad (10.168)$$

just as for the field theoretic Green functions in the vacuum. Now it is easy to see the periodicity. For the interval $\tau - \tau' \in (-\hbar/k_B T, 0)$ we calculate

$$\begin{aligned} G(\mathbf{x} - \mathbf{x}', \tau - \tau') &= \pm \text{Tr} \left[e^{-\beta H_G} \psi^\dagger(\mathbf{x}', \tau') \psi(\mathbf{x}, \tau) \right] / \text{Tr}(e^{-\beta H_G}) \\ &= \pm \text{Tr} \left[\psi(\mathbf{x}, \tau) e^{-\beta H_G} \psi^\dagger(\mathbf{x}', \tau') \right] / \text{Tr}(e^{-\beta H_G}) \\ &= \pm \text{Tr} \left[e^{-\beta H_G} \psi(\mathbf{x}, \tau + \beta) \psi^\dagger(\mathbf{x}', \tau') \right] / \text{Tr}(e^{-\beta H_G}) \\ &= \pm G(\mathbf{x} - \mathbf{x}', \tau - \tau' + \beta), \end{aligned} \quad (10.169)$$

thus showing that interacting Boson and Fermion thermal Green functions are periodic and antiperiodic under the replacement $\tau \rightarrow \tau + \beta$, just as in the free case in Eq. (2.413).

Notes and References

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11

Extracting Finite Results from Perturbation Series. Regularization and Renormalization

The Feynman integrals introduced in the last chapter suffer from a serious defect: Most of them are divergent. Fortunately, there exists a certain class of field theories, called *renormalizable field theories*, for which it is nevertheless possible to extract finite predictions for physically observable quantities. All infinities can be absorbed into a few divergent prefactors in any relation between input parameters of the theory and their observed physical values. The price to pay is the impossibility of predicting these parameters, but all other observable properties of the theory can be expressed in terms of their physical values. Typically, these parameters are masses and coupling constants, as well as the normalization of field operators.

The action of a scalar field with a ϕ^4 -interaction in four dimensions defines such a renormalizable field theory and allows for a good demonstration for this procedure. It will now be discussed in detail.

11.1 Vacuum Diagrams

The Lagrangian of the scalar ϕ^4 -theory is

$$\mathcal{L} = \frac{1}{2} (\partial\phi)^2 - \frac{m^2}{2} \phi^2 - \frac{g}{4!} \phi^4. \quad (11.1)$$

Their Feynman diagrams are composed of lines

$$\text{——} = \frac{i}{q^2 - m^2}, \quad (11.2)$$

and vertices

$$\times = -\frac{g}{4!}. \quad (11.3)$$

The Green functions of the theory

$$\begin{aligned} G^{(n)}(x_1, \dots, x_n) &= \langle 0 | T e^{-i \frac{g}{4!} \int dx \phi^4(x)} \phi(x_1) \dots \phi(x_n) | 0 \rangle / \langle 0 | T e^{-i \frac{g}{4!} \int dx \phi^4(x)} | 0 \rangle \\ &\equiv G_N^{(n)}(x_1, \dots, x_n) / Z[0] \end{aligned} \quad (11.4)$$

can be calculated perturbatively by expanding numerator and denominator on the right-hand side in powers of the coupling constant g . The resulting time-ordered products of free-field operators are treated according to Wick's rule, by expanding them into a sum of all Wick contractions. The denominator is a pure phase factor $e^{2i\phi_\pm^\eta}$, as we know from the Gell-Mann-Low formula (9.73). Its diagrammatic expansion has been given in Section 10.3.1, where it was shown to consist of a sum of all vacuum graphs. Here we are interested in the size of the individual terms. Using translational invariance in space and time, we may rewrite (10.34) as

$$\begin{aligned} Z[0] &= \langle 0 | T e^{-i\frac{g}{4!} \int dx \phi^4(x)} | 0 \rangle \\ &= 1 - iT \left\{ \frac{g}{4!} \langle 0 | \phi^4(0) | 0 \rangle - \frac{1}{2!} \left(\frac{g}{4!} \right)^2 \int dx \langle 0 | \phi^4(x) \phi^4(0) | 0 \rangle + \dots \right\}. \end{aligned} \quad (11.5)$$

This expansion runs into an immediate difficulty: the first-order term does not exist in an infinite spacetime volume.¹ Such an infinity can rather trivially be avoided by restricting the discussion to a finite-size system in a finite-time interval. A finite product VT , however, is not yet enough to produce finite results on the right-hand side of (11.5). The typical problem that is still present can be illustrated by considering the first-order Feynman integral (10.36) appearing in the evaluation of (11.5). In momentum space it reads

$$-3i \frac{g}{4!} VT \left(\int \frac{d^4 q}{(2\pi)^4} \frac{i}{q^2 - m^2 + i\eta} \right)^2, \quad (11.6)$$

where 3 is the multiplicity factor of the diagram. The energy integrals have a singularity when q^0 hits the physical mass shell at $q^0 = \omega_{\mathbf{q}} = \sqrt{\mathbf{q}^2 + m^2}$. The $i\eta$ -term in the denominator specifies how to go around this. The singularity can be removed by performing a Wick rotation in the q^0 -plane according to the rules explained in Fig. 7.2. After this the energy integral is completely regular, so that the $i\eta$ -term may be omitted, and (11.6) is expressed in terms of a euclidean integral:

$$-i \frac{g}{4!} VT \left(\int \frac{d^4 q_E}{(2\pi)^4} \frac{1}{q_E^2 + m^2} \right)^2. \quad (11.7)$$

The integral has a quadratic divergence at large momenta. In order to obtain a finite result we have to modify the system in such a way that, in addition to the finite spacetime volume VT , its Wick-rotated energy-momentum space is finite as well. Thus we restrict all euclidean momenta q_E to lie within a sphere of radius Λ :

$$q_E^2 \leq \Lambda^2. \quad (11.8)$$

¹Recall that a similar overall time factor T was found before in the general discussion in Chapter 9. There it appeared in the $\eta \rightarrow 0$ -limit of the switching parameter η [see (9.106)]. In that general derivation we did not find a spatial volume factor, since we considered merely quantum mechanics, not local quantum field theory.

The integration radius Λ is called an *ultraviolet cutoff*, or shorter *UV cutoff*, since it eliminates the very short wavelengths of the field. Such a UV cutoff would have arisen naturally if the physical phenomena would have taken place on a 4-dimensional lattice with spacing of the order $l = \pi/\Lambda$ between the lattice points rather than a continuous spacetime. On such a lattice, each term in the perturbation expansion would have a finite value. If the lattice spacing can be chosen much finer than the regions explored by presently available experiments, this would not present any practical handicap. Any perturbation expansion containing a UV cutoff is of course unable to describe the physics taking place *between* the lattice points.

Hopefully, this is a purely technical problem. If we could resum infinitely many diagrams, the series might define a function which can be used also beyond the cutoff (11.8). A simple model function to illustrate such a hope is given for example by

$$\left(\frac{q^2}{\mu^2}\right)^g, \quad (11.9)$$

where μ is some characteristic mass parameter of the problem. In a perturbation expansion, this function would appear in the form of a series

$$\sum_{n=1}^{\infty} g^n \left[\log(q^2/\mu^2)\right]^n. \quad (11.10)$$

This expansion makes sense only if the momenta of the system are contained within a sphere (11.8) whose size is smaller than

$$\Lambda^2 = \mu^2 e^{1/g}. \quad (11.11)$$

The unexpanded expression (11.9), on the other hand, is defined in the entire complex q^2 -plane, except for a cut from $q^2 = 0$ to $-\infty$. This characteristic behavior will indeed emerge in some partial resummation procedures of many perturbation series. In general, however, the divergences may be of a much more violent nature. The coefficients of the higher-order terms grow in general with $n!$, and the series have a zero radius of convergence. The physical significance of this violent divergence will be discussed later.

To second order in g , the Wick expansion of the second expectation value on the right-hand side of (11.5) yields the Feynman integrals (10.42). In momentum space they read

$$\begin{aligned} \frac{1}{2!} 9 \text{ (two circles)} &= \frac{1}{2!} 9 \left(\frac{g}{4!}\right)^2 \left[\int d^4 q \frac{1}{q^2 - m^2 + i\eta} \right]^2, \\ \frac{1}{2!} 72 \text{ (three circles)} &= \frac{1}{2!} 72 \left(\frac{g}{4!}\right)^2 \left[\int d^4 q_1 \frac{i}{q_1^2 - m^2 + i\eta} \right]^2 \int d^4 q_2 \left(\frac{i}{q_2^2 - m^2 + i\eta} \right)^2, \\ \frac{1}{2!} 24 \text{ (figure-eight)} &= \frac{1}{2!} 24 \left(\frac{g}{4!}\right)^2 \int d^4 q_1 d^4 q_2 d^4 q_3 \frac{i}{q_1^2 - m^2 + i\eta} \frac{i}{q_2^2 - m^2 + i\eta} \frac{i}{q_3^2 - m^2 + i\eta}. \end{aligned} \quad (11.12)$$

After performing again Wick rotations and introducing the euclidean momentum cutoff (11.8), we see that these expressions diverge as $\Lambda^8, \Lambda^4 \log \Lambda, \Lambda^4$, respectively. Analogous statements hold for higher orders.

Thus the infinite phase caused by the vacuum diagrams diverges quite catastrophically for two reasons, both deriving from fundamental properties of spacetime: one is homogeneity (i. e., translational invariance) which causes the overall factors VT . The other is the continuity of spacetime. It is responsible for the fact that the Fourier representations of the fields contain euclidean momentum integrals running over an infinite momentum volume. It is a pleasant feature of the Gell-Mann–Low formula that the divergence of the phase arising from the vacuum diagrams is irrelevant. In Section 9.1.3 it was demonstrated order by order in a perturbation expansion that the phase in the denominator cancels against an identical phase arising in the numerator when expanding (11.4) in powers of g [recall (10.12)]. In graphical terms this amounts to a cancellation of all Feynman diagrams in the numerator, which contain a disconnected part, against corresponding vacuum diagrams of the denominator. This cancellation removes all vacuum diagrams from the numerator, together with their unpleasant VT - and Λ -divergences. In quantum mechanics, this was sufficient to obtain finite results in the limit of a vanishing switching parameter η .

We are thus confronted with only those Feynman graphs which are free of vacuum contributions. Let us demonstrate the treatment in some detail.

11.2 Two- and Four-Point Functions

In Eq. (10.62) we have derived the first terms of the perturbation series for the two-point function:

$$G^{(2)}(x_1, x_2) = \text{---} x_1 \text{---} x_2 + 12 \text{---} \bigcirc \text{---} x_1 \text{---} x_2 + 144 \text{---} \bigcirc \text{---} x_1 \text{---} x_2 + 144 \text{---} \bigcirc \text{---} x_1 \text{---} x_2 + 96 \text{---} \bigcirc \text{---} x_1 \text{---} x_2, \quad (11.13)$$

which amounts to the geometric series (10.85) in momentum space:

$$\begin{aligned} G^{(2)}(q) &= \frac{i}{q^2 - m^2 - \Sigma(q)} \\ &= G_0(q) + G_0(q) [-i\Sigma(q)] G_0(q) + G_0(q) [-i\Sigma(q)] G_0(q) [-i\Sigma(q)] G_0(q) + \dots, \end{aligned} \quad (11.14)$$

with $\Sigma(q)$ being the sum of proper self-energy diagrams (= one-particle irreducible diagrams with two amputated legs)

$$-i\Sigma(q) = 12 \text{---} \bigcirc \text{---} + 144 \text{---} \bigcirc \text{---} + 96 \text{---} \bigcirc \text{---} . \quad (11.15)$$

The Feynman integrals associated with these diagrams can be written in momentum space as follows:

$$\begin{aligned} \text{Diagram 1} &= -\frac{ig}{4!} \int d^4k \frac{i}{k^2 - m^2 + i\eta}, \\ \text{Diagram 2} &= \left(-\frac{ig}{4!}\right)^2 \int d^4k_1 \left(\frac{i}{k_1^2 - m^2 + i\eta}\right)^2 \int d^4k_2 \frac{i}{k_2^2 - m^2 + i\eta}, \end{aligned} \quad (11.16)$$

$$\text{Diagram 3} = \left(-\frac{ig}{4!}\right)^2 \int d^4k_2 d^4k_1 \frac{i}{k_1^2 - m^2 + i\eta} \frac{i}{k_2^2 - m^2 + i\eta} \frac{i}{(q - k_1 - k_2)^2 - m^2 + i\eta}. \quad (11.17)$$

The four-point Green function is reduced to the vertex function $\Gamma^{(4)}$ by factorizing out the four Green functions associated with the external legs:

$$G^{(4)}(p_1, \dots, p_4) = G^{(2)}(p_1)G^{(2)}(p_2)G^{(2)}(p_3)G^{(2)}(p_4)i\Gamma^{(4)}(p_1, \dots, p_4). \quad (11.18)$$

The vertex function $\Gamma^{(4)}$ collects all one-particle irreducible graphs with four amputated legs [see (10.6.1) and (10.89)]:

$$\begin{aligned} i\Gamma^{(4)} &= 4! \times \text{Diagram 4} + (4!)^2 \left\{ \frac{1}{2} \left(\text{Diagram 5} + 2\text{perm} \right) \right. \\ &\quad + (4!)^3 \left\{ \frac{1}{4} \left(\text{Diagram 6} + 2\text{perm} \right) \right. \\ &\quad \left. + \frac{1}{2} \left(\text{Diagram 7} + 2\text{perm} \right) \right. \\ &\quad \left. \left. + \frac{1}{2} \left(\text{Diagram 8} + 5\text{perm} \right) \right\} + \dots \right\} \end{aligned} \quad (11.19)$$

In momentum space, these diagrams correspond to the Feynman integrals:

$$\text{Diagram 4} = \left(-\frac{ig}{4!}\right)^2 \int d^4k \frac{i}{k^2 - m^2 + i\eta} \frac{i}{(k + q_1 + q_2)^2 - m^2 + i\eta}, \quad (11.20)$$

$$\text{Diagram 5} = \left(-\frac{ig}{4!}\right)^3 \left[\int d^4k \frac{i}{k^2 - m^2 + i\eta} \frac{i}{(k + q_1 + q_2)^2 - m^2 + i\eta} \right]^2, \quad (11.21)$$

$$\begin{aligned} \text{Diagram 6} &= \left(-\frac{ig}{4!}\right)^3 \int d^4k \frac{i}{k^2 - m^2 + i\eta} \left[\frac{i}{(k + q_1 + q_2)^2 - m^2 + i\eta} \right]^2 \\ &\quad \times \int d^4k' \frac{i}{k'^2 - m^2 + i\eta}, \end{aligned} \quad (11.22)$$

$$\begin{aligned}
& \left(-\frac{ig}{4!} \right)^3 \int \bar{d}^4 k_1 \bar{d}^4 k_2 \frac{i}{k_1^2 - m^2 + i\eta} \\
& \times \frac{i}{(k_1 + q_2 + q_4)^2 - m^2 + i\eta} \frac{i}{k_2^2 - m^2 + i\eta} \frac{i}{(k_1 - k_2 - q_1)^2 - m^2 + i\eta}.
\end{aligned} \tag{11.23}$$

We may perform the Wick rotation in the loop integrals so that now $\bar{d}^4 q$ goes over into i times the euclidean volume elements $d^4 q_E / (2\pi)^4$, and q^2 becomes $-q_E^2 = -(\mathbf{q}^2 + q_4^2)$. Then we find the following analytic expressions for self-energy and four-point vertex function:

$$\Sigma(q) = \frac{g}{2} D_1 - \frac{g^2}{4} D_2 D_1 - \frac{g^2}{6} D_3(q), \tag{11.24}$$

$$\begin{aligned}
\Gamma^{(4)}(q_i) = & g - \frac{g^2}{2} [I(q_1 + q_2) + 2 \text{ perm}] + \frac{g^3}{4} [I^2(q_1 + q_2) + 2 \text{ perm}] \\
& + \frac{g^3}{2} [I_3(q_1 + q_2) D_1 + 2 \text{ perm}] + \frac{g^3}{2} [I_4(q_i) + 5 \text{ perm}].
\end{aligned} \tag{11.25}$$

Here, $D_{1,2,3}$ and I, I_3, I_4 are the following Feynman integrals

$$D_1 = \int \bar{d}^4 k \frac{1}{k^2 + m^2}, \tag{11.26}$$

$$D_2 = \int \bar{d}^4 k \frac{1}{(k^2 + m^2)^2}, \tag{11.27}$$

$$D_3(q) = \int \bar{d}^4 k_1 \bar{d}^4 k_2 \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)[(q - k_1 - k_2)^2 + m^2]}, \tag{11.28}$$

$$I(q) = \int \bar{d}^4 k \frac{1}{(k^2 + m^2)} \frac{1}{[(k + q)^2 + m^2]}, \tag{11.29}$$

$$I_3(q) = \int \bar{d}^4 k \frac{1}{(k^2 + m^2)^2} \frac{1}{[(k + q)^2 + m^2]}, \tag{11.30}$$

$$\begin{aligned}
I_4(q_i) = & \int \bar{d}^4 k_1 \bar{d}^4 k_2 \frac{1}{(k_1^2 + m^2)[(k_1 + q_2 + q_4)^2 + m^2]} \\
& \times \frac{1}{(k_2^2 + m^2)[(k_1 - k_2 - q_1)^2 + m^2]}.
\end{aligned} \tag{11.31}$$

11.3 Divergences, Cutoff, and Counterterms

The trouble with these expressions is that, except for I_3 , all integrals diverge. In order to extract physical information from the divergent expressions, we introduce an ultraviolet cutoff in euclidean momentum space (11.8) and integrate all momenta only over a spherical range $q^2 \leq \Lambda^2$. Then for large Λ , the different expressions diverge like $D_{1,3} \sim \Lambda^2$, $D_2, I \sim \log \Lambda^2 / m^2$, $I_4 \sim \log^2 \Lambda^2 / m^2$.

In the presence of such a cutoff we must watch out that the size of the coupling constant remains small enough to justify an expansions in powers of g . In the present case we have to require at first that the quantities

$$g \Lambda^2/m^2, \quad g \log \Lambda^2/m^2, \quad g^2 \log^2 \Lambda^2/m^2 \quad (11.32)$$

are all very much smaller than unity. As far as the first term is concerned, this severely restricts the size of g for narrow lattices with $\Lambda^2 \gg m^2$. The other contributions involving logarithms are not so restrictive and permit somewhat more sizable couplings, since the logarithm grows very slowly with Λ/m .

Before proceeding it is useful to separate each momentum integral into a term which diverges for $\Lambda \rightarrow \infty$, and a remainder which remains finite in this limit, and thus becoming independent of Λ . A standard procedure to do this consists in expanding the diverging integrals in a power series of the external momenta. After a few diverging expansion terms, all coefficients are finite. We collect the remaining finite powers and call their sum the *regular part* of the diagram. For the diagrams under consideration this treatment leads to

$$D_3(q) = D_3(0) + D'_3(0)q^2 + D_3^R(q), \quad (11.33)$$

$$I(q) = I(0) + I^R(q), \quad (11.34)$$

where a prime denotes the derivative with respect to q^2 . Only the lowest coefficients $D_3(0)$, $D'_3(0)$ and $I(0)$ are divergent for $\Lambda \rightarrow \infty$. The remainders $D^R(q)$, $I^R(q)$ are cutoff-independent functions of the momenta in the $\Lambda \rightarrow \infty$ -limit.

The Feynman amplitude $I_4(q_i)$ involves two integrations. Since the expansion (11.25) contains all 6 permutations of the momenta q_1, q_2, q_3 , the fourth being fixed by energy-momentum conservation, $q_4 = -q_1 - q_2 - q_3$, we may freely permute the momenta in the integral (11.23) and calculate

$$I_4(q_i) = \int d^4k \frac{1}{(k^2 + m^2) [(q_1 + q_2 - k)^2 + m^2]} I(q_3 + k), \quad (11.35)$$

where $I(q)$ is the integral (11.29) which is expanded as in (11.34). Thus we can write

$$I_4(q_i) = I(q_1 + q_2)I(0) + \int d^4k \frac{1}{(k^2 + m^2) [(q_1 + q_2 - k)^2 + m^2]} I^R(q_3 + k). \quad (11.36)$$

Performing the subtraction in $I(q_1 + q_2)$ we have

$$\begin{aligned} I_4(q_i) &= I^2(0) + I^R(q_1 + q_2)I(0) \\ &\quad + \int d^4k \frac{1}{(k^2 + m^2) [(q_1 + q_2 - k)^2 + m^2]} I^R(q_3 + k). \end{aligned} \quad (11.37)$$

The last term can now be subtracted at $q_i = 0$, leaving a finite remainder. Since $I^R(0) = 0$, we may also write

$$I_4(q_i) = I_4(0) + I^R(q_1 + q_2) I(0) + I_4^R(q_i). \quad (11.38)$$

There are two types of cutoff dependences: One which is momentum-independent and one which is accompanied by the regularized amplitude $I^R(q_1 + q_2)$. This structure will be important in achieving a finite vertex function. With this separation we can rewrite Σ and $\Gamma^{(4)}$ as

$$\Sigma(q) = \Sigma(0) + \Sigma'(0)q^2 + \Sigma^R(q) + \dots, \quad (11.39)$$

$$\begin{aligned} \Gamma^{(4)}(q_i) = & g - \frac{g^2}{2} \left\{ 3I(0) + [I^R(q_1 + q_2) + 2 \text{ perm}] \right\} \\ & + \frac{g^3}{4} \left\{ 3I^2(0) + 2 [I^R(q_1 + q_2) + 2 \text{ perm}] I(0) + [(I^R(q_1 + q_2))^2 + 2 \text{ perm}] \right\} \\ & + \frac{g^3}{2} [I_3(q_1 + q_2) + 2 \text{ perm}] D_1 \\ & + \frac{g^3}{2} \left\{ 6I_4(0) + [I_4^R(q_i) + 5 \text{ perm}] \right\} + \dots, \end{aligned} \quad (11.40)$$

with the Λ -dependent quantities

$$\Sigma(0) = \frac{g}{2} D_1 - \frac{g^2}{4} D_2 D_1 - \frac{g^2}{6} D_3(0), \quad (11.41)$$

$$\Sigma'(0) = -\frac{g^2}{6} D_3'(0). \quad (11.42)$$

Let us interpret this separation physically. For this we consider the full single-particle propagator (11.14). It has the form

$$G^{(2)}(q) = \frac{1}{q^2 + m^2 + \Sigma(0) + \Sigma'(0)q^2 + \Sigma^R(q)}. \quad (11.43)$$

The pole of this propagator corresponds to the mass of the particle after the perturbative corrections. If the cutoff is sufficiently large we may, for a moment, neglect $\Sigma^R(q)$. Then $G^{(2)}$ can be rewritten as

$$\begin{aligned} G^{(2)}(q) &= \frac{1}{q^2 [1 + \Sigma'(0)] + [m^2 + \Sigma(0)]} \\ &= \frac{[1 + \Sigma'(0)]^{-1}}{q^2 + m^2 [1 + \Sigma(0)/m^2] / [1 + \Sigma'(0)]}. \end{aligned} \quad (11.44)$$

This looks like the propagator of a free field $\langle 0 | T \phi_R(x) \phi_R(y) | 0 \rangle$, with

$$\phi_R \equiv \sqrt{1 + \Sigma'(0)} \phi, \quad (11.45)$$

and a mass

$$m_R^2 = m^2 \frac{1 + \Sigma(0)/m^2}{1 + \Sigma'(0)}. \quad (11.46)$$

Experimentally, only the renormalized mass m_R is observable; there is no way of detecting the original mass parameter m in the Lagrangian.

Thus, in all amplitudes calculated from the Lagrangian, the mass m_R has to be used in the final expression rather than m . Technically, this turns out to be slightly inconvenient. There is a more economic method due to Bogoliubov which is based on adding, to the Lagrangian, a set of counterterms which have the same form as the terms of the original Lagrangian. First the free parts:

$$\mathcal{L}_c = c^\phi \frac{1}{2} (\partial\phi)^2 - c^{m^2} \frac{m^2}{2} \phi^2. \quad (11.47)$$

The coefficient functions are expanded in a power series in g starting with g :

$$c^\phi = \sum_{n=1}^{\infty} c_n^\phi g^n, \quad c^{m^2} = \sum_{n=1}^{\infty} c_n^{m^2} g^n. \quad (11.48)$$

They are supposed to be small enough to be treated as a perturbation. If we now calculate the self-energy $\Sigma(q)$ up to order g^2 we find the additional OPI Feynman graphs

$$\begin{aligned} \text{---}\times\text{---} &= (c_1^{m^2} g + c_2^{m^2} g^2) m^2, \\ \text{---}\text{+}\text{---} &= (c_1^\phi g + c_2^\phi g^2) p^2, \end{aligned} \quad (11.49)$$

and loops of the form

$$\text{---}\bigcirc\text{---} = \frac{1}{2} c_1^{m^2} g^2 m^2 D_2, \quad (11.50)$$

$$\text{---}\bigcirc\text{---} = \frac{1}{2} c_1^\phi g^2 \int d^4k \frac{k^2}{(k^2 + m^2)^2} = \frac{1}{2} c_1^\phi g^2 (D_1 - m^2 D_2).$$

The crosses and little circles are called *mass-* and *wave function insertions*, respectively. When adding these terms to the cutoff-dependent parts of the self-energy, they become

$$\begin{aligned} \Sigma^{\text{sg}}(q) &= \frac{g}{2} D_1 - \frac{g^2}{4} D_2 D_1 - \frac{g^2}{6} D_3(0) - \frac{g^2}{6} D_3'(0) q^2 \\ &\quad + (c_1^{m^2} g + c_2^{m^2} g^2) m^2 + (c_1^\phi g + c_2^\phi g^2) q^2 \\ &\quad + \frac{1}{2} c_1^{m^2} g^2 m^2 D_2 + \frac{1}{2} c_1^\phi g^2 (D_1 - m^2 D_2). \end{aligned} \quad (11.51)$$

The point is now that we can always choose the counterterms in such a way that the physical mass arrives at the physical value m we started out with. This can be done order by order in perturbation theory:

To order g we determine

$$c_1^{m^2} m^2 = -\frac{1}{2} D_1, \quad c_1^\phi = 0. \quad (11.52)$$

Inserting this into (11.51), we see that the second and 9th term cancel each other. To second order we determine

$$c_2^{m^2} m^2 = \frac{1}{6} D_3(0), \quad (11.53)$$

$$c_2^\phi = \frac{1}{6} D'_3(0). \quad (11.54)$$

With these choices, no cutoff-dependent parts are left in $\Sigma(q)$ and

$$\Sigma(q) \equiv \Sigma_R(q) = -\frac{g^2}{6} [D_3(q) - D_3(0) - D'_3(0)q^2]. \quad (11.55)$$

As far as the physical results are concerned, this procedure is completely equivalent to the first. The only difference is that by using counterterms, the initial mass parameter in the Lagrangian winds up directly in the final observable expressions, whereas in the first method all expressions must be brought to the renormalized form at the end of all calculations.

The counterterm method really means that instead of the original Lagrangian we have worked with the modified Lagrangian

$$\mathcal{L} + \mathcal{L}_c = \frac{1 + c^\phi}{2} (\partial\phi)^2 - \frac{1 + c^{m^2}}{2} m^2 \phi^2, \quad (11.56)$$

where ϕ and m are the renormalized field and masses, respectively. This is equivalent to starting out with

$$\mathcal{L}_0 \equiv \mathcal{L} + \mathcal{L}_c = \frac{1}{2} (\partial\phi_0)^2 - \frac{m_0^2}{2} \phi_0^2, \quad (11.57)$$

where

$$\phi_0 \equiv \sqrt{1 + c^\phi} \phi, \quad m_0^2 \equiv m^2 (1 + c^{m^2}) (1 + c^\phi)^{-1}. \quad (11.58)$$

Identifying this ϕ_0 with the previous ϕ and the new ϕ with the previous ϕ_R we see that to lowest order in g , we have $c^\phi = -\Sigma'(0)$, $c^{m^2} = -\Sigma(0)$. To higher orders, an additional change from m to m_R is necessary in the normalization factors (11.45), (11.46). To compare the earlier treatment with the counterterm equations (11.58), the integrals $\Sigma(0)$, $\Sigma'(0)$ in (11.41), (11.42) must be expressed in terms of the unrenormalized mass, while c^ϕ , c^{m^2} in (11.54) and (11.53) contain the renormalized mass.

The counterterm method has the obvious advantage that only cutoff-independent quantities appear at every stage of the calculation.

Note that the physical mass is not quite equal to the Lagrangian parameter m^2 . The propagator is

$$G^{(2)}(q) = \frac{1}{q^2 + m^2 + \Sigma_R(q)}, \quad (11.59)$$

and the renormalized quantity $\Sigma_R(q)$ will cause a shift of the pole position to order g in the coupling constant. This finite shift may, however, be easily calculated.

At this point we realize that the finite shift can also be avoided by expanding the loop integrals not around zero but around $q^2 = m^2$. Then

$$D_3(q) = D_3(q)|_{q^2=m^2} + (q^2 + m^2)D'_3(m^2) + \tilde{D}_3^R(q). \quad (11.60)$$

Now the counterterms would be (11.52), together with

$$c_2^{m^2} m^2 = -\frac{1}{6} [D_3(m^2) - m^2 D'_3(m^2)], \quad (11.61)$$

$$c_2^\phi = -\frac{1}{6} D'_3|_{q^2=-m^2}, \quad (11.62)$$

leading to a propagator

$$G^{(2)}(q) = \frac{1}{q^2 + m^2 + \tilde{\Sigma}_R(q)}, \quad (11.63)$$

where the regular part starts out with the second power in $q^2 + m^2$ and therefore leaves the pole at its initial place $q^2 = -m^2$.

Let us now turn to the four-point vertex $\Gamma^{(4)}$. To make it finite we have to include the additional graphs caused by the counterterms (11.47). The lowest contribution enters to order g^3 :

$$\text{Diagram 1} = g^3 c_1^{m^2} m^2 [I_3(q_1 + q_2) + 2 \text{ perm}], \quad (11.64)$$

$$\text{Diagram 2} = g^3 c_1^\phi \{ [I(q_1 + q_2) - m^2 I_3(q_1 + q_2)] + 2 \text{ perm} \}.$$

Using (11.52), this gives

$$-\frac{g^3}{2} D_1 [I_3(q_1 + q_2) + 2 \text{ perm}], \quad (11.65)$$

thus canceling the second-last line in (11.40).

To regularize the remaining Λ -dependent quantities, we introduce a counterterm of the interaction type

$$\mathcal{L}_c = -\frac{g}{4!} c^g \phi^4, \quad (11.66)$$

where c^g has an expansion:

$$c^g = \sum_{n=1}^{\infty} c_n^g g^n. \quad (11.67)$$

This adds to the four-point vertex $\Gamma^{(4)}$ the diagrams

$$\times + \text{circle with cross on left} + \text{circle with cross on right}, \quad (11.68)$$

where the small circles denote the coupling constant counterterms. These insertions amount to replacing $g \rightarrow g(1 + c_1^g g + c_2^g g^2)$ in the first and second term of the expansion (11.40) (the others receive corrections $\mathcal{O}(g^4)$).

It remains to combine mass and coupling constant insertions. To order g^3 , there are none. The corrected expression for $\Gamma^{(4)}$ is therefore

$$\begin{aligned} \Gamma^{(4)} &= g(1 + c_1^g g + c_2^g g^2) \\ &- \frac{1}{2} (g^2 + 2 c_1^g g^3) \{3I(0) + [I^R(q_1 + q_2) + 2 \text{ perm}]\} \\ &+ \frac{g^3}{4} \{3I^2(0) + 2 [I^R(q_1 + q_2) + 2 \text{ perm}] I(0) + [(I^R(q_1 + q_2))^2 + 2 \text{ perm}]\} \\ &+ \frac{g^3}{2} \{6I_4(0) + [I_4^R(q_i) + 5 \text{ perm}]\} + \dots \end{aligned} \quad (11.69)$$

We now determine c^g order by order to cancel the remaining infinities:

$$c_1^g = \frac{3}{2} I(0), \quad (11.70)$$

$$c_2^g = \frac{15}{4} I^2(0) - 3I_4(0). \quad (11.71)$$

The result is the renormalized $\Gamma^{(4)}$:

$$\begin{aligned} \Gamma_R^{(4)}(q_i) &= g - \frac{g^2}{2} [I^R(q_1 + q_2) + 2 \text{ perm}] \\ &+ \frac{g^3}{4} [I^{R^2}(q_1 + q_2) + 2 \text{ perm}] + \frac{g^3}{2} [I_4^R(q_i) + 5 \text{ perm}] + \dots \end{aligned} \quad (11.72)$$

Finally, we have to consider the effects of the coupling constant counterterms upon the self energy. There are the additional graphs

$$\text{circle with dot on bottom} + \text{circle with dot on top} + \text{circle with dot on left} + \text{circle with dot on right} + \dots, \quad (11.73)$$

of which only the first contributes to the second-order expression (11.51), with an amplitude

$$\frac{g^2}{2} c_1^g D_1 = \frac{3}{4} g^2 I(0) D_1.$$

Adding this to (11.51), the quadratic mass counterterm is modified to

$$c_2^{m^2} = \frac{1}{6} D_3(0) - \frac{3}{4} I(0) D_1. \quad (11.74)$$

In this way we have arrived at cutoff-independent expressions for Σ and $\Gamma^{(4)}$. Note, in particular, that the unpleasant terms in the vertex function (11.69) which depend on both, cutoff and momenta, have dropped out.

The total counterterms to second order in g are

$$c^{m^2} m^2 = -\frac{1}{2} g D_1 + \frac{g^2}{6} D_3(0) - \frac{3}{4} g^2 I(0) D_1, \quad (11.75)$$

$$c^\phi = \frac{1}{6} D_3'(0) g^2, \quad (11.76)$$

$$c^g = g \frac{3}{2} I(0) + g^2 \left[\frac{15}{4} I^2(0) - 3 I_4(0) \right] - \frac{g^2}{3}. \quad (11.77)$$

This procedure can be extended to any order in perturbation theory. Moreover, if more general vertex functions are calculated with an arbitrary number of legs the counterterms regularizing the two and four point vertices are sufficient to guarantee also their cutoff independence. The general argument will be formulated in the next chapter.

11.4 Bare Theory and Multiplicative Renormalization

There is one important aspect of the counterterms which has to be stressed: All counterterms have the same form as the terms in the original Lagrangian. Thus one may rewrite $\mathcal{L} + \mathcal{L}_c$ as

$$\mathcal{L} + \mathcal{L}_c = \frac{1 + c^\phi}{2} (\partial\phi)^2 - \frac{1 + c^{m^2}}{2} m^2 (\partial\phi)^2 - \frac{g}{4!} (1 + c^g) \phi^4. \quad (11.78)$$

Therefore we can return to the original form by a multiplicative renormalization. We define the so-called bare fields, mass, and coupling constant

$$\phi_B \equiv \phi Z_\phi^{1/2} = \phi(1 + c^\phi)^{1/2}, \quad (11.79)$$

$$m_B^2 = m^2 Z_m Z_\phi^{-1} = m^2 (1 + c^{m^2}) / (1 + c^\phi), \quad (11.80)$$

$$g_B = g Z_g Z_\phi^{-2} = g (1 + c^g) / (1 + c^\phi)^2, \quad (11.81)$$

and the total Lagrangian becomes

$$\mathcal{L} + \mathcal{L}_c \equiv \mathcal{L}_B = \frac{1}{2} (\partial\phi_B)^2 - \frac{m_B^2}{2} \phi_B^2 - \frac{g_B}{4!} \phi_B^4. \quad (11.82)$$

In this bare Lagrangian, all quantities depend on the physical parameters m, g , and the cutoff Λ . However, due to the renormalizability of the theory, all Λ -dependence drops out and only functions of m and g remain.

It is instructive to see the renormalization work if one uses the bare Lagrangian (11.82) as a basis for a perturbation expansion, without constructing counterterms order by order in g . Thus we calculate the self-energy (11.24) and vertex function (11.25) from the original graphs (11.15) and (11.19), now expressed in terms of the bare parameters g_B and m_B instead of g, m . We find renormalized Green functions by multiplying the bare Green functions with a factor $Z_\phi^{-1/2}$ for each field, i.e.,

$$G_R^{(2)} = Z_\phi^{-1} G_B, \quad (11.83)$$

$$G_R^{(4)} = Z_\phi^{-2} G_B^{(4)}. \quad (11.84)$$

The bare vertex functions

$$\Gamma_B^{(4)} \equiv G_B^{-1} G_B^{-1} G_B^{-1} G_B^{-1} G_B^{(4)}$$

become finite via the inverse factors

$$\Gamma_R^{(2)} = \Gamma_B^{(2)} Z_\phi, \quad (11.85)$$

$$\Gamma_R^{(4)} = \Gamma_B^{(4)} Z_\phi^2. \quad (11.86)$$

In the previous scheme, the renormalized two-point vertex took the form

$$\Gamma_R^{(2)}(q) = q^2 + m^2 + \Sigma^R(q), \quad (11.87)$$

where m is the renormalized mass defined before. Thus we may identify m from

$$\Gamma_R^{(2)}(0) = \Gamma_B^{(2)}(q)|_{q^2=0} Z_\phi = [m_B^2 + \Sigma_B(0)] Z_\phi = m^2. \quad (11.88)$$

The wave function renormalization is fixed by making the slope of $\Gamma_R^{(2)}$ equal to unity at the origin [note that $\Sigma_R(q)$ starts out with q^4 because of the double subtraction in (11.55)]. Hence

$$\left. \frac{\partial}{\partial q^2} \Gamma_R^{(2)}(q^2) \right|_{q^2=0} = \left. \frac{\partial}{\partial q^2} \Gamma_B^{(2)}(q) \right|_{q^2=0} Z_\phi = \left[1 + \frac{\partial}{\partial q^2} \Sigma^B(0) \right] Z_\phi = 1. \quad (11.89)$$

Finally, the renormalized coupling is given by

$$\Gamma_R^{(4)}(0) = g_B \Gamma_B^{(4)}(0) Z_\phi^2 = g. \quad (11.90)$$

This leads to the three equations:

$$m_R^2 = \left[m_B^2 + \frac{g_B}{2} D_1^B - \frac{g_B^2}{4} D_2^B D_1^B - \frac{g_B^2}{6} D_3^B(0) \right] Z_\phi, \quad (11.91)$$

$$g_R = \left[g_B - \frac{3}{2} g_B^2 I^B(0) + \frac{3}{4} g_B^3 I^{B^2}(0) + \frac{3}{2} g_B^3 I_3^B(0) D_1^B + 3 g_B^3 I_4^B(0) \right] Z_\phi^2, \quad (11.91)$$

$$1 = \left[1 - \frac{g_B^2}{6} D_3^{B'}(0) \right] Z_\phi. \quad (11.92)$$

We now solve these three equations for g_B , m_B in terms of g , m by inserting on the right-hand sides the power series expansions

$$\begin{aligned} g_B &= \sum_{n=1}^{\infty} a_n g^n, \\ m_B^2 &= m_R^2 \sum_{n=1}^{\infty} b_n g^n, \\ Z_\phi &= 1 + \sum_{n=1}^{\infty} c_n g^n, \end{aligned} \quad (11.93)$$

and by determining the coefficients a_n , b_n , c_n order by order in g . To first order in g there are only few terms, and we can proceed less systematically in two steps. First, we forget for a moment (11.92), set $Z_\phi = 1$, and call the masses and coupling constants emerging from (11.91) and (11.91) $\bar{m}^2$ and $\bar{g}$, respectively. Inverting (11.91) we have

$$m_B^2 = \bar{m}^2 - \frac{g_B}{2} \bar{D}_1 + \mathcal{O}(g_B^2), \quad (11.94)$$

where $\bar{D}_1$ is the same expression as D_1 , except with m^2 replaced by $\bar{m}^2$. Inserting this into (11.91), we may replace m_B by m_R in all functions I , D . The only exception is $I^B(0)$ where a first-order correction (11.94) must be taken into account, leading to

$$I^B(0) = I^R(0) + g_B I_3^R(0) D_1^R + \mathcal{O}(g_B^2). \quad (11.95)$$

In this way we have accounted for all terms of order g_B^2 , and Eq. (11.91) yields

$$\bar{g} = g_B - \frac{3}{2} g_B^2 \bar{I}(0) + \frac{3}{4} g_B^3 \bar{I}(0)^2 + 3 g_B^3 \bar{I}_4(0). \quad (11.96)$$

Inverting this gives

$$g_B = \bar{g} + \frac{3}{2} \bar{g}^2 \bar{I}(0) + \frac{15}{4} \bar{g}^3 \bar{I}(0)^2 - 3 \bar{g}^3 \bar{I}_4(0). \quad (11.97)$$

Now we observe that with (11.94), the term D_1^B in (11.91) can be re-expanded as

$$D_1^B = \bar{D}_1 + \frac{g_B}{2} \bar{D}_1 \bar{D}_2, \quad (11.98)$$

so that (11.91) takes the form

$$\bar{m}^2 = m_B^2 + \frac{g_B}{2} \bar{D}_1(0) - \frac{g_B^2}{6} \bar{D}_3(0). \quad (11.99)$$

Together with (23.35), this yields

$$m_B^2 = \bar{m}^2 - \frac{g_1}{2} \bar{D}_1 - \frac{3}{4} \bar{g}^2 \bar{I}(0) \bar{D}_1 + \frac{1}{6} \bar{g}^2 \bar{D}_3(0). \quad (11.100)$$

On the right-hand sides of this and (23.35) we recognize precisely the counterterms (11.75) calculated with the barred parameters $\bar{g}, \bar{m}$ of Eqs. (11.96) and (11.99) instead of g, m . This is in agreement with the multiplicative renormalization laws (11.80), since we assumed for the moment $Z_\phi = 1$ or $c^\phi = 0$, in which case Eqs. (11.79)–(11.81) take the form

$$\begin{aligned}\phi_B &= \phi_1, \\ m_B^2 &= \bar{m}^2 Z_m, \\ g_B &= \bar{g} Z_g.\end{aligned}\tag{11.101}$$

Let us finally include the effect of Z_ϕ and go from $\bar{m}, \bar{g}$ to m, g . Since

$$Z^\phi = \left[1 - \frac{g^2}{6} D_3^{R'}(0) \right]^{-1}\tag{11.102}$$

is of second order in g_B , we have to this order

$$Z^\phi = 1 + \frac{\bar{g}^2}{6} \bar{D}_3'(0) + \dots = 1 + c_R^\phi + \dots\tag{11.103}$$

We now determine m, g from

$$\bar{m}^2(1 + c_1^{m^2}) = m_R^2(1 + c_R^{m^2})(1 + c_R^\phi)^{-1},\tag{11.104}$$

$$\bar{g}(1 + c_1^g) = g_R(1 + c_R^g)(1 + c_R^\phi)^{-2}.\tag{11.105}$$

The first of these equations shows that m^2 and m_1^2 differ by a term quadratic in g_1^2 :

$$m_1^2 = m_R^2 \left[1 - \frac{g_1^2}{6} D_3^1(0) + \dots \right],\tag{11.106}$$

which can be written as

$$m_1^2 = m_R^2 \left[1 - \frac{g_R^2}{6} D_3^{R'}(0) + \dots \right],\tag{11.107}$$

without changing terms of order g^2 . Inserting this into (11.100) yields

$$m_B^2 = m_R^2 - \frac{g_R}{2} D_1^R - \frac{3}{4} g_R^2 I^R(0) D_1^R + \frac{1}{6} g_R^2 D_3^R(0) - m_R^2 \frac{g_R^2}{6} D_3^{R'}(0).\tag{11.108}$$

Inserting (11.107) into (23.35), we can replace m_1 by m without mistake up to order g_1^3 . But then we see from (11.105) that

$$g_1 = g_R \left[1 - \frac{g_R^2}{3} D_3^{R'}(0) + \dots \right],\tag{11.109}$$

i.e., g_1 differs from g_R only by a correction term of second order. Combined with (11.96), this implies

$$g_B = g_R + \frac{3}{2} g_R^2 I^R(0) + \frac{15}{4} g_R^3 I^R(0)^2 - 3 g_R^3 I_4^R(0) - \frac{g_R^3}{3} D_3^{R'}(0).\tag{11.110}$$

Again we find precisely the same counterterms as in (11.77). This completes the renormalization program with the bare quantities as a starting point and an application of the normalization conditions (11.91), (11.91), (11.92).

As we mentioned before, the finite values g_R, m_R do not correspond to what we would experimentally identify as the physical coupling constants of the particles. The mass would be defined by the pole of the renormalized propagator $G_R^{(2)}(q)$, which lies at the zero of the renormalized vertex function $\Gamma_R^{(2)}(q)$

$$\Gamma^{(2)}(q) \Big|_{q^2 = -m_R^2} = 0. \quad (11.111)$$

The physical coupling is given by

$$\Gamma^{(4)}(q_i) \Big|_{\text{MS}} = g_R, \quad (11.112)$$

where the subscript MS denotes the point where all legs are on the mass shells of physical particles. These satisfy

$$\begin{aligned} q_i^2 &= m_R^2, \\ q_i q_j &= \frac{m_R^2}{3} (4\delta_{ij} - 1), \end{aligned} \quad (11.113)$$

such that $(q_i + q_j)^2 = \frac{4}{3}m^2$.

The wave function normalization at the physical pole is set equal to unity:

$$\frac{\partial \Gamma_R(q)}{\partial q^2} \Big|_{q^2 = -m_R^2} = 1. \quad (11.114)$$

Then all vertex functions can be directly expressed in terms of these physical values. The difference between these and the previous m, g are calculable in terms of a multiplicative renormalization whose factors are power series in g with only *finite* coefficients.

11.5 Dimensional Regularization of Integrals

There is another method for making Feynman integrals finite that allows for a specific control over the divergences. It has the advantage of not needing the specification of a subtraction point in momentum space. Moreover, in field theories other than ϕ^4 , which contain massless particles and are gauge invariant, it preserves most symmetry relations between the Green functions. This is an important advantage over other regularization methods. In particular, the *Ward identities* of gauge theories are preserved which are essential for proving renormalizability.

Some classical symmetries, however, cannot be salvaged into the quantum field theory. If this happens, one speaks of an *anomaly* with respect to this symmetry. Famous examples are the *chiral anomaly* of massless quark theories, or the *conformal anomaly* of the two-dimensional quantum field theory of strings. Instead of

employing a cutoff, it is possible to analytically continue the Feynman integrals to a continuous spacetime dimension in the neighborhood of the physical dimension $D = 4$.

Starting point of this continuation procedure is the observation that a Feynman propagator can be written as

$$\frac{1}{k^2 + 2kq + m^2} = \int_0^\infty d\tau e^{-\tau(k^2 + 2kq + m^2)}, \quad k^2 + 2kq + m^2 > 0. \quad (11.115)$$

This can be generalized to an arbitrary power:

$$\frac{1}{(k^2 + 2kq + m^2)^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{d\tau}{\tau} \tau^\nu e^{-\tau(k^2 + 2kq + m^2)}, \quad k^2 + 2kq + m^2 > 0, \quad (11.116)$$

valid for all real $\nu > 0$.

Let us insert this representation into a typical Feynman integral

$$\int d^D k \frac{1}{(k^2 + 2kq + m^2)^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{d\tau}{\tau} \tau^\nu \int d^D k e^{-\tau(k^2 + 2kq + m^2)}. \quad (11.117)$$

where $D = 1, 2, 3, \dots$, and

$$d^D k \equiv \frac{d^D k}{(2\pi)^D}. \quad (11.118)$$

For integer D , the D -dimensional momentum integral on the right-hand side evaluated as

$$\begin{aligned} \int d^D k e^{-\tau(k^2 + 2kq + m^2)} &= \left(\int d^1 k e^{-\tau(k+q)^2} \right)^D e^{-\tau(m^2 - q^2)} \\ &= \frac{1}{(2\pi)^D} \left(\frac{\pi}{\tau} \right)^{D/2} e^{-\tau(m^2 - q^2)}, \end{aligned} \quad (11.119)$$

since after a quadratic completion of the exponential it factorizes into D products of one-dimensional Gaussian integrals. This equation forms the basis for the definition of Feynman diagrams in a continuous number of spacetime dimensions. We simply *define* the left-hand side of (11.119) for *all complex* D via the analytic continuation of the right-hand side of (11.119). After this, we perform in (11.117) the integral over τ , using the formula

$$\int_0^\infty d\tau \tau^{\nu-D/2-1} e^{-\tau a} = \Gamma(\nu - D/2) \frac{1}{a^{\nu-D/2}}, \quad a > 0. \quad (11.120)$$

Note that although the integral on the left-hand side exists only for $D < 2\nu$, the right-hand side provides an analytic continuation to larger $D > 2\nu$ if one goes around the singularities at $D = 2\nu, 2\nu + 2, 2\nu + 4, \dots$. The extension can be shown explicitly by rewriting the left-hand side as follows:

$$\int_0^\infty d\tau \tau^{\nu-D/2-1} e^{-\tau a} = \int_c^\infty d\tau \tau^{\nu-D/2-1} e^{-\tau a} + \int_0^c d\tau \tau^{\nu-D/2-1} (e^{-\tau a} - 1) + \frac{c^{\nu-D/2}}{\nu - D/2}, \quad (11.121)$$

with some parameter $c > 0$, on which the right-hand side does not depend. In contrast to the original integral, the right-hand side is now defined for $2\nu < D < 2\nu + 2$. In the limit $c \rightarrow 0$, we fall back to the original integral. For $2\nu < D < 2\nu + 2$, however, we can take the limit $c \rightarrow \infty$ and we obtain the continuation rule

$$\int_0^\infty d\tau \tau^{\nu-D/2-1} e^{-\tau a} \equiv \int_0^\infty d\tau \tau^{\nu-D/2-1} (e^{-\tau a} - 1). \quad (11.122)$$

If D approaches 2ν from above, the decomposition (11.121) for $c > 0$ shows that the integral is singular like $1/(\nu - D/2)$. The precise result is

$$\int d^D k \frac{1}{(k^2 + 2kq + m^2)^\nu} = \frac{1}{(2\pi)^D} \frac{\pi^{D/2}}{(m^2 - q^2)^{\nu-D/2}} \frac{\Gamma(\nu - D/2)}{\Gamma(\nu)}. \quad (11.123)$$

This equation is valid by analytic continuation in the entire complex D -plane, except at the singularities $D = 2\nu, 2\nu + 2, 2\nu + 4, \dots$ of the Gamma function.

The analytic continuation has a peculiar feature that is worth emphasizing since it has important applications in massless theories (in particular gauge theories): For all D which do not lie at the above singular points, the limit $\nu \rightarrow 0$ is well-defined, and yields

$$\int d^D k = 0. \quad (11.124)$$

If one defines the integral at the singular points by analytic continuation from the neighborhood it vanishes identically for all D . Let us split (11.124) into an angular and radial integral, and rewrite it as

$$S_D \int dk k^{D-1} = 0, \quad (11.125)$$

where S_D is the surface of a sphere in D dimensions:

$$S_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}, \quad (11.126)$$

so that $S_1 = 2$, $S_2 = 2\pi$, $S_3 = 4\pi$, $S_4 = 2\pi^2, \dots$. Since D is arbitrary, we deduce from (11.123) that the general homogeneous integral

$$\frac{S_D}{(2\pi)^D} \int dk k^{D-1} k^{-2\nu} = 0 \quad (11.127)$$

vanishes for all ν . We may also write this in the form

$$\int d^D k k^{-2\nu} = 0, \quad (11.128)$$

known as *Veltman's integral rule*.

If we take $q = 0$ and the limit $m \rightarrow 0$ directly in the integral formula (11.123) for $\nu \neq 0$, the same result is obviously true for D if it is larger than 2ν . Then the integral is proportional to $m^{D-2\nu}$. Indeed, for $D > 2\nu$, the integral $\int d^D k k^{-2\nu} = 0$ is regular at $k = 0$. In (11.127) we show how that integral can be continued to the singular regime $D \leq 2\nu$.

The integral contains a prefactor which will occur in all Feynman integrals. It will be useful to call it, by analogy with the measure of integration (11.118), the *reduced surface* of a unit sphere

$$\bar{S}_D \equiv \frac{S_D}{(2\pi)^D} = \frac{1}{(2\pi)^D} \frac{2\pi^{D/2}}{\Gamma(D/2)} = \frac{1}{(4\pi)^{D/2}} \frac{2}{\Gamma(D/2)}, \quad (11.129)$$

for example $\bar{S}_1 = 1/\pi$, $\bar{S}_2 = 1/2\pi$, $\bar{S}_3 = 1/2\pi^2$, $\bar{S}_4 = 1/8\pi^2, \dots$. In the perturbation expansions to be derived, the factor $\bar{S}_D$ will accompany each loop integral and may be absorbed into the coupling constants [see (11.216)].

With the reduced surface of a sphere, the Feynman integral (11.123) may be rewritten as

$$\int d^D k \frac{1}{(k^2 + 2kq + m^2)^\nu} = \bar{S}_D \frac{\Gamma(D/2)\Gamma(\nu - D/2)}{2} \Gamma(\nu) \frac{1}{(m^2 - q^2)^{\nu-D/2}}. \quad (11.130)$$

This integral is now used to derive several related Feynman integrals, by forming successive derivatives with respect to the momentum four-vector k . In this way, we obtain the formulas

$$\int d^D k \frac{k_\mu}{(k^2 + 2kq + m^2)^\nu} = \bar{S}_D \frac{\Gamma(D/2)\Gamma(\nu - D/2)}{2\Gamma(\nu)} \frac{1}{(m^2 - q^2)^{\nu-D/2}} (-q_\mu), \quad (11.131)$$

$$\begin{aligned} \int d^D k \frac{k_\mu k_\nu}{(k^2 + 2kq + m^2)^\nu} &= \bar{S}_D \frac{\Gamma(D/2)}{2\Gamma(\nu)} \frac{1}{(m^2 - q^2)^{\nu-D/2}} \\ &\times \left[\Gamma(\nu - D/2) q_\mu q_\nu + \Gamma(\nu - 1 - D/2) \frac{1}{2} \delta_{\mu\nu} (m^2 - q^2) \right], \end{aligned} \quad (11.132)$$

$$\begin{aligned} \int d^D k \frac{k_\mu k_\nu k_\lambda}{(k^2 + 2kq + m^2)^\nu} &= \bar{S}_D \frac{\Gamma(D/2)}{2\Gamma(\nu)} \frac{1}{(m^2 - q^2)^{\nu-D/2}} \\ &\times \left[-\Gamma(\nu - D/2) k_\mu k_\nu k_\lambda - \Gamma(\nu - 1 - D/2) \frac{1}{2} (\delta_{\mu\nu} k_\lambda + \delta_{\mu\lambda} k_\nu + \delta_{\nu\lambda} k_\mu) (m^2 - q^2) \right]. \end{aligned} \quad (11.133)$$

By expanding (11.123) in powers of ν and comparing the coefficients, we find a further important integral from the linear term in ν :

$$\int d^D k \log(k^2 + 2kq + m^2) = \bar{S}_D \frac{1}{D} \Gamma(D/2) \Gamma(1 - D/2) (m^2 - q^2)^{D/2}. \quad (11.134)$$

Strictly speaking, the logarithm on the left-hand side does not make sense since its argument has the dimension of a square mass. It should therefore always be written

as $\log[(k^2 + 2kq + m^2)/\mu^2]$ with some auxiliary mass μ . If $m \neq 0$, the auxiliary mass μ can, of course, be set equal to m . In dimensional regularization, however, this proper way of writing the logarithm does not change the integral at all, since it merely amounts to adding an integral over a constant, and this vanishes by the Veltman rule (11.128).

Note that we obtain the same result from a direct calculation with k^2 in the numerator, when forming the trace of (11.132) over the indices μ and ν . The result is consistent with the trivial trace formula

$$\delta_{\mu\mu} \equiv D, \quad (11.135)$$

which is initially valid only for integer D , but which is applicable in an arbitrary continuous dimension D .

Because of this, and for symmetry reasons, we can replace in a rotationally invariant integral the product of momentum vectors as follows:

$$k_\mu k_\nu \rightarrow \frac{k^2}{D} \delta_{\mu\nu}, \quad k_\mu k_\nu k_\lambda k_\kappa \rightarrow \frac{(k^2)^2}{D(D+2)} (\delta_{\mu\nu} \delta_{\lambda\kappa} + \delta_{\mu\lambda} \delta_{\nu\kappa} + \delta_{\mu\kappa} \delta_{\nu\lambda}). \quad (11.136)$$

In a general dimension D , all the above Feynman integrals are finite without a cutoff Λ , except for certain integer values of D . A typical example is the physical spacetime dimension $D = 4$. To control the divergences in four spacetime dimensions we set $D = 4 - \varepsilon$ with some small number ε . The divergences for D close to $D = 4$ appears now as a pole term in $1/\varepsilon^n$ with some finite power $n > 0$. This way of controlling the divergences of Feynman integrals is called the method of *dimensional regularization*, or of *analytic regularization*.

Let us study the small- ε singularities of the Feynman integrals in Eqs. (11.26)–(11.31) for real D near the physical dimension $D = 4$. The first integral in the list is

$$D_1 = \int d^D k \frac{1}{k^2 + m^2} = S_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) (m^2)^{-1+D/2}. \quad (11.137)$$

The divergence of this integral manifests itself in the pole of the Gamma function at the physical dimension $D = 4$. In the neighborhood of this dimension we set

$$D \equiv 4 - \varepsilon, \quad (11.138)$$

and express the integral in terms of ε . The singularity at small ε may be isolated by using the identity

$$\Gamma(x) = \frac{1}{x} \Gamma(1+x), \quad (11.139)$$

and the expansion

$$\Gamma(1+x) \Gamma(1-x) = \frac{\pi x}{\sin \pi x} = 1 + \frac{\pi^2}{6} x^2 + \dots \quad (11.140)$$

Note that the second relation has only quadratic correction terms ε^2 . There is a useful generalization of this,

$$\frac{\prod_n \Gamma(1 + a_n \varepsilon)}{\prod_m \Gamma(1 + a'_m \varepsilon)} = 1 + \mathcal{O}(\varepsilon^2), \quad (11.141)$$

if

$$\sum_n a_n - \sum_m a'_m = 0. \quad (11.142)$$

This relation ensures the cancellation of all terms proportional to ε when expanding $\Gamma(1 + a\varepsilon) = 1 - \gamma\varepsilon + \mathcal{O}(\varepsilon^2)$. With (11.140), we have

$$\begin{aligned} \Gamma(D/2)\Gamma(1 - D/2) &= \Gamma\left(2 - \frac{\varepsilon}{2}\right)\Gamma\left(-1 + \frac{\varepsilon}{2}\right) = -\frac{2}{\varepsilon}\Gamma\left(1 - \frac{\varepsilon}{2}\right)\Gamma\left(1 + \frac{\varepsilon}{2}\right) \\ &= -\frac{2}{\varepsilon} + \mathcal{O}(\varepsilon), \end{aligned} \quad (11.143)$$

and therefore

$$D_1 = S_D m^2 \cdot (m^2)^{-\varepsilon/2} \left[-\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon) \right]. \quad (11.144)$$

This expression has a mass dimension $(m^2)^{1-\varepsilon/2}$ and a singularity proportional to $1/\varepsilon$. It may be separated into a singular and a regular expression

$$D_1 \equiv D_1^{\text{sg}} + D_1^{\text{reg}}, \quad (11.145)$$

with

$$D_1^{\text{sg}} \equiv -S_D (m^2)^{1-\varepsilon/2} \frac{1}{\varepsilon}. \quad (11.146)$$

The singular part is not uniquely defined. It may be modified by an arbitrary regular term. For instance, we may introduce an arbitrary fixed mass scale μ and choose as a singular part

$$D_1^{\text{sg}} \equiv -S_D m^2 (\mu^2)^{-\varepsilon/2} \frac{1}{\varepsilon}. \quad (11.147)$$

The two choices differ by a regular term $\frac{1}{2}S_D \log(m^2/\mu^2)$. The latter choice has the form m^2 times a function that is independent of the mass m . We shall see below that this property persists to higher orders in perturbation theory. This property will later be of great advantage in studying the theory in the limit $m \rightarrow 0$. The scale parameter μ is unavoidable when taking this limit.

This parameter will play an important role in studying the scale properties of the perturbation expansion via the so-called *renormalization group* in Chapter 20. That group governs all critical phenomena observed in second-order phase transitions.

By comparing the singular term (11.147) with the previous cutoff divergence which was

$$D_1 = \frac{1}{(4\pi)^2} \Lambda^2, \quad (11.148)$$

we realize that the quantity $1/\varepsilon$ plays the same role as before Λ^2/m^2 .

A similar subtraction procedure is applied to the other Feynman integrals in the list (11.26)–(11.31). Consider, for example, the second one (11.27):

$$D_2 = \int d^D k \frac{1}{(k^2 + m^2)^2} = S_D \frac{1}{2} \frac{\Gamma(D/2) \Gamma(2 - D/2)}{\Gamma(2)} (m^2)^{D/2-2} \quad (11.149)$$

Now

$$\Gamma(D/2) \Gamma(2 - D/2) = (1 - D/2) \left[-\frac{2}{\varepsilon} + \mathcal{O}(\varepsilon) \right] \quad (11.150)$$

$$= \frac{2}{\varepsilon} - 1 + \mathcal{O}(\varepsilon) \quad (11.151)$$

so that

$$D_2 = S_D (m^2)^{-\varepsilon/2} \left[\frac{1}{\varepsilon} - \frac{1}{2} + \mathcal{O}(\varepsilon) \right] \equiv D_2^{\text{sg}} + D_2^{\text{reg}}. \quad (11.152)$$

Here we choose the expression

$$D_2^{\text{sg}} \equiv S_D \mu^{-\varepsilon} \frac{1}{\varepsilon} \quad (11.153)$$

as a singular part, with the mass parameter μ ensuring the correct dimension of both singular and regular terms. This makes the singular term independent of the mass m . This is again useful for a study of the theory in the massless limit.

Another advantage of introducing the mass parameter μ in the singular parts (11.147) and (11.153) is that D_2^{sg} is related to D_1^{sg} by a derivative $-\partial/\partial m^2$:

$$D_2^{\text{sg}} = \frac{\partial}{\partial m^2} D_1^{\text{sg}}. \quad (11.154)$$

Note that the pole term $1/\varepsilon$ replaces a logarithmic divergence that would appear in a cutoff regularization. Since also the quadratic divergence in D_1 had a $1/\varepsilon$ -pole, one may wonder how the singularities in ε can reflect the difference between quadratic and logarithmic divergence in the cutoff method: Comparison with D_1 shows that while D_2 has its lowest singularity at $D = 4$, i.e., at $\varepsilon = 0$, D_1 has it at $D = 2$, i.e., at $\varepsilon = 2$.

An example for the more involved treatment of singularities, consider the fourth Feynman integral in the list (11.26)–(11.31):

$$I(q) = \int d^D k \frac{1}{(k^2 + m^2) [(k - q)^2 + m^2]}. \quad (11.155)$$

It may be evaluated with the help of Feynman's formula

$$\frac{1}{AB} = \int_0^1 dx \frac{1}{[Ax + B(1-x)]^2} = \int_0^1 dx \frac{1}{[A(1-x) + Bx]^2} \quad (11.156)$$

which follows from the trivial relation

$$\frac{1}{AB} = \frac{1}{B-A} \left(\frac{1}{A} - \frac{1}{B} \right) = \frac{1}{B-A} \int_A^B dz \frac{1}{z^2}. \quad (11.157)$$

For n denominators, Feynman's formula reads²

$$\frac{1}{A_i \cdots A_n} = (n-1)! \int_0^1 \int_0^1 dx_1 \cdots dx_n \frac{\delta(\sum_{i=1}^n x_i - 1)}{(A_1 x_1 + \cdots + A_n x_n)^n}, \quad (11.158)$$

as can be proved by induction. By differentiating both sides α_i times with respect to A_i , one finds more generally

$$\frac{1}{A_1^{\alpha_1} \cdots A_n^{\alpha_n}} = \frac{\Gamma(\sum_{i=1}^n \alpha_i)}{\prod_{i=1}^n \Gamma(\alpha_i)} \prod_{i=1}^n \int_0^1 dx_i \frac{\prod_{i=1}^n x_i^{\alpha_i-1} \delta(\sum_{i=1}^n x_i - 1)}{[\sum_{i=1}^n x_i A_i]^{\sum_{i=1}^n \alpha_i}}. \quad (11.159)$$

By analytic continuation, this formula remains valid for complex values of α_i .

Using (11.156) and the substitution $z = Ax + B(1-x)$, we rewrite (11.155) as

$$\begin{aligned} I(q) &= \int_0^1 dx \int d^D k \frac{1}{\{(k^2 + m^2)(1-x) + [(k+q)^2 + m^2]x\}^2} \\ &= \int_0^1 dx \int d^D k \frac{1}{[k^2 + 2kqx + q^2x + m^2]^2}. \end{aligned} \quad (11.160)$$

The momentum integration gives

$$I(q) = S_D \frac{1}{2} \Gamma(D/2) \Gamma(2-D/2) \int_0^1 dx \frac{1}{[q^2x(1-x) + m^2]^{2-D/2}}. \quad (11.161)$$

Going over to the variable ε , we rewrite this as

$$I(q) = S_D \frac{1}{2} \Gamma(2-\varepsilon/2) \Gamma(\varepsilon/2) \mu^{-\varepsilon} \int_0^1 dx \frac{(\mu^2)^{\varepsilon/2}}{[q^2x(1-x) + m^2]^{\varepsilon/2}}. \quad (11.162)$$

We have used once more the mass parameter μ to make the integral dimensionless. The integral is regular at $\varepsilon = 1$. A singularity comes only from the prefactor, which possesses a $1/\varepsilon$ -behavior to be extracted with the help of formula (11.140):

$$\begin{aligned} \Gamma(2-\varepsilon/2) \Gamma(\varepsilon/2) &= \left(1 - \frac{\varepsilon}{2}\right) \frac{2}{\varepsilon} \Gamma\left(1 - \frac{\varepsilon}{2}\right) \Gamma\left(1 + \frac{\varepsilon}{2}\right) \\ &= \frac{2}{\varepsilon} - 1 + \mathcal{O}(\varepsilon). \end{aligned} \quad (11.163)$$

²For a proof of this formula see Vol. I of E. Goursat and E.R. Hedrick, *A Course in Mathematical Analysis*, Ginn and Co., Boston, 1904.

Hence we obtain

$$I(q) = S_D \frac{1}{\varepsilon} \left(1 - \frac{\varepsilon}{2}\right) \mu^{-\varepsilon} \left(\frac{\mu^2}{q^2}\right)^{\varepsilon/2} J_\varepsilon^m(q), \quad (11.164)$$

with the integral

$$J_\varepsilon^m(q) = \int_0^1 dx \left[x(1-x) + \frac{m^2}{q^2} \right]^{-\varepsilon/2}. \quad (11.165)$$

For $m = 0$, the integral can immediately be done:

$$J_\varepsilon^m(q) \equiv J_\varepsilon^0 = \int_0^1 x^a (1-x)^b = \frac{\Gamma(a+1)\Gamma(b+1)}{\Gamma(a+b+2)}, \quad (11.166)$$

with

$$J_\varepsilon^0 = \frac{\Gamma^2(1-\varepsilon/2)}{\Gamma(2-\varepsilon)} = 1 + \varepsilon + \mathcal{O}(\varepsilon^2). \quad (11.167)$$

We may therefore expand

$$I(q) = S_D \left(\frac{1}{\varepsilon} + \frac{1}{2}\right) \mu^{-\varepsilon} \left(\frac{\mu^2}{q^2}\right)^{\varepsilon/2} + \mathcal{O}(\varepsilon). \quad (11.168)$$

The residue at the pole is independent of q , as a manifestation of the renormalizability of the theory. For $m \neq 0$, we can expand (11.165) in powers of m and find the same pole term in ε . This property is a special feature of this regularization procedure.

We now choose the singular part

$$I^{\text{sg}} \equiv S_D \frac{\mu^{-\varepsilon}}{\varepsilon}, \quad (11.169)$$

to form the subtracted Feynman integral

$$I^{\text{reg}}(q) = I(q) - I^{\text{sg}}, \quad (11.170)$$

which is smooth in the limit $\varepsilon \rightarrow 0$. As before, we have included the factor $\mu^{-\varepsilon}$ in (11.169) for dimensional reasons.

For $m \neq 0$, we expand $J_\varepsilon^m(q)$ in powers of ε and find an additional factor

$$1 - \frac{\varepsilon}{2} [L^m(q) - L^0], \quad (11.171)$$

where

$$\begin{aligned} L^m(q) &= \int_0^1 dx \log \left[x(1-x) + \frac{m^2}{q^2} \right] \\ &= -2 + \log \frac{m^2}{q^2} + \frac{\sqrt{q^2 + 4m^2}}{\sqrt{q^2}} \log \frac{\sqrt{q^2 + 4m^2} + \sqrt{q^2}}{\sqrt{q^2 + 4m^2} - \sqrt{q^2}}. \end{aligned} \quad (11.172)$$

This can also be written as

$$L^m(q) = -2 + \log \frac{m^2}{q^2} + 2\theta \coth \theta, \quad (11.173)$$

with

$$\sinh^2 \theta \equiv \frac{q^2}{4m^2} \quad (11.174)$$

or

$$\theta \equiv \operatorname{atanh} \frac{\sqrt{q^2}}{\sqrt{q^2 + 4m^2}} = \frac{1}{2} \log \frac{\sqrt{q^2 + 4m^2} + \sqrt{q^2}}{\sqrt{q^2 + 4m^2} - \sqrt{q^2}}. \quad (11.175)$$

For $m = 0$, $L^0(q)$ becomes a constant: $L^0(q) \equiv L^0 = -2$.

Altogether, we obtain for any mass m :

$$I(q) = S_D \mu^{-\varepsilon} \left[\frac{1}{\varepsilon} - \frac{1}{2} - \frac{1}{2} L^m(q) - \frac{1}{2} \log \frac{q^2}{\mu^2} \right] + \mathcal{O}(\varepsilon). \quad (11.176)$$

The singularity is the same as in the $m = 0$ -expression (11.168), so that the subtraction (11.170) regularizes the integral for all m . Note that the subtraction constant of $D_2(q)$ is the same as that of $I(q)$:

$$I^{\text{sg}} = D_2^{\text{sg}}. \quad (11.177)$$

This is obvious from the definitions (11.27) and (11.29) and the mass and momentum independence of the singular parts.

The result (11.176) can now be applied to the calculation of the third Feynman integral in the list (11.26)–(11.31):

$$D_3(q) = \int d^D k_1 d^D k_2 \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)} \frac{1}{[(q + k_1 + k_2)^2 + m^2]}. \quad (11.178)$$

In $D = 4$ dimensions, this integral contains 8 momentum integrations and only 6 powers of momenta in the denominator, so that it diverges formally like Λ^2 . Before applying Feynman's formula (11.159), we decrease the degree of divergence by the so-called *partial integration trick* due to 't Hooft and Veltman.³

To derive this, we observe that the process of partial differentiation with respect to the momentum variables satisfies the trivial identity:

$$\frac{\partial k^\mu}{\partial k^\nu} = \delta^\mu_\nu. \quad (11.179)$$

Contracting the indices in D dimensions as in (11.135) gives

$$\frac{\partial k^\mu}{\partial k^\mu} = D, \quad (11.180)$$

³G. 't Hooft and M.T. Veltman, Nucl. Phys. B 44, 189 (1972). See also T. Curtright and G. Ghandour, Ann. Phys. 106, 209 (1977).

which amounts to the *trick* relation

$$\frac{1}{D} \frac{\partial k^\mu}{\partial k^\nu} = 1. \quad (11.181)$$

Generalizing this we may insert the trivial identity

$$1 = \frac{1}{2D} \left(\frac{\partial k_1^\mu}{\partial k_1^\mu} + \frac{\partial k_2^\mu}{\partial k_2^\mu} \right) \quad (11.182)$$

into the integral (11.178) and, after an integration by parts and neglecting the surface terms, we may write

$$\begin{aligned} D_3(q) = & -\frac{1}{2D} \int d^D k_1 d^D k_2 \left(k_1^\mu \frac{\partial}{\partial k_1^\mu} + k_2^\mu \frac{\partial}{\partial k_2^\mu} \right) \\ & \times \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)} \frac{1}{[(q + k_1 + k_2)^2 + m^2]}. \end{aligned} \quad (11.183)$$

Performing the differentiations leads to the following sum of two integrals

$$\begin{aligned} D_3(q) = & -\frac{1}{D-3} \int d^D k_1 d^D k_2 \frac{3m^2 + q(q + k_1 + k_2)}{(k_1^2 + m^2)(k_2^2 + m^2) [(q + k_1 + k_2)^2 + m^2]^3} \\ = & -\frac{1}{D-3} [3m^2 A(q) + B(q)], \end{aligned} \quad (11.184)$$

where

$$A(q) = \int d^D k_1 d^D k_2 \frac{1}{(k_1^2 + m^2)^2 (k_2^2 + m^2) [(q + k_1 + k_2)^2 + m^2]}, \quad (11.185)$$

and

$$B(q) = \int d^D k_1 d^D k_2 \frac{q(q + k_1 + k_2)}{(k_1^2 + m^2)(k_2^2 + m^2) [(q + k_1 + k_2)^2 + m^2]^2}. \quad (11.186)$$

The first integral is only logarithmically divergent, the second diverges linearly. These integrals are now evaluated with the help of Feynman's formula (11.156). We begin with $A(q)$, which can obviously be rewritten as

$$\begin{aligned} A(q) = & \int d^D k_1 \frac{1}{(k_1^2 + m^2)^2} I(k_1 + q) \\ = & S_D \frac{1}{2} \Gamma(D/2) \Gamma(2 - D/2) \\ & \times \int_0^1 dx \int d^D k \frac{1}{(k^2 + m^2)^2} \frac{1}{[(q + k)^2 x(1 - x) + m^2]^{2-D/2}}. \end{aligned} \quad (11.187)$$

We remove a factor $[x(1-x)]^{2-D/2}$ from the denominator and apply to the remaining integrand the generalized Feynman formula (11.159) as

$$\frac{1}{A^\alpha} \frac{1}{B^\beta} = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \Gamma(\beta)} \int_0^1 dy \frac{y^{\alpha-1} (1-y)^{\beta-1}}{[Ay + B(1-y)]^{\alpha+\beta}}. \quad (11.188)$$

This leads to

$$A(q) = S_D \frac{1}{2} \Gamma(D/2) \Gamma(2 - D/2) \frac{\Gamma(4 - D/2)}{\Gamma(2) \Gamma(2 - D/2)} \\ \times \int_0^1 dx [x(1-x)]^{D/2-2} \int_0^1 dy \int d^D k \frac{y(1-y)^{1-D/2}}{f^{4-D/2}(q; k, x, y)}, \quad (11.189)$$

with

$$f(q; k, x, y) = y(k^2 + m^2) + (1-y) \left[(q+k)^2 + \frac{m^2}{x(1-x)} \right] \\ = k^2 + (2kq + q^2)(1-y) + m^2 \left[y + \frac{1-y}{x(1-x)} \right]. \quad (11.190)$$

By performing the integral over $d^D k$ in (11.189), we obtain

$$A(q) = S_D^2 \frac{1}{2} \Gamma(D/2) \Gamma(2 - D/2) \frac{\Gamma(4 - D/2)}{\Gamma(2) \Gamma(2 - D/2)} \\ \times \frac{1}{2} \frac{\Gamma(D/2) \Gamma(4 - D)}{\Gamma(4 - D/2)} \int_0^1 dx [x(1-x)]^{D/2-2} \\ \times \int_0^1 dy y (1-y)^{1-D/2} \left\{ q^2 y (1-y) + m^2 \left[y + \frac{1-y}{x(1-x)} \right] \right\}^{D-4}, \quad (11.191)$$

which reads in terms of ε :

$$A(q) = S_D^2 \frac{1}{4} \Gamma^2(2 - \varepsilon/2) \Gamma(\varepsilon) (m^2)^{-\varepsilon} \int_0^1 dx [x(1-x)]^{-\varepsilon/2} \\ \times \int_0^1 dy y (1-y)^{\varepsilon/2-1} \left\{ \frac{q^2}{m^2} y (1-y) + \left[y + \frac{1-y}{x(1-x)} \right] \right\}^{-\varepsilon}. \quad (11.192)$$

Defining the dimensionless expression in curly brackets as

$$F(q; x, y) \equiv \frac{q^2}{m^2} y (1-y) + \left[y + \frac{1-y}{x(1-x)} \right], \quad (11.193)$$

we expand

$$F^{-\varepsilon}(q; x, y) = 1 - \varepsilon \log F(q; x, y) + \mathcal{O}(\varepsilon^2). \quad (11.194)$$

The first term gives [via (11.166)]

$$S_D^2 \frac{1}{4} \Gamma^2(2 - \varepsilon/2) \Gamma(\varepsilon) (m^2)^{-\varepsilon} \frac{\Gamma^2(1 - \varepsilon/2)}{\Gamma(2 - \varepsilon)} \frac{\Gamma(2) \Gamma(\varepsilon/2)}{\Gamma(2 + \varepsilon/2)}. \quad (11.195)$$

This can be rewritten as

$$S_D^2 (m^2)^{-\varepsilon} \frac{1}{4} (1 - \varepsilon/2)^2 \frac{2}{\varepsilon^2} \frac{1}{1 - \varepsilon} \frac{1}{1 + \varepsilon/2} \frac{\Gamma^4(1 - \varepsilon/2) \Gamma(1 + \varepsilon) \Gamma(1 + \varepsilon/2)}{\Gamma(1 - \varepsilon) \Gamma(1 + \varepsilon/2)}. \quad (11.196)$$

The ratio of Gamma-functions has the general form (11.141) with (11.142), and can be replaced by $1 + \mathcal{O}(\varepsilon^2)$. Thus we obtain the first contribution to $A(q)$:

$$A(q) = S_D^2 \frac{(m^2)^{-\varepsilon}}{4\varepsilon} \left[\frac{2}{\varepsilon} - 1 + \mathcal{O}(\varepsilon) \right]. \quad (11.197)$$

We now turn to the second contribution in (11.192) due to the logarithm in the expansion (11.194). A singular term at $\varepsilon = 0$ can only come from the end-point singularity in the y -integral of (11.192) at $y = 1$. Near that point, the logarithm goes to zero like

$$\log F(q; x, y) = \mathcal{O}(1 - y), \quad (11.198)$$

so that the integral has no end-point singularity after all. Thus there is no further singular contribution to $A(q)$ in Eq. (11.240).

To complete the calculation of the pole terms in $D_3(q)$ we have to study the second integral $B(q)$ in Eq. (11.184). After applying again the Feynman formula twice we arrive at an expression of the type (11.192):

$$\begin{aligned} B(q) &= S_D^2 \frac{1}{4} \Gamma^2(2 - \varepsilon/2) \Gamma(\varepsilon) q^2 (m^2)^{-\varepsilon} \int_0^1 dx [x(1-x)]^{-\varepsilon/2} \\ &\quad \times \int_0^1 dy y (1-y)^{\varepsilon/2} [F(q; x, y)]^{-\varepsilon}. \end{aligned} \quad (11.199)$$

Here both the x - and the y -integrals are free of endpoint singularities and converge. At $\varepsilon = 0$, the integrals are equal to $1/2$. Thus we find the pole term of $B(q)$:

$$B(q) = S_D^2 \frac{(m^2)^{-\varepsilon}}{4\varepsilon} \Gamma^2(2 - \varepsilon/2) \Gamma(1 + \varepsilon) \frac{q^2}{2} = S_D^2 \frac{(m^2)^{-\varepsilon}}{4\varepsilon} \frac{q^2}{2} [1 + \mathcal{O}(\varepsilon)]. \quad (11.200)$$

Inserting this and (11.197) into (11.184), we obtain for the singular part of $D_3(q)$:

$$D_3^{\text{sg}}(q) = -S_D^2 m^2 \mu^{-2\varepsilon} \frac{6}{4\varepsilon} \left[\frac{1}{\varepsilon} - 2 \log \frac{m}{\mu} + \frac{1}{2} + \frac{q^2}{12m^2} \right], \quad (11.201)$$

where we have introduced the mass parameter μ to make the singular term proportional to m^2 as in D_1^{sg} and D_2^{sg} in (11.145) and (11.152). Apart from the overall factor m^2 , the singular term contains a logarithmic dependence on m , in contrast to D_1^{sg} and D_2^{sg} , which had only the overall factor m^2 . It will turn out that in the present subtraction scheme all terms $m^2 \log(m/\mu)$ will eventually cancel in the divergent parts of self-energy and vertex functions. Observe that the singular term has only a linear q^2 -dependence. This is necessary for the renormalizability of the theory, since a q^2 -term can be compensated by a counterterm of the gradient type $\partial\phi(x)\partial\phi(x)$ in the Lagrangian density.

Consider finally the last Feynman integral in the list (11.27)–(11.31):

$$\begin{aligned} I_4(q_i) &= \int d^D k_1 d^D k_2 \frac{1}{(k_1^2 + m^2) [(q_1 + q_{12} - k_1)^2 + m^2]} \\ &\quad \times \frac{1}{(k_2^2 + m^2) [(k_1 - k_2 + q_3)^2 + m^2]}. \end{aligned} \quad (11.202)$$

This can be written as

$$I_4(q_i) = \int d^D k \frac{1}{k^2 + m^2} \frac{1}{(q_1 + q_2 - k)^2 + m^2} I(k + q_3), \quad (11.203)$$

which becomes, using (11.162),

$$\begin{aligned} I_4(q_i) &= S_D \frac{1}{2} \Gamma\left(2 - \frac{\varepsilon}{2}\right) \Gamma\left(\frac{\varepsilon}{2}\right) \int_0^1 dx \\ &\times \int d^D k \frac{1}{k^2 + m^2} \frac{1}{(q_1 + q_2 - k)^2 + m^2} \frac{1}{[(q_3 + k)^2 x(1-x) + m^2]^{\varepsilon/2}}. \end{aligned} \quad (11.204)$$

The denominators are combined via (11.188), and we obtain

$$\begin{aligned} I_4(q_i) &= S_D^2 \frac{1}{2} \Gamma\left(2 - \frac{\varepsilon}{2}\right) \Gamma(2 + \varepsilon/2) \int_0^1 dx [x(1-x)]^{-\varepsilon/2} \int_0^1 dy (1-y)^{\varepsilon/2-1} y \\ &\times \frac{1}{2} \frac{\Gamma(2 - \varepsilon/2) \Gamma(\varepsilon)}{\Gamma(2 + \varepsilon/2)} \int_0^1 dz \left\{ yz(1-yz)(q_1 + q_2)^2 + y(1-y)q_3^2 \right. \\ &\quad \left. - 2yz(1-y)q_3(q_1 + q_2) + m^2 \left[y + \frac{1-y}{x(1-x)} \right] \right\}^{-\varepsilon}. \end{aligned} \quad (11.205)$$

The only pole term comes from the end-point singularity in the integral at $y = 1$. For $y = 1$, the curly bracket can be expanded as

$$\begin{aligned} \{\dots\} &= [(q_1 + q_2)^2]^{-\varepsilon} \left\{ 1 - \varepsilon \log \left[z(1-z) + \frac{m^2}{(q_1 + q_2)^2} \right] \right. \\ &\quad \left. - \varepsilon \log \frac{[\dots]}{z(1-z)(q_1 + q_2)^2 + m^2} + \mathcal{O}(\varepsilon^2) \right\}. \end{aligned} \quad (11.206)$$

Using formula (11.141) with (11.142), the pre-factor of (11.205) is seen to have an expansion

$$\frac{1}{4\varepsilon}(1 - \varepsilon) + \mathcal{O}(\varepsilon),$$

so that

$$\begin{aligned} I_4(q_i) &= S_D^2 \frac{1}{4\varepsilon} (1 + \varepsilon) \int_0^1 dx [x(1-x)]^{-\varepsilon/2} \int_0^1 dy (1-y)^{\frac{\varepsilon}{2}-1} y \\ &\times [(q_1 + q_2)^2]^{-\varepsilon} \int_0^1 dz \left\{ 1 - \varepsilon \log \left[z(1-z) + \frac{m^2}{(q_1 + q_2)^2} \right] \right. \\ &\quad \left. - \varepsilon \log \frac{[\dots]}{z(1-z)(q_1 + q_2)^2 + m^2} \right\} + \mathcal{O}(\varepsilon). \end{aligned} \quad (11.207)$$

The first two terms in the integral are independent of x and y , and give

$$\frac{\Gamma^2(1 - \varepsilon/2) \Gamma(\varepsilon/2) \Gamma(2)}{\Gamma(2 - \varepsilon) \Gamma(2 + \varepsilon/2)} [1 - \varepsilon L^m(q_1 + q_2)], \quad (11.208)$$

where $L^m(q)$ is the integral (22.49) which occurred in the evaluation of $I(q)$ of Eq. (11.164)]. Thus, up to here the singular part of $I_4(q_i)$ is

$$I_4(q_i) = S_D^2 \frac{\mu^{-2\varepsilon}}{2\varepsilon^2} \left[1 - \frac{\varepsilon}{2} - \varepsilon L^m(q_1 + q_2) - \varepsilon \log \frac{(q_1 + q_2)^2}{\mu^2} \right] + \mathcal{O}(\varepsilon^0), \quad (11.209)$$

where we have used the mass parameter μ to make the logarithm dimensionless. We now look at the effect of the last logarithm in (11.206). It is accompanied by a factor ε and it vanishes at $y = 1$ such that it fails to lead to an end-point singularity at $y = 1$, $\varepsilon = 0$. Therefore it contributes to order $\mathcal{O}(\varepsilon^0)$ and can be neglected as far as the singular parts are concerned. Thus Eq. (11.208) remains unchanged.

Let us decompose this into singular and regular terms in accordance with the decomposition (11.38), using the singular term I^{sg} calculated in (11.169) of the Feynman integral (11.162):

$$\begin{aligned} I_4(q_i) &\equiv I_4^{\text{sg}} + I_4^{\text{reg}}(q_i) \\ &= \Delta I_4^{\text{sg}} + I^{\text{reg}}(q_1 + q_2) I^{\text{sg}} + I_4^{\text{reg}}(q_i), \end{aligned} \quad (11.210)$$

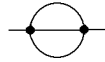
with the momentum-independent term

$$\Delta I_4^{\text{sg}} = S_D^2 \frac{\mu^{-2\varepsilon}}{2\varepsilon^2} \left(1 + \frac{\varepsilon}{2} \right). \quad (11.211)$$

11.6 Renormalization of Amplitudes

Let us now apply these formulas. Consider at first the self-energy up to second order where we have found it useful to recall the origin of the different contributions graphically:

$$\begin{aligned} \Sigma(q) = & \frac{1}{2}gD_1 & - \frac{1}{4}g^2D_2D_1 & - & \frac{1}{6}g^2D_3 \\ & \text{---}\bullet\text{---} & \text{---}\bullet\text{---} & & \text{---}\bullet\text{---} \\ & \text{---}\times\text{---} & \text{---}+ \text{---} & & \\ & + \left(c_1^{m^2}g + c_2^{m^2}g^2 \right) m^2 & + & \left(c_1^\phi g + c_2^\phi g^2 \right) q^2 & \\ & - \frac{1}{2} c_1^{m^2} g^2 D_2 & - \frac{1}{2} c_1^\phi g^2 (D_1 - m^2 D_2) & + \frac{1}{2} c_1^g g^2 D_1 & . \end{aligned} \quad (11.212)$$



Obviously, we can regularize this expression in the same way as before by just choosing the singular parts of $D_1, D_2, D_2 D_1$, and D_3 for the counterterms

$$c_1^{m^2} = -\frac{1}{2}D_1^{\text{sg}}, \quad c_2^{m^2} = \frac{1}{4}(D_2 D_1)^{\text{sg}} - \frac{1}{4}(D_1^{\text{sg}} D_2)^{\text{sg}} - \frac{3}{4}(D_2^{\text{sg}} D_1)^{\text{sg}} + \frac{1}{6}D_3^{\text{sg}}(0), \quad (11.213)$$

$$c_1^\phi = 0, \quad c_2^\phi = \frac{1}{6}D_3'^{\text{sg}}. \quad (11.214)$$

Care has to be taken to distinguish between the singular parts of $D_2^{\text{sg}} D_1$, $D_1^{\text{sg}} D_2$, and $(D_2 D_1)^{\text{sg}}$, and we find from (11.145), (11.147), (11.152), (11.153), and (11.201)

$$\begin{aligned} (D_1^{\text{sg}} D_2)^{\text{sg}} &= S_D^2 \left\{ -m^2 \mu^{-\varepsilon} \frac{1}{\varepsilon} \cdot (m^2)^{-\varepsilon/2} \left[\frac{1}{\varepsilon} - \frac{1}{2} + \mathcal{O}(\varepsilon) \right] \right\}^{\text{sg}}, \\ &= S_D^2 m^2 \mu^{-2\varepsilon} \left[-\frac{1}{\varepsilon^2} + \frac{1}{\varepsilon} \log \frac{m}{\mu} + \frac{1}{2\varepsilon} \right], \\ (D_2^{\text{sg}} D_1)^{\text{sg}} &= S_D^2 \left\{ \frac{\mu^{-\varepsilon}}{\varepsilon} \cdot (m^2)^{1-\varepsilon/2} \left[-\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon) \right] \right\}^{\text{sg}} \\ &= S_D^2 m^2 \mu^{-2\varepsilon} \left[-\frac{1}{\varepsilon^2} + \frac{1}{\varepsilon} \log \frac{m}{\mu} \right], \\ (D_2 D_1)^{\text{sg}} &= S_D^2 \left\{ (m^2)^{-\varepsilon/2} \left[\frac{1}{\varepsilon} - \frac{1}{2} + \mathcal{O}(\varepsilon) \right] (m^2)^{1-\varepsilon/2} \left[-\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon) \right] \right\}^{\text{sg}} \\ &= S_D^2 m^2 \mu^{-2\varepsilon} \left[-\frac{1}{\varepsilon^2} + \frac{2}{\varepsilon} \log \frac{m}{\mu} + \frac{1}{2\varepsilon} \right], \\ D_3^{\text{sg}}(0) &= S_D^2 m^2 \mu^{-2\varepsilon} \frac{6}{4\varepsilon} \left[-\frac{1}{\varepsilon^2} + \frac{2}{\varepsilon} \log \frac{m}{\mu} - \frac{1}{2\varepsilon} \right]. \end{aligned} \quad (11.215)$$

In writing (11.214), we have used $I^{\text{sg}} = D_2^{\text{sg}}$ according to (11.177). Due to the non-integer dimension all Feynman integrals carry a factor $\mu^{-\varepsilon}$ for each order in g . It is convenient to absorb these factors, together with the surface factor S_D , into the coupling constant and introduce the dimensionless *reduced coupling constant*

$$\lambda \equiv g S_D \mu^{-\varepsilon}. \quad (11.216)$$

This considerably simplifies all expressions.

Collecting the different terms in (11.213) and (11.214), we obtain

$$\begin{aligned} c^{m^2} &= \lambda \frac{1}{2\varepsilon} + \lambda^2 \frac{1}{4} \left(\frac{2}{\varepsilon^2} - \frac{1}{2\varepsilon} \right) \\ c^\phi &= -\lambda^2 \frac{1}{48\varepsilon}. \end{aligned} \quad (11.217)$$

Note the pleasant cancellation of all mass factors! This happens at all higher-orders in the coupling constant.

Some people do not include the factor S_D into the definition of λ , but only its $D = 4$ -value $S_4 = 2/(4\pi)^2$. The relation between the two is obtained from the expansion

$$\Gamma(D/2) = \Gamma(2 - \varepsilon/2) = 1 + (\gamma - 1)\varepsilon/2 + \mathcal{O}(\varepsilon^2), \quad (11.218)$$

implying that the factor $\mathcal{S}_D$ in (11.216) can be expanded as

$$\mathcal{S}_D = (2/(4\pi)^2)[1 + (\log 4\pi - \gamma + 1)\varepsilon/2 + \mathcal{O}(\varepsilon^2)]. \quad (11.219)$$

Then (11.201) may be expanded as

$$D_3^{\text{sg}}(q) = -\frac{1}{(4\pi)^4} \frac{(m^2)^{1-\varepsilon}}{\varepsilon} \left[\frac{6}{\varepsilon} + 9 - 6\gamma + 6 \log 4\pi + \frac{q^2}{2m^2} + \mathcal{O}(\varepsilon) \right]. \quad (11.220)$$

Consider now the coupling-constant counterterms. Recalling the full vertex function

$$\begin{aligned} \Gamma^{(4)}(q_i) = & g - \frac{1}{2}g^2 [I(q_1 + q_2) + 2 \text{ perm}] + \frac{1}{4}g^3 [I^2(q_1 + q_2) + 2 \text{ perm}] \\ & \times \quad \quad \quad \times \quad \quad \quad \times \\ & + \frac{1}{2}g^3 [I_3(q_1 + q_2) D_1 + 2 \text{ perm}] + \frac{1}{2}g^3 [I_4(q_i) + 5 \text{ perm}] \\ & \quad \quad \quad \times \quad \quad \quad \times \\ & + (c_1^g g + c_2^g g^2) g - c_1^g g^3 [I(q_1 + q_2) + 2 \text{ perm}] \\ & \quad \quad \quad \times \quad \quad \quad \times \\ & + c_1^{m^2} g^3 [I_3(q_1 + q_2) + 2 \text{ perm}] + c_1^\phi g^3 [I_3(q_1 + q_2) + 2 \text{ perm}] \\ & \quad \quad \quad \times \quad \quad \quad \times \end{aligned} \quad (11.221)$$

we may identify

$$c_1^g = \frac{3}{2} I^{\text{sg}} \quad (11.222)$$

$$\begin{aligned} c_2^g = & -\frac{1}{4} [(I^2)^{\text{sg}} + 2 \text{ perm}] - \frac{1}{2} [(I_3 D_1)^{\text{sg}} + 2 \text{ perm}] - \frac{1}{2} [I_4^{\text{sg}} + 5 \text{ perm}] \\ & + \frac{3}{2} [(I^{\text{sg}} I)^{\text{sg}} + 2 \text{ perm}] + \frac{1}{2} [(D_1^{\text{sg}} I_3)^{\text{sg}} + 2 \text{ perm}]. \end{aligned} \quad (11.223)$$

Inserting (11.210) into (11.223) we separate $I = I^{\text{sg}} + I^{\text{reg}}$, $D_1 = D_1^{\text{sg}} + D_1^{\text{reg}}$ and use the fact that $I_3(q_i)$ is regular to cancel the term $(I_3 D_1)^{\text{sg}}$ against the term $-(D_1^{\text{sg}} I_3)^{\text{sg}}$, so that

$$\begin{aligned} c_2^g = & -\frac{3}{4} [(I^{\text{sg}})^2 + 2 I^{\text{sg}} I^{\text{reg}}] - 3 (\Delta I_4^{\text{sg}} + I^{\text{sg}} I^{\text{reg}}) \\ & + \frac{9}{2} [(I^{\text{sg}})^2 + I^{\text{sg}} I^{\text{reg}}]. \end{aligned} \quad (11.224)$$

The terms containing I^{reg} are seen to cancel each other, and we arrive at

$$c_2^g = \frac{15}{4} (I^{\text{sg}})^2 - 3\Delta I_4^{\text{sg}}. \quad (11.225)$$

We now insert (11.177), (11.211), and obtain

$$\begin{aligned} c^g &= \lambda \frac{3}{2\varepsilon} + \lambda^2 \left[\frac{15}{4} \frac{1}{\varepsilon^2} - 3 \left(\frac{1}{2\varepsilon^2} + \frac{1}{4\varepsilon} \right) \right] \\ &= \lambda \frac{3}{2\varepsilon} + \lambda^2 \frac{1}{4} \left(\frac{9}{\varepsilon^2} - \frac{3}{\varepsilon} \right). \end{aligned} \quad (11.226)$$

Here we have to pause for a very important observation. Nowhere in the formulas for c^{m^2} , c^ϕ , c^g does the physical mass appear. There is only the arbitrary mass scale μ that has been used to make the coupling constant dimensionless. If this situation prevails to all orders in perturbation theory we can conclude that the counterterms calculated according to the rules of this section serve to renormalize massive as well as massless theories. The multiplicative renormalization constants depend only on the dimensionless coupling constant g .

The finite regularized vertex functions depend on the choice of g, m , and the parameter μ . For massive theories μ can be set equal to m , and only the two parameters g and m are necessary to specify the manifold of all perturbative solutions to the ϕ^4 field theory. For zero physical mass, the parameter μ can no longer be eliminated. Now the vertex functions will depend on g and μ . Since the parameter μ has been introduced in a completely arbitrary manner, we have the suspicion that it cannot represent a true degree of freedom in the calculation of both massive and massless theories. In fact we shall see in the next section that there is only a two-parameter manifold in g, m, μ -space which corresponds to different sets of vertex functions. As far as the renormalization is concerned, however, μ is absolutely necessary to obtain finite expressions if the physical mass m is taken to zero.

11.7 Additive Renormalization of Vacuum Energy

The renormalization of the two- and four-point functions discussed above does not remove *all* infinities of the theory. A further important infinity in many-body theories and cosmology is the infinity associated with the sum over all vacuum diagrams. They emerge in the calculation of $Z[0]$ of Eq. (11.5) which may be used to define the total vacuum energy due to the interaction

$$Z[0] = e^{-TE_{\text{int}}^{\text{vac}}}. \quad (11.227)$$

The energy $E_{\text{int}}^{\text{vac}}$ has to be added to the total energy of all zero-point oscillations of the field $\phi(x)$ which is

$$E_0^{\text{vac}} = \sum_{\mathbf{p}} \frac{\hbar\omega_{\mathbf{p}}}{2}. \quad (11.228)$$

Recall Eqs. (7.670) and (7.434), and the discussion of the Casimir effect in Section 7.12. This and the contribution from all vacuum diagrams are divergent, and this infinity must be subtracted from the total energy to ensure that the physical vacuum has zero total energy. This is necessary for the final theory to be Lorentz invariant.

11.8 Generalization to $O(N)$ -Symmetric Models

In many physical systems, the field ϕ has several degrees of freedom: In the superconductor it is a complex field which may be considered as a two-component object with ϕ^2 , ϕ^4 replaced by

$$\phi^2 \rightarrow |\phi|^2 = \phi_1^2 + \phi_2^2, \quad \phi^4 \rightarrow |\phi|^4 \rightarrow (\phi_1^2 + \phi_2^2)^2. \quad (11.229)$$

A magnetic system, on the other hand, is characterized by a vector field (ϕ_1, ϕ_2, ϕ_3) and the Lagrangian contains the invariants

$$\phi^2 \rightarrow \phi_1^2 + \phi_2^2 + \phi_3^2, \quad \phi^4 \rightarrow (\phi_1^2 + \phi_2^2 + \phi_3^2)^2. \quad (11.230)$$

It is therefore useful to generalize all results to the case of an $O(N)$ -vector ϕ_a such that instead of ϕ^2 , ϕ^4 we have:

$$\phi^2 \rightarrow \sum_{a=1}^N \phi_a^2, \quad \phi^4 \rightarrow \left(\sum_{a=1}^N \phi_a^2 \right)^2. \quad (11.231)$$

The propagator is the same as before except that it is accompanied by a Kronecker δ_{ab} . The vertex function, on the other hand, carries a symmetric tensor

$$T_{abcd} = \frac{1}{3} (\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}). \quad (11.232)$$

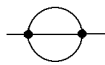
When calculating the Feynman diagrams, all integrations remain the same except that each integral is accompanied by a product of T -tensors with a contraction of indices for every internal line. For the previous diagrams these may be given as follows:



$$D_1 \rightarrow D_1 T_{\underline{abcc}}, \quad (11.233)$$



$$D_2 D_1 \rightarrow D_2 D_1 T_{\underline{abcd}} T_{cdee}, \quad (11.234)$$



$$D_3 \rightarrow D_3 T_{\underline{acde}} T_{\underline{bcde}}, \quad (11.235)$$

$$\begin{array}{c} \diagup \quad \diagdown \\ \circlearrowleft \end{array} \quad I \rightarrow IT_{\underline{a}b\bar{e}f}T_{\underline{c}d\bar{e}f}, \quad (11.236)$$

$$\begin{array}{c} \diagup \quad \diagdown \\ \circlearrowleft \quad \circlearrowleft \end{array} \quad I^2 \rightarrow I^2T_{\underline{a}b\bar{e}f}T_{efgh}T_{gh\bar{c}d}, \quad (11.237)$$

$$\begin{array}{c} \circlearrowleft \\ \diagup \quad \diagdown \end{array} \quad I_3D_1 \rightarrow I_3D_1T_{\underline{a}b\bar{e}f}T_{\underline{c}d\bar{e}g}T_{fghh}, \quad (11.238)$$

$$\begin{array}{c} \diagup \quad \diagdown \\ \circlearrowleft \quad \circlearrowleft \end{array} \quad I_4 \rightarrow I_4T_{\underline{a}b\bar{e}f}T_{\underline{e}c\bar{g}h}T_{f\bar{d}gh}. \quad (11.239)$$

For greater transparency we have underlined the external indices.

It is convenient to introduce the reduced matrix elements of the contracted tensors as follows

$$\begin{aligned} T_{abcc} &= \delta_{ab}T_{D_1}, \\ T_{abcd}T_{cdee} &= \delta_{ab}T_{D_2D_1} = \delta_{ab}T_{D_1}^2, \\ T_{acde}T_{bcde} &= \delta_{ab}T_{D_3}, \\ T_{abef}T_{cdef} \Big|_{\text{symm}} &= T_{abcd}T_I, \\ T_{abef}T_{efgh}T_{cdgh} \Big|_{\text{symm}} &= T_{abcd}T_{I^2}, \\ T_{abef}T_{cdeg}T_{fghh} \Big|_{\text{symm}} &= T_{abcd}T_{I_3D_1} \equiv T_{abcd}T_IT_{D_1}, \\ T_{abef}T_{ecgh}T_{fdgh} \Big|_{\text{symm}} &= T_{abcd}T_{I_4}. \end{aligned} \quad (11.240)$$

The subscript $_{\text{symm}}$ denotes symmetrization in the indices $abcd$, thereby replacing each $\delta_{ab}\delta_{cd}$ by T_{abcd} . In order to calculate the irreducible matrix elements we observe that

$$T_{abcc} = \frac{N+2}{3}\delta_{ab}, \quad (11.241)$$

$$T_{aefg}T_{befg} = \frac{N+2}{3}\delta_{ab}, \quad (11.242)$$

so that

$$T_{D_1} = \frac{N+2}{3}, \quad (11.243)$$

$$T_{D_3} = \frac{N+2}{3}. \quad (11.244)$$

In order to calculate T_I we first note that

$$T_{abef}T_{cdef} = \frac{1}{9}[(N+4)\delta_{ab}\delta_{cd} + 2\delta_{ac}\delta_{bd} + 2\delta_{ad}\delta_{bc}]. \quad (11.245)$$

It is useful to abbreviate the three tensors in the brackets as A_1 , A_2 , A_3 , i.e., we write

$$T_{abef}T_{cdef} = \left[\frac{N+4}{9}A_1 + \frac{2}{9}A_2 + \frac{2}{9}A_3 \right]_{abcd}. \quad (11.246)$$

The symmetrization of the tensors A_1 , A_2 , A_3 gives each time T_{abcd} so that

$$T_{abcf}T_{cdef}|_{\text{symm}} = \frac{N+8}{9}T_{abcd} \quad (11.247)$$

and hence

$$T_I = \frac{N+8}{9}. \quad (11.248)$$

For the other products in (11.240) we observe the multiplication rules

$$\begin{aligned} & (p_1A_1 + p_2A_2 + p_3A_3)_{abef} (q_1A_1 + q_2A_2 + q_3A_3)_{efcd} \\ &= \{[p_1(q_1N + q_2 + q_3) + p_2q_1 + p_3q_1]A_1 + (p_2q_2 + p_3q_3)A_2 + (p_2q_3 + p_3q_2)A_3\}_{abcd}. \end{aligned} \quad (11.249)$$

If we want to form $T_{abef}T_{efgh}T_{cdgh}$, we have to multiply $A_1 + A_2 + A_3$ by $\frac{N+4}{9}A_1 + \frac{2}{9}A_2 + \frac{2}{9}A_3$, and symmetrize the result, which gives

$$\frac{1}{3} \left(\frac{N+4}{9}N + \frac{4}{9} \right) + \frac{2}{3} \left(\frac{N+4}{9} + \frac{2}{9} + \frac{2}{9} \right) T_{abcd}. \quad (11.250)$$

This implies that

$$T_{I^2} = \frac{1}{27} (N^2 + 6N + 20). \quad (11.251)$$

The last product in (11.240) is found by using the general rule

$$\begin{aligned} & (p_1A_1 + p_2A_2 + p_3A_3)_{abcd} (q_1A_1 + q_2A_2 + q_3A_3)_{cedf} \\ &= \{[p_1(q_1 + Nq_2 + q_3) + (p_2 + p_3)q_2]A_1 + (p_2q_1 + p_3q_3)A_2 + (p_3q_1 + p_2q_3)A_3\}_{abef}. \end{aligned} \quad (11.252)$$

Applying this to $\frac{1}{3}(A_1 + A_2 + A_3)$ and $\frac{N+4}{9}A_1 + \frac{2}{9}A_2 + \frac{2}{9}A_3$, we find after symmetrization:

$$\begin{aligned} T_{I_4} &= \frac{1}{3} \left(\frac{N+4}{9} + N\frac{2}{9} + \frac{2}{9} \right) + \frac{1}{3} \left(\frac{2}{9} + \frac{2}{9} \right) + 2\frac{1}{3} \left(\frac{N+4}{9} + \frac{2}{9} \right) \\ &= \frac{1}{27} (5N + 22). \end{aligned} \quad (11.253)$$

The diagrams D_2D_1 and I_3D_1 in Eq. (11.233) have only a single loop attached to a line. Any such attachment inserts a tensor (11.241) into one of the index contractions, producing merely a factor $(N+2)/3$. Thus we obtain

$$T_{D_2D_1} = \left(\frac{N+2}{3} \right)^2, \quad (11.254)$$

$$T_{I_3D_1} = \left(\frac{N+8}{9} \right) \left(\frac{N+2}{3} \right). \quad (11.255)$$

Let us now consider the counterterms (11.213) and (11.214) in the presence of T -tensors (11.240). They become

$$(c_1^{m^2})_{\alpha\beta} = -\frac{1}{2}D_1^{\text{sg}}T_{D_1}\delta_{\alpha\beta}, \quad (c_2^{m^2})_{\alpha\beta} = \frac{1}{4}(D_2D_1)^{\text{sg}}T_{D_2D_1}\delta_{\alpha\beta} - \frac{1}{4}(D_1^{\text{sg}}D_2)^{\text{sg}}T_{D_1}T_{\alpha\beta\gamma\gamma} \\ - \frac{3}{4}(D_2^{\text{sg}}D_1)^{\text{sg}}T_IT_{\alpha\beta\gamma\gamma} + \frac{1}{6}D_3^{\text{sg}}(0)T_{D_3}\delta_{\alpha\beta}, \quad (11.256)$$

$$(c_1^\phi)_{\alpha\beta} = 0, \quad (c_2^\phi)_{\alpha\beta} = \frac{1}{6}D_3'^{\text{sg}}T_{D_3}\delta_{\alpha\beta}. \quad (11.257)$$

Inserting into (11.257) the relations $T_{D_1}T_{\alpha\beta\gamma\gamma} = T_{D_1}^2\delta_{\alpha\beta}$, $T_IT_{\alpha\beta\gamma\gamma} = T_{D_2}T_{D_1}\delta_{\alpha\beta}$, and going over to the dimensionless coupling constant $\lambda = gS_D\mu^{-\varepsilon}$ of Eq. (11.216), we obtain the generalization of Eqs. (11.217):

$$c^{m^2} = \lambda \frac{1}{2\varepsilon}T_{D_1} + \frac{\lambda^2}{4} \left[\frac{1}{\varepsilon^2}T_{D_2D_1} + \left(\frac{1}{\varepsilon^2} - \frac{1}{2\varepsilon} \right) T_{D_3} \right], \\ c^\phi = -\lambda^2 \frac{1}{48\varepsilon}T_{D_3}, \\ c^g = \frac{3}{2\varepsilon}\lambda T_I + \lambda^2 \left[\frac{3}{4} \frac{1}{\varepsilon^2}T_{I^2} + 3 \left(\frac{1}{2\varepsilon^2} + \frac{1}{4\varepsilon} \right) T_{I_4} \right]. \quad (11.258)$$

For the counterterms (11.222) and (11.225) we find similarly

$$(c_1^g)_{\alpha\beta\gamma\delta} = \frac{3}{2}I^{\text{sg}}T_IT_{\alpha\beta\gamma\delta} \quad (11.259)$$

$$(c_2^g)_{\alpha\beta\gamma\delta} = \left\{ -\frac{3}{4}(I^2)^{\text{sg}}T_{I^2} - \frac{3}{2}(I_3D_1)^{\text{sg}}T_IT_{D_1} - 3(I_4)^{\text{sg}}T_{I_4} \right. \\ \left. + \frac{9}{2}(I^{\text{sg}}I)^{\text{sg}}T_{I^{\text{sg}}I} + \frac{3}{2}(D_1^{\text{sg}}I_3)^{\text{sg}}T_{D_1^{\text{sg}}I_3} \right\} T_{\alpha\beta\gamma\delta}, \quad (11.260)$$

where

$$T_{I^{\text{sg}}I}T_{\alpha\beta\gamma\delta} = T_IT_{\alpha\beta\sigma\tau}T_{\sigma\tau\gamma\delta} = T_I^2T_{\alpha\beta\gamma\delta}, \quad T_{D_1^{\text{sg}}I_3} = T_{D_1}T_{\alpha\beta\sigma\tau}T_{\sigma\tau\gamma\delta} = T_{D_1}T_IT_{\alpha\beta\sigma\tau}. \quad (11.261)$$

The resulting generalization of (11.222) is

$$c_2^g = -\frac{3}{4} \left[(I^{\text{sg}})^2 + 2I^{\text{sg}}I^{\text{reg}} \right] T_{I^2} - 3(\Delta I_4^{\text{sg}} + I^{\text{sg}}I^{\text{reg}})T_{I_4} \\ + \frac{9}{2} \left[(I^{\text{sg}})^2 + I^{\text{sg}}I^{\text{reg}} \right] T_I^2. \quad (11.262)$$

With the reduced matrix elements (11.248) and (11.253), the regular terms I^{reg} cancel as before (here somewhat more miraculously), and c_2^g simplifies to

$$c_2^g = (I^{\text{sg}})^2 \left(\frac{9}{2}T_{I_4} - \frac{3}{4}T_I^2 \right) - 3\Delta I_4^{\text{sg}}T_{I_4}. \quad (11.263)$$

Inserting the reduced matrix elements (11.247)–(11.253), and the reduced coupling constant $\lambda = \tilde{g}S_D\mu^{-\varepsilon}$ of Eq. (11.216), the counterterms become, finally,

$$\begin{aligned} c^{m^2} &= \lambda \frac{1}{2\varepsilon} \frac{N+2}{3} + \lambda^2 \left[\frac{1}{4\varepsilon^2} \left(\frac{N+2}{3} \right)^2 - \frac{1}{4} \left(\frac{1}{\varepsilon^2} - \frac{1}{2\varepsilon} \right) \frac{N+2}{3} \right], \\ c^\phi &= -\lambda^2 \frac{1}{48\varepsilon} \frac{N+2}{3}, \\ c^g &= \lambda \frac{3}{2\varepsilon} \frac{N+8}{9} + \lambda^2 \left\{ \frac{3}{4\varepsilon^2} \frac{N^2+6N+20}{27} + 3 \left(\frac{1}{2\varepsilon^2} + \frac{1}{4\varepsilon} \right) \frac{5N+22}{27} \right\}. \end{aligned} \quad (11.264)$$

A further generalization, that is sometimes encountered in the literature useful for applications, is the case of n fields ϕ_i^α ($i = 1, \dots, n$), each of which occurring in an $O(q)$ -symmetric combination

$$\mathcal{L} = \frac{1}{2} \sum_{i,\alpha}^{n,q} [(\partial\phi_i^\alpha)^2 + m^2(\phi_i^\alpha)^2] + \frac{1}{4!} \sum_{i,j,k,l=1}^n g_{ijkl} \sum_{\alpha=1}^q \phi_i^\alpha \phi_j^\alpha \sum_{\beta=1}^q \phi_k^\beta \phi_l^\beta. \quad (11.265)$$

Among these, the case of a cubic symmetry in the indices is of special interest when there are only two independent couplings

$$\sum_{i,i'=1}^n g_{ii'} \sum_{\alpha=1}^q (\phi_i^\alpha)^2 \sum_{\beta=1}^q (\phi_{i'}^\beta)^2 = g_1 \left(\sum_{i=1}^n \sum_{\alpha=1}^q (\phi_i^\alpha)^2 \right)^2 + g_2 \sum_{i=1}^n \left(\sum_{\alpha=1}^q (\phi_i^\alpha)^2 \right)^2. \quad (11.266)$$

The special case of n complex fields (where ϕ_i^α with $\alpha = 1, 2$) governs the statistical mechanics of ensembles of dislocation lines in a crystal. Such fields are also used to describe phase transformations in cubic crystals. The interaction (11.272) corresponds to the tensor (11.232) being replaced by

$$\begin{aligned} T_{i\alpha,i\beta,k\gamma,l\delta} &= g_1 S_{i\alpha,j\beta,k\gamma,l\delta} + g_2 F_{i\alpha,j\beta,k\gamma,l\delta} \\ &= \frac{g_1}{3} (\delta_{ij}\delta_{kl}\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{ik}\delta_{jl}\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{il}\delta_{jk}\delta_{\alpha\delta}\delta_{\beta\gamma}) \\ &\quad + \frac{g_2}{3} (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) \delta_{ij}\delta_{ik}\delta_{il}. \end{aligned} \quad (11.267)$$

It is then straightforward to generalize the previous results. Take, for example, T_I arising from

$$T_{abef}T_{cdef}|_{\text{symm}} = T_{abcd}T_I. \quad (11.268)$$

Multiplying the tensors S , F with each other we find

$$\begin{aligned} SS|_{\text{symm}} &= \frac{nq+8}{9}S, \\ FF|_{\text{symm}} &= \frac{q+8}{9}F, \\ FS|_{\text{symm}} &= \frac{2}{3}F + \frac{q+2}{9}S. \end{aligned} \quad (11.269)$$

Hence, the lowest-order counterterms $c^g = \frac{2}{3}\lambda T_I$ are replaced by

$$\begin{aligned} c^{g_1} &= \frac{3}{2\varepsilon} \left(\frac{pq+8}{9} \lambda_1 + 2 \frac{q+2}{9} \lambda_2 \right), \\ c^{g_2} &= \frac{3}{2\varepsilon} \left(\frac{q+8}{9} \lambda_1 + \frac{4}{3} \lambda_2 \right). \end{aligned} \quad (11.270)$$

11.9 Finite S-Matrix Elements

We are now in a position to calculate also finite S matrix elements. Again we shall, for simplicity, consider here only elastic scattering between two ϕ -particles, the generalization being straight-forward.

Recalling Eq. (10.86), the four-point function $G^{(4)}(x_1, \dots, x_n)$ has the following structure: It consists of disconnected and connected parts with the disconnected ones being the product of two interacting single-particle Green functions: We may write

$$G^{(4)}(x_4, x_3, x_2, x_1) = \left[G^{(2)}(x_4, x_3) G^{(2)}(x_2, x_1) + 2 \text{ perm} \right] + G_c^{(4)}(x_4, x_3, x_2, x_1). \quad (11.271)$$

The two-particle Green functions were obtained by summing the one-particle irreducible graphs of the self-energy [see (11.26)] and by forming the geometric series in momentum space

$$G^{(2)}(q) = \frac{i}{q^2 - m^2 - \Sigma(q) + i\eta}. \quad (11.272)$$

The connected four-point function is then obtained as

$$G^{(4)}(q_4, q_3, q_2, q_1) = G^{(2)}(q_4) G^{(2)}(q_3) \Gamma^{(4)}(q_4, q_3, q_2, q_1) G^{(2)}(q_2) G^{(2)}(q_1), \quad (11.273)$$

where the vertex function $\Gamma^{(4)}(q_4, q_3, q_2, q_1)$ is the sum of all one-particle irreducible vertex graphs. We now prove that this vertex function gives directly the scattering amplitude if the momenta q_4, q_3, q_2, q_1 , are evaluated on the physical mass shells of the incoming and outgoing particles where the energies are given by $q_0 = \sqrt{\mathbf{q}^2 + m^2}$.⁴ The argument proceeds very similar to the previous discussion in Section (10.7). We form again the limit (10.111) but with the energies q_i^0 on the physical mass shells (rather than the bare mass shells used there). We are then confronted with studying the limit (10.112) with the fully interacting two-point function $G^{(2)}(q)$,

$$\lim_{x_1^0 \rightarrow -\infty} \sqrt{\frac{2q_1^0}{V}} e^{-i(q_1^0 x_1^0 - \mathbf{q}_1 \cdot \mathbf{x}_1)} \int \frac{d^4 q}{(2\pi)^4} e^{-iq(z-x)} \frac{i}{q^2 - m^2 - \Sigma(q) + i\eta}, \quad (11.274)$$

rather than the free one. The integrand has poles at the physical energy value $q^0 = \pm \sqrt{\mathbf{q}^2 + m^2} \mp i\eta$. In addition, there are cuts from the higher Feynman amplitudes, the lowest starting at $q_0 = \sqrt{\mathbf{q}^2 + (3m)^2}$ from the second-order graph $\ominus$. The

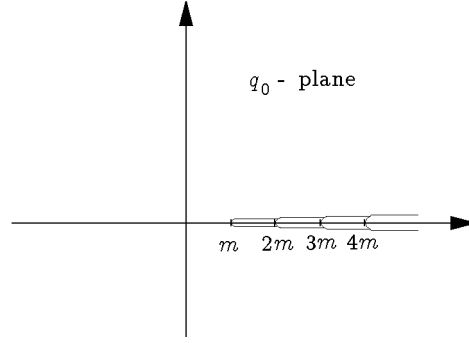


FIGURE 11.1 Singularities in the complex q_0 -plane of a Feynman propagator. There are poles and cuts due to three- and more-particle intermediate states in the diagram.

cuts are slightly displaced in the imaginary direction due to the $i\eta$ attached to each mass. Thus the complex q_0 -plane looks as shown in Fig. 11.1.

If we now distort the contour of the q^0 -integration, we may pick up the contribution of the pole at $q^0 = \sqrt{\mathbf{q}^2 + m^2}$ as well as the multi-particle cuts. In the limit $x_1^0 \rightarrow -\infty$, only the pole contributes. The contributions of its neighborhood disappear due to their infinitely rapid oscillations. These are equivalent to zero by the standard *Lebesgue lemma*. Thus we obtain the same rules as before but now for the interacting Green functions $G^{(2)}$ rather than $G_0^{(2)}$, and with the particles on the physical mass shell. As a consequence, the four-point function (11.273) gives the following S -matrix element

$$S(q_4, q_3 | q_2, q_1) = \delta_{q_3 q_1} \delta_{q_4 q_2} + \delta_{q_3 q_2} \delta_{q_4 q_1} + (2\pi)^4 \delta^{(4)}(q_4 + q_3 - q_2 - q_1) \prod_{i=1}^4 \frac{1}{\sqrt{2V q_i^0}} \Gamma^{(4)}(q_1, q_3, q_2, q_1), \quad (11.275)$$

with $\Gamma^{(4)}(q_1, q_3, q_2, q_1)$ being the amputated OPI four-point function evaluated for the on-shell momenta q_1, q_3, q_2, q_1 , with $q^0 = \sqrt{\mathbf{q}^2 + m^2}$ for the incoming and $q^0 = -\sqrt{\mathbf{q}^2 + m^2}$ for the outgoing particles. The first two terms in (11.275) correspond to the particles running past each other without scattering (the so-called *direct beam* right behind the sample in the experiment). The symmetrization in q_3, q_4 is a reflection of particle identity. The second term contains the amplitude for true scattering. The factor after the total momentum conservation $(2\pi)^4 \delta^{(4)}(p_f - p_i)$ function is $-i$ times the t -matrix defined in Section 10.7 [recall Eq. (9.293)].

In a scattering process where two particles enter and four emerge (a so-called *production process*), the disconnected parts are absent and we have directly

$$S(q_6, q_5, q_4, q_3 | q_2, q_1) = (2\pi)^4 \delta^{(4)}\left(\sum_{i=3}^6 q_i - \sum_{i=1}^2 q_i\right) i\Gamma^{(6)}(q_6, q_5, q_4, q_3, q_2, q_1) \prod_{i=1}^6 \frac{1}{\sqrt{2V q_i^0}}. \quad (11.276)$$

⁴Remember that the n -point vertex functions $\Gamma^{(n)}(q_n, q_{n-1}, \dots, q_4, q_3, q_2, q_1)$ are defined for any off-shell values of the energies.

Appendix 11A Second Proof of Veltman's Integral Rule

Here we shall convince ourselves in another way of the consistency of Veltman's integral rule (11.128):

$$\int d^D k k^{-2\nu} = 0, \quad D < 2\nu. \quad (11A.1)$$

In Eq. (11.226), this was derived by taking the limit $m \rightarrow 0$ in the dimensionally regularized integral (11.123) for $D > 2\nu$. Instead of the integral (11A.1), we shall discuss the more general integral

$$\int d^D k f(k), \quad (11A.2)$$

with a rotationally invariant $f(k)$ which is bound for large k by

$$|f(k)| < A k^{-2\nu}. \quad (11A.3)$$

Then the integral exists for $0 < D < 2\nu$, whereas it is not immediately defined for $-2 < D < 0$, since after integrating out the angular variables, the integrand has an IR-singularity at $k = 0$:

$$\int d^D k f(k) \equiv S_D \int_0^\infty dk k^{D-1} f(k).$$

This singularity can be circumvented by the same trick as the singularity at $\tau = 0$ in the integral (11.121). With some $c > 0$ we rewrite

$$\begin{aligned} \int d^D k f(k) &= S_D \left\{ \int_c^\infty dk k^{D-1} f(k) \right. \\ &\quad \left. + \int_0^c dk k^{D-1} [f(k) - f(0)] \right\} + f(0) \frac{c^D}{D}. \end{aligned} \quad (11A.4)$$

This is independent of c and defined for $-2 < D < 2\alpha$. In the limit $c \rightarrow 0$ it gives back the previous integral defined only for $0 < D < 2\alpha$. For $-2 < D < 0$ we can take the opposite limit $c \rightarrow \infty$ and only the second term survives:

$$\int d^D k f(k) = \int d^D k [f(k) - f(0)]. \quad (11A.5)$$

For $D \rightarrow 0$, the third term gives

$$\int d^0 k f(k) = f(0). \quad (11A.6)$$

Repeated application of this procedure permits a continuation of the integral to arbitrarily low dimensions $-2l - 2 < D < -2l$ ($l = 0, 1, 2, \dots$) via the formula

$$\int d^D k f(k) = \int d^D k \left\{ [f(k) - f(0)] - k^2 f'(0) - \dots - k^{2l} f^{(l)}(0) \right\}, \quad (11A.7)$$

with

$$\int d^{-2l} k f(k) = (-\pi)^{-l} f^{(l)}(0). \quad (11A.8)$$

Note that if an integral has initially no range of D where it exists, for instance if it runs over the function $f(k) = k^{-2\nu}(k^2 + a)/(k^2 + b)$, the above procedure serves to define it for $-2l + 2\nu < D < 2\nu$ ($l = 1, 2, 3, \dots$). With $l = 1$, for example, we define

$$\begin{aligned} \int d^D k k^{-2\nu} \frac{k^2 + a}{k^2 + b} &\equiv \int d^D k k^{-2\nu} \left(\frac{k^2 + a}{k^2 + b} - \frac{a}{b} \right) \\ &= \int d^D k k^{-2\nu} \frac{b - a}{b} \frac{k^2}{k^2 + b}, \end{aligned} \quad (11A.9)$$

with the right-hand side existing for $-2 + 2\nu < D < 2\nu$.

We now observe that this continuation procedure can make sense only if the difference between the two sides is formally equal to zero, i.e., if

$$\int d^D k k^{2\nu} = 0, \quad D < 2\nu. \quad (11A.10)$$

The basic reason for this identity is, of course, the fundamental requirement of dimensional regularization which implies that the Gaussian integral (11.119) holds for all D , positive and negative values. Setting q and m equal to zero this implies

$$\int d^D k e^{-\tau k^2} = \left(\frac{\pi}{\tau}\right)^{D/2}. \quad (11A.11)$$

For $D < 0$ the limit $\tau \rightarrow 0$ gives once more (11.124) while for $D = 0$ we obtain (11A.6). Inserting a factor $k^{-2\nu}$ we have

$$\int d^D k k^{-2\nu} e^{-\tau k^2} = \frac{\Gamma(D/2 - \nu)}{\Gamma(D/2)} \pi^{D/2} \tau^{\nu - D/2}. \quad (11A.12)$$

For $D < 2\nu$ the limit $\tau \rightarrow 0$ gives

$$\int d^D k k^{-2\nu} = 0, \quad (11A.13)$$

in agreement with (11A.10).

Note that this relation implies a specific choice of a small- k cutoff. Suppose we had regularized the small- k regime of the Gaussian integral by an exponential cutoff $e^{-\delta/k^2}$. Then we would have obtained

$$\int d^D k k^{-2\nu} e^{-\tau k^2 - \delta/k^2} = \frac{\Gamma(D/2 - \nu)}{\Gamma(D/2)} \frac{\pi^{D/2}}{\tau^{D/2 - \nu}} 2\sqrt{\tau\delta} K_{D/2 - \nu}(2\sqrt{\tau\delta}), \quad (11A.14)$$

where $K_\nu(z)$ is the modified Bessel function. For small z this behaves like

$$K_\nu(z) = K_{-\nu}(z) \approx \frac{1}{2} \Gamma(\nu) \left(\frac{z}{2}\right)^\nu, \quad (11A.15)$$

so that for small τ and δ , the integral would have been

$$\int d^D k k^{-2\nu} e^{-\tau k^2 - \delta/k^2} \approx \frac{\Gamma(D/2 - \nu)}{\Gamma(D/2)} \pi^{D/2} \begin{cases} \frac{\pi^{D/2}}{\tau^{D/2 - \nu}}, & D > 2\nu, \\ \frac{\pi^{D/2}}{\delta^{D/2 - \nu}}, & D < 2\nu, \end{cases} \quad (11A.16)$$

with the limit $\tau \rightarrow 0$ no longer giving zero for $D < 2\nu$ but a very large number. In a renormalizable massless theory this infinity must cancel order by order in perturbation theory. It is this property which makes it possible to use the infrared cutoff implied by the integral formula $\int d^D k k^{-2\nu} = 0$ also for $D > 2\nu$.

Notes and References

A detailed account of the techniques for extracting finite results from higher-order perturbation expansions up to five loops can be found in the books:

H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4 -Theories*, World Scientific, Singapore 2001, pp. 1–489 (klnrt.de/b8).

M.E. Peskin and D.V. Schroeder, *An Introduction to Quantum Field Theory*, Westview Press, N.Y. (1995).

J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, Clarendon Press, London 1969.

Higher-loop calculations are discussed in detail in the first of the above textbooks. See also:

H. Kleinert, J. Neu, V. Schulte-Frohlinde, K.G. Chetyrkin, and S.A. Larin, *Five-Loop Renormalization Group Functions of $O(n)$ -symmetric ϕ^4 -Theory and ε -Expansions of Critical Exponents up to ε^5* , Phys. Lett. B **272**, 39 (1991);

H. Kleinert and V. Schulte-Frohlinde, *Exact Five-Loop Renormalization Group Functions of ϕ^4 -Theory with $O(N)$ -Symmetric and Cubic Interactions. Critical Exponents up to ε^5* , Phys. Lett. B **342**, 284 (1995).

D.B. Murray and B.G. Nickel, (unpublished); preprint available from the last link on the webpage <http://klnrt.de/b8>.

*Nothing is mightier than an idea
whose time has come.*
V. M. HUGO (1802-1885)

12

Quantum Electrodynamics

In Chapter 7 we have learned how to quantize relativistic free fields and in Chapters 10 and 11 how to deal with interactions if the coupling is small. So far, this was only done perturbatively. Fortunately, there is a large set of physical phenomena for which perturbative techniques are sufficient to supply theoretical results that agree with experiment. In particular, there exists one theory, where the agreement is extremely good. This is the quantized theory of interacting electrons and photons called *quantum electrodynamics*, or shortly QED.

12.1 Gauge Invariant Interacting Theory

The free Lagrangians of electrons and photons are known from Chapter 5 as

$$\mathcal{L}(x) = \overset{\text{e}}{\mathcal{L}}(x) + \overset{\gamma}{\mathcal{L}}(x), \quad (12.1)$$

with

$$\overset{\text{e}}{\mathcal{L}}(x) = \bar{\psi}(x) (i\not{\partial} - m) \psi(x), \quad (12.2)$$

$$\overset{\gamma}{\mathcal{L}}(x) = -\frac{1}{4} F_{\mu\nu}(x) F^{\mu\nu}(x) = -\frac{1}{4} [\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)] [\partial^\mu A^\nu(x) - \partial^\nu A^\mu(x)]. \quad (12.3)$$

When quantizing the photon field, there were subtleties due to the gauge freedom in the choice of the gauge fields A_μ :

$$A_\mu(x) \rightarrow A_\mu(x) + \partial_\mu \Lambda(x). \quad (12.4)$$

For this reason, there were different ways of constructing a Hilbert space of free particles. The first, described in Subsection 7.5.1, was based on the quantization of only the two physical transverse degrees of freedom. The time component of the gauge field A^0 and the spatial divergence $\nabla \cdot \mathbf{A}(x)$ had no canonically conjugate field and were therefore classical fields, with no operator representation in the Hilbert space. The two fields are related by Coulomb's law which reads, in the absence of charges:

$$\nabla^2 A^0(x) = -\partial^0 \nabla \cdot \mathbf{A}(x). \quad (12.5)$$

Only the *transverse components*, defined by

$$A_{\perp}^i(x) \equiv \left(\delta^{ij} - \nabla^i \nabla^j / \nabla^2 \right) A^j(\mathbf{x}, t), \quad (12.6)$$

were operators. These components represent the proper dynamical variables of the system. After fulfilling the canonical commutation rules, the positive- and negative-frequency parts of these fields define creation and annihilation operators for the electromagnetic quanta. These are the photons of right and left circular polarization.

This method had an esthetical disadvantage that two of the four components of the vector field $A^{\mu}(x)$ require a different treatment. The components which become operators change with the frame of reference in which the canonical quantization procedure is performed.

To circumvent this, a covariant quantization procedure was developed by Gupta and Bleuler in Subsection 7.5.3. In their quantization scheme, the propagator took a pleasant covariant form. But this happened at the expense of another disadvantage, that this Lagrangian describes the propagation of four particles of which only two correspond to physical states. Accordingly, the Hilbert space contained two kinds of unphysical particle states, those with negative and those with zero norm. Still, a physical interpretation of this formalism was found with the help of a subsidiary condition that selects the physical subspace in the Hilbert space of free particles.

The final and most satisfactory successful quantization was developed by Faddeev and Popov [1] and was described in Subsection 7.5.2. It started out by modifying the initial photon Lagrangian by a gauge-fixing term

$$\mathcal{L}_{\text{GF}}(x) = -D\partial^{\mu}A_{\mu}(x) + \alpha D^2(x)/2. \quad (12.7)$$

After that, the quantization can be performed in the usual canonical way.

12.1.1 Reminder of Classical Electrodynamics of Point Particles

In this chapter we want to couple electrons and photons with each other by an appropriate interaction and study the resulting interacting field theory, the famous *quantum electrodynamics* (QED). Since the coupling should not change the two physical degrees of freedom described by the four-component photon field A^{μ} , it is important to preserve the gauge invariance, which was so essential in assuring the correct Hilbert space of free photons. The prescription how this can be done has been known for a long time in the context of classical electrodynamics of point particles. In that theory, a free relativistic particle moving along an arbitrarily parametrized path $x^{\mu}(\tau)$ in four-space is described by an action

$$\mathcal{A} = -mc^2 \int d\tau \sqrt{\frac{dx^{\mu}}{d\tau} \frac{dx_{\mu}}{d\tau}} = -mc^2 \int dt \left[1 - \frac{\mathbf{v}^2(t)}{c^2} \right]^{1/2}, \quad (12.8)$$

where $x^0(\tau) = t$ is the time and $d\mathbf{x}/dt = \mathbf{v}(t)$ the velocity along the path. If the particle has a charge e and lies at rest at position $\mathbf{x}$, its potential energy is

$$V(t) = e\phi(\mathbf{x}, t), \quad (12.9)$$

where

$$\phi(\mathbf{x}, t) = A^0(\mathbf{x}, t). \quad (12.10)$$

In our convention, the charge of the electron e has a negative value to agree with the sign in the historic form of the Maxwell equations

$$\begin{aligned} \nabla \cdot \mathbf{E}(x) &= -\nabla^2 \phi(x) = \rho(x), \\ \nabla \times \mathbf{B}(x) - \dot{\mathbf{E}}(x) &= \nabla \times \nabla \times \mathbf{A}(x) - \dot{\mathbf{E}}(x) \\ &= -[\nabla^2 \mathbf{A}(x) - \nabla \cdot \nabla \mathbf{A}(x)] - \dot{\mathbf{E}}(x) = \frac{1}{c} \mathbf{j}(x). \end{aligned} \quad (12.11)$$

If the electron moves along a trajectory $\mathbf{x}(t)$, the potential energy becomes

$$V(t) = e\phi(\mathbf{x}(t), t). \quad (12.12)$$

In the Lagrangian $L = T - V$, this contributes with the opposite sign

$$L^{\text{int}}(t) = -eA^0(\mathbf{x}(t), t), \quad (12.13)$$

adding a potential term to the interaction

$$\mathcal{A}^{\text{int}}|_{\text{pot}} = -e \int dt A^0(\mathbf{x}(t), t). \quad (12.14)$$

Since the time t coincides with $x^0(t)/c$ of the trajectory, this can be expressed as

$$\mathcal{A}^{\text{int}}|_{\text{pot}} = -\frac{e}{c} \int dx^0 A^0(x). \quad (12.15)$$

In this form it is now quite simple to write down the complete electromagnetic interaction purely on the basis of relativistic invariance. The minimal Lorentz-invariant extension of (12.15) is obviously

$$\mathcal{A}^{\text{int}} = -\frac{e}{c} \int dx^\mu A_\mu(x). \quad (12.16)$$

Thus, the full action of a point particle can be written, more explicitly, as

$$\begin{aligned} \mathcal{A} &= \int dt L(t) = -mc \int ds - \frac{e}{c} \int dx^\mu A_\mu(x) \\ &= -mc^2 \int dt \left[1 - \frac{\mathbf{v}^2}{c^2} \right]^{1/2} - e \int dt \left(A^0 - \frac{1}{c} \mathbf{v} \cdot \mathbf{A} \right). \end{aligned} \quad (12.17)$$

The canonical formalism supplies the canonically conjugate momentum

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = m \frac{\mathbf{v}}{\sqrt{1 - \mathbf{v}^2/c^2}} + \frac{e}{c} \mathbf{A} \equiv \mathbf{p} + \frac{e}{c} \mathbf{A}. \quad (12.18)$$

Thus the velocity is related to the canonical momentum and external vector potential via

$$\frac{\mathbf{v}}{c} = \frac{\mathbf{P} - \frac{e}{c}\mathbf{A}}{\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2}}. \quad (12.19)$$

This can be used to calculate the Hamiltonian as the Legendre transform

$$H = \frac{\partial L}{\partial \mathbf{v}} \mathbf{v} - L = \mathbf{P} \cdot \mathbf{v} - L, \quad (12.20)$$

with the result

$$H = c\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2} + eA^0. \quad (12.21)$$

At nonrelativistic velocities, this has the expansion

$$H = mc^2 + \frac{1}{2m}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + eA^0 + \dots. \quad (12.22)$$

The rest energy mc^2 is usually omitted in this limit.

12.1.2 Electrodynamics and Quantum Mechanics

When going over from quantum mechanics to second-quantized field theory in Chapter 2, we found the rule that a nonrelativistic Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \quad (12.23)$$

becomes an operator

$$H = \int d^3x \psi^\dagger(\mathbf{x}, t) \left[-\frac{\nabla^2}{2m} + V(\mathbf{x}) \right] \psi(\mathbf{x}, t). \quad (12.24)$$

For brevity, we have omitted a hat on top of H and the fields $\psi^\dagger(\mathbf{x}, t), \psi(\mathbf{x}, t)$. Following the rules of Chapter 2, we see that the second-quantized form of the interacting nonrelativistic Hamiltonian in a static $A(\mathbf{x})$ field with the Hamiltonian (12.22) (minus mc^2),

$$H = \frac{(\mathbf{P} - e\mathbf{A})^2}{2m} + eA^0, \quad (12.25)$$

is given by

$$H = \int d^3x \psi^\dagger(\mathbf{x}, t) \left[-\frac{1}{2m} \left(\nabla - i\frac{e}{c}\mathbf{A} \right)^2 + eA^0 \right] \psi(\mathbf{x}, t). \quad (12.26)$$

The action of this theory reads

$$\mathcal{A} = \int dt L = \int dt \int d^3x \left[\psi^\dagger(\mathbf{x}, t) \left(i\partial_t + eA^0 \right) \psi(\mathbf{x}, t) + \frac{1}{2m} \psi^\dagger(\mathbf{x}, t) \left(\nabla - i\frac{e}{c}\mathbf{A} \right)^2 \psi(\mathbf{x}, t) \right]. \quad (12.27)$$

It is easy to verify that (12.26) reemerges from the Legendre transform

$$H = \frac{\partial L}{\partial \dot{\psi}(\mathbf{x}, t)} \dot{\psi}(\mathbf{x}, t) - L. \quad (12.28)$$

The action (12.27) holds also for time-dependent $A^\mu(x)$ -fields.

These equations show that electromagnetism is introduced into a free quantum theory of charged particles following the minimal substitution rule

$$\begin{aligned} \nabla &\rightarrow \nabla - i\frac{e}{c}\mathbf{A}(\mathbf{x}, t), \\ \partial_t &\rightarrow \partial_t + ieA^0(\mathbf{x}, t), \end{aligned} \quad (12.29)$$

or covariantly:

$$\partial_\mu \rightarrow \partial_\mu - i\frac{e}{c}A_\mu(x). \quad (12.30)$$

The substituted action has the important property that the gauge invariance of the free photon action is preserved by the interacting theory: If we perform the gauge transformation

$$A^\mu(x) \rightarrow A^\mu(x) + \partial^\mu \Lambda(x), \quad (12.31)$$

i.e.,

$$\begin{aligned} A^0(\mathbf{x}, t) &\rightarrow A^0(\mathbf{x}, t) + \partial_t \Lambda(\mathbf{x}, t), \\ \mathbf{A}(\mathbf{x}, t) &\rightarrow \mathbf{A}(\mathbf{x}, t) - \nabla \Lambda(\mathbf{x}, t), \end{aligned} \quad (12.32)$$

the action remains invariant provided that we simultaneously change the fields $\psi(\mathbf{x}, t)$ of the charged particles by a spacetime-dependent phase

$$\psi(\mathbf{x}, t) \rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \psi(\mathbf{x}, t). \quad (12.33)$$

Under this transformation, the space and time derivatives of the field change like

$$\begin{aligned} \nabla \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left[\nabla - i\frac{e}{c}\nabla \Lambda(\mathbf{x}, t) \right] \psi, \\ \partial_t \psi &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} (\partial_t - ie\partial_t \Lambda) \psi(\mathbf{x}, t). \end{aligned} \quad (12.34)$$

The covariant derivatives in the action (12.27) have therefore the following simple transformation law:

$$\begin{aligned} \left(\nabla - i\frac{e}{c}\mathbf{A} \right) \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left(\nabla - i\frac{e}{c}\mathbf{A} \right) \psi(\mathbf{x}, t), \\ \left(\partial_t + i\frac{e}{c}A^0 \right) \psi(\mathbf{x}, t) &\rightarrow e^{-i(e/c)\Lambda(\mathbf{x}, t)} \left(\partial_t + ieA^0 \right) \psi(\mathbf{x}, t). \end{aligned} \quad (12.35)$$

These combinations of derivatives and gauge fields are called *covariant derivatives* and are written as

$$\begin{aligned}\mathbf{D}\psi(\mathbf{x}, t) &\equiv \left(\nabla - i\frac{e}{c}\mathbf{A} \right) \psi(\mathbf{x}, t), \\ D_t\psi(\mathbf{x}, t) &\equiv \left(\partial_t + ieA^0 \right) \psi(\mathbf{x}, t),\end{aligned}\tag{12.36}$$

or, in four-vector notation, as

$$D_\mu\psi(x) = \left(\partial_\mu + i\frac{e}{c}A_\mu \right) \psi(x).\tag{12.37}$$

Here the adjective “covariant” does not refer to the Lorentz group but to the gauge group. It records the fact that $D_\mu\psi$ transforms under local gauge changes (12.29) of ψ in the same way as ψ itself in (12.33):

$$D_\mu\psi(x) \rightarrow e^{-i(e/c)\Lambda(x)} D_\mu\psi(x).\tag{12.38}$$

With the help of such covariant derivatives, any action which is invariant under global phase changes by a constant phase angle [i.e., $U(1)$ -invariant in the sense discussed in Section 8.11.1]

$$\psi(x) \rightarrow e^{-i\alpha}\psi(x),\tag{12.39}$$

can easily be made invariant under *local* gauge transformations (12.31). We merely have to replace all derivatives by covariant derivatives (12.37), and add to the field Lagrangian the gauge-invariant photon expression (12.3).

12.1.3 Principle of Nonholonomic Gauge Invariance

The minimal substitution rule can be viewed as a consequence of a more general principle of *nonholonomic gauge invariance*. The physics of the initial action (12.17) is trivially invariant under the addition of a term

$$\Delta\mathcal{A} = -\frac{e}{c} \int dt \dot{x}^\mu(t) \partial_\mu \Lambda(x).\tag{12.40}$$

The integral runs over the particle path and contributes only a pure surface term from the endpoints:

$$\Delta\mathcal{A} = -\frac{e}{c} [\Lambda(x_b) - \Lambda(x_a)].\tag{12.41}$$

This does not change the particle trajectories. If we now postulate that the dynamical laws of physics remain also valid when we admit *multivalued* gauge functions $\Lambda(x)$ for which the Schwarz integrability criterion is violated, i.e., which possess noncommuting partial derivatives:

$$(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu)\Lambda(x) \neq 0.\tag{12.42}$$

Then the derivatives

$$A_\mu(x) = \partial_\mu \Lambda(x) \quad (12.43)$$

have a nonzero curl $F_{\mu\nu} = (\partial_\mu A_\nu - \partial_\nu A_\mu) = (\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) \Lambda(x) \neq 0$, and the action (12.41) coincides with the interaction (12.16).

Similarly we can derive the equations of motion of a wave function in an electromagnetic field from that in field-free space by noting the trivial invariance of quantum mechanics without fields under gauge transformations (12.33), and by extending the set of permissible gauge functions $\Lambda(x)$ to multivalued functions for which the partial derivatives do not commute as in (12.42).

In either case, the nonholonomic gauge transformations convert the physical laws obeyed by a particle in Euclidean spacetime without electromagnetism into those with electromagnetic fields.

This principle is discussed in detail in the literature [11]. It can be generalized to derive the equations of motion in a curved spacetime from those in flat spacetime by nonholonomic coordinate transformations which introduce defects in spacetime.

12.1.4 Electrodynamics and Relativistic Quantum Mechanics

Let us follow this rule for relativistic electrons and replace, in the Lagrangian (12.2), the differential operator $\not{\partial} = \gamma^\mu \partial_\mu$ by

$$\gamma^\mu \left(\partial_\mu + i \frac{e}{c} A_\mu \right) = \left(\not{\partial} + i \frac{e}{c} \not{A} \right) \equiv \not{D}. \quad (12.44)$$

In this way we arrive at the Lagrangian of quantum electrodynamics (QED)

$$\mathcal{L}(x) = \bar{\psi}(x) (i\not{D} - m) \psi(x) - \frac{1}{4} F_{\mu\nu}^2. \quad (12.45)$$

The classical field equations can easily be found by extremizing the action with respect to all fields, which gives

$$\frac{\delta \mathcal{A}}{\delta \bar{\psi}(x)} = (i\not{D} - m) \psi(x) = 0, \quad (12.46)$$

$$\frac{\delta \mathcal{A}}{\delta A_\mu(x)} = \partial_\nu F^{\nu\mu}(x) - \frac{1}{c} j^\mu(x) = 0, \quad (12.47)$$

where $j^\mu(x)$ is the *current density*:

$$j^\mu(x) \equiv ec \bar{\psi}(x) \gamma^\mu \psi(x). \quad (12.48)$$

Equation (12.47) coincides with the Maxwell equation for the electromagnetic field around a classical four-dimensional vector current $j^\mu(x)$:

$$\partial_\nu F^{\nu\mu}(x) = \frac{1}{c} j^\mu(x). \quad (12.49)$$

In the Lorenz gauge $\partial_\mu A^\mu(x) = 0$, this equation reduces to

$$-\partial^2 A^\mu(x) = \frac{1}{c} j^\mu(x). \quad (12.50)$$

The current density j^μ combines the charge density $\rho(x)$ and the spatial current density $\mathbf{j}(x)$ of particles of charge e in a four-vector:

$$j^\mu = (c\rho, \mathbf{j}). \quad (12.51)$$

In terms of electric and magnetic fields $E^i = F^{i0}$, $B^i = -F^{jk}$, the field equations (12.49) turn into the Maxwell equations

$$\nabla \cdot \mathbf{E} = \rho = e\bar{\psi}\gamma^0\psi = e\psi^\dagger\psi, \quad (12.52)$$

$$\nabla \times \mathbf{B} - \dot{\mathbf{E}} = \frac{1}{c} \mathbf{j} = \frac{e}{c} \bar{\psi}\boldsymbol{\gamma}\psi. \quad (12.53)$$

The first is Coulomb's law, the second is Ampère's law in the presence of charges and currents.

Note that the physical units employed here differ from those used in many books of classical electrodynamics [12], by the absence of a factor $1/4\pi$ on the right-hand side. The Lagrangian used in those books is

$$\begin{aligned} \mathcal{L}(x) &= -\frac{1}{8\pi} F_{\mu\nu}^2(x) - \frac{1}{c} j^\mu(x) A_\mu(x) \\ &= \frac{1}{4\pi} [\mathbf{E}^2(x) - \mathbf{B}^2(x)] - \left[\rho(x)\phi(x) - \frac{1}{c} \mathbf{j}(x) \cdot \mathbf{A}(x) \right], \end{aligned} \quad (12.54)$$

which leads to Maxwell's field equations

$$\begin{aligned} \nabla \cdot \mathbf{E} &= 4\pi\rho, \\ \nabla \times \mathbf{B} - \dot{\mathbf{E}} &= \frac{4\pi}{c} \mathbf{j}. \end{aligned} \quad (12.55)$$

The form employed conventionally in quantum field theory arises from this by replacing $A \rightarrow \sqrt{4\pi}A$ and $e \rightarrow -\sqrt{4\pi}e^2$. The charge of the electron in our units has therefore the numerical value

$$e = -\sqrt{4\pi\alpha} \approx -\sqrt{4\pi/137} \quad (12.56)$$

rather than $e = -\sqrt{\alpha}$.

12.2 Noether's Theorem and Gauge Fields

In electrodynamics, the conserved charge resulting from the U(1)-symmetry of the matter Lagrangian by Noether's theorem (recall Chapter 8) is the source of a massless particle, the photon. This is described by a gauge field which is minimally coupled to the conserved current. A similar structure will be seen in Chapters 27

and 28 to exist for many internal symmetries giving rise to nonabelian versions of the photon, for instance the famous W - and Z -vector mesons, which mediate the weak interactions, or the gluons which give rise to strong interactions. It is useful to recall Noether's derivation of conservation laws in such theories.

For a locally gauge invariant theory, the conserved matter current can no longer be found by the rule (8.118), which was so useful in the globally invariant theory. Indeed, in quantum electrodynamics, the derivative with respect to the local field transformation $\epsilon(x)$ would be simply given by

$$j_\mu = \frac{\delta \mathcal{L}}{\partial \partial_\mu \Lambda}, \quad (12.57)$$

since this would be identically equal to zero, due to local gauge invariance. We may, however, subject *just* the matter field to a local gauge transformation at *fixed* gauge fields. Then we obtain the correct current

$$j_\mu \equiv \left. \frac{\partial \mathcal{L}}{\partial \partial_\mu \Lambda} \right|_\gamma. \quad (12.58)$$

Since the complete change under local gauge transformations $\delta_s^x \mathcal{L}$ vanishes identically, we can alternatively vary *only* the gauge fields and keep the electron field fixed

$$j_\mu = - \left. \frac{\partial \mathcal{L}}{\partial \partial_\mu \Lambda} \right|_e. \quad (12.59)$$

This is done most simply by forming the functional derivative with respect to the gauge field, and by omitting the contribution of $\tilde{\mathcal{L}}$:

$$j_\mu = - \frac{\partial \mathcal{L}^e}{\partial \partial_\mu \Lambda}. \quad (12.60)$$

An interesting consequence of local gauge invariance can be found for the gauge field itself. If we form the variation of the pure gauge field action

$$\delta_s^\gamma \mathcal{A} = \int d^4x \operatorname{tr} \left[\delta_s^x A_\mu \frac{\gamma \mathcal{A}^\epsilon}{\delta A_\mu} \right], \quad (12.61)$$

and insert, for $\delta_s^x A$, an infinitesimal pure gauge field configuration

$$\delta_s^x A_\mu = -i \partial_\mu \Lambda(x), \quad (12.62)$$

the variation must vanish for all $\Lambda(x)$. After a partial integration, this implies the local conservation law $\partial_\mu j^\mu(x) = 0$ for the current

$$j^\mu(x) = -i \frac{\delta \mathcal{A}^\gamma}{\delta A_\mu}. \quad (12.63)$$

In contrast to the earlier conservation laws derived for matter fields which were valid only if the matter fields obey the Euler-Lagrange equations, the current conservation law for gauge fields is valid for *all* field configurations. It is an *identity*, often called *Bianchi identity* due to its close analogy with certain identities in Riemannian geometry.

To verify this, we insert the Lagrangian (12.3) into (12.63) and find $j^\nu = \partial_\mu F^{\mu\nu}/2$. This current is trivially conserved for any field configuration due to the antisymmetry of $F^{\mu\nu}$.

12.3 Quantization

The canonical formalism can be used to identify canonical momenta of the fields $\psi(x)$ and $A^i(x)$:

$$\pi_\psi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}(x)} = \psi^\dagger(x), \quad (12.64)$$

and

$$\pi_{A^i}(x) \equiv \pi^i(x) = F^{0i}(x) = -E^i(x), \quad (12.65)$$

and to find the Hamiltonian density

$$\begin{aligned} \mathcal{H}(x) &= \frac{\partial L}{\partial \dot{\psi}(x)} \dot{\psi}(x) + \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^k(x)} \dot{A}^k(x) - \mathcal{L}(x) \\ &= \bar{\psi}(-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + m)\psi + \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) + \boldsymbol{\nabla} A^0 \cdot \mathbf{E} + e\bar{\psi}\gamma_\mu\psi A^\mu. \end{aligned} \quad (12.66)$$

Here, and in all subsequent discussions, we use natural units in which the light velocity is equal to unity.

The quantization procedure in the presence of interactions now goes as follows: The Dirac field of the electron has the same equal-time anticommutation rules as in the free case:

$$\begin{aligned} \{\psi_a(\mathbf{x}, t), \psi_b^\dagger(\mathbf{x}', t)\} &= \delta^{(3)}(\mathbf{x}' - \mathbf{x})\delta_{ab}, \\ \{\psi(\mathbf{x}, t), \psi(\mathbf{x}', t)\} &= 0, \\ \{\psi^\dagger(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)\} &= 0. \end{aligned} \quad (12.67)$$

For the photon field we first write down the naive commutation rules of the spatial components:

$$-[E_i(\mathbf{x}, t), A_j(\mathbf{x}', t)] = -i\delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta_{ij} \quad (12.68)$$

$$[A_i(\mathbf{x}, t), A_j(\mathbf{x}', t)] = 0, \quad (12.69)$$

$$[E_i(\mathbf{x}, t), E_j(\mathbf{x}', t)] = 0. \quad (12.70)$$

As in Eq. (7.346), the first commutator cannot be true here, since by Coulomb's law (12.52):

$$\begin{aligned}\nabla \cdot \mathbf{E} &= -\nabla \cdot \dot{\mathbf{A}} - \nabla^2 A^0 \\ &= e\psi^\dagger\psi,\end{aligned}\tag{12.71}$$

and we want the canonical fields A_i to be independent of $\psi, \psi^\dagger$, and thus to commute with them. The contradiction can be removed just as in the free case by postulating (12.68) only for the transverse parts of E_i , and using $\delta_{ij}^T(\mathbf{x} - \mathbf{x}')$ as in (7.347), while letting the longitudinal part $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$ be a c -number field, since it commutes with all $A^i(\mathbf{x}, t)$. The correct commutation rules are the following:

$$\begin{aligned}\left[\dot{A}_j(\mathbf{x}, t), A_j(\mathbf{x}', t)\right] &= -i\delta_{ij}^T(\mathbf{x} - \mathbf{x}'), \\ \left[A_j(\mathbf{x}, t), A_j(\mathbf{x}', t)\right] &= 0, \\ \left[\dot{A}_i(\mathbf{x}, t), \dot{A}_j(\mathbf{x}', t)\right] &= 0.\end{aligned}\tag{12.72}$$

To calculate the temporal behavior of an arbitrary observable composed of $\psi, \psi^\dagger$, and of $A_i, \dot{A}_i$ fields, only one more set of commutation rules has to be specified which are those with A^0 . This field occurs in the Hamiltonian density (12.66) and is not one of the canonical variables. Moreover, in contrast to the free-field case in Section 7.5, it is no longer a c -number. To see this, we express A^0 in terms of the dynamical fields using Coulomb's law (12.71):

$$A^0(\mathbf{x}, t) = \frac{1}{4\pi} \int d^3x' \frac{1}{|\mathbf{x}' - \mathbf{x}|} \left(e\psi^\dagger\psi + \nabla \cdot \dot{\mathbf{A}} \right)(\mathbf{x}', t).\tag{12.73}$$

This replaces Eq. (4.268) in the presence of charges. In an infinite volume with asymptotically vanishing fields, there is no freedom of adding a solution of the homogeneous Poisson equation (4.269). Hence, whereas $\nabla \cdot \mathbf{A}$ is a c -number field, the time component of the gauge field A^0 is now a non-local operator involving the fermion fields. Since these are independent of the electromagnetic field, A^0 still commutes with the canonical $A_i, \dot{A}_j$ fields:

$$\left[A^0(\mathbf{x}, t), A^i(\mathbf{x}')\right] = \left[A^0(\mathbf{x}, t), \dot{A}^i(\mathbf{x}', t)\right] = 0.\tag{12.74}$$

The commutator with the Fermi fields, on the other hand, is nonzero:

$$\left[A^0(\mathbf{x}, t), \psi(\mathbf{x}', t)\right] = -\frac{e}{4\pi|\mathbf{x} - \mathbf{x}'|}\psi(\mathbf{x}, t).\tag{12.75}$$

Note the peculiar property of A^0 : It does not commute with the electron field, no matter how large the distance between the space points is. This property is called *nonlocality*. It is a typical property of the present transverse covariant quantization procedure.

Certainly, the arbitrary c -number function $\nabla \cdot \mathbf{A}(\mathbf{x}, t)$ can be made zero by an appropriate gauge transformation, as in (4.257).

In the Hamiltonian, the field A^0 can be completely removed by a partial integration:

$$\int d^3x \nabla A^0 \cdot \mathbf{E} = - \int d^3x A^0 \nabla \cdot \mathbf{E}, \quad (12.76)$$

if we set the surface term equal to zero. Using now the field equation

$$\nabla \cdot \mathbf{E} = e\psi^\dagger \psi, \quad (12.77)$$

we derive

$$\begin{aligned} H &= \int d^3x \mathcal{H} \\ &= \int d^3x \left\{ \bar{\psi} \left[-i\boldsymbol{\gamma} \cdot (\nabla - i\frac{e}{c}\mathbf{A}) + m \right] \psi + \frac{1}{2} (\mathbf{E}^2 + \mathbf{B}^2) \right\}. \end{aligned} \quad (12.78)$$

When looking at this expression, one may wonder where the electrostatic interaction has gone. The answer is found by decomposing the electric field

$$E^i = -\partial^0 A^i + \partial^i A^0 \quad (12.79)$$

into longitudinal and transverse parts E_L^i and E_T^i with $\mathbf{E}_L \cdot \mathbf{E}_T = 0$:

$$\begin{aligned} E_L^i &= \partial^i \left(A^0 - \frac{\partial^i \partial^j}{\nabla^2} A^j \right), \\ E_T^i &= -\partial^0 \left(\delta^{ij} - \frac{\partial^i \partial^j}{\nabla^2} \right) A^j. \end{aligned} \quad (12.80)$$

Then the field energy becomes

$$\frac{1}{2} \int d^3x (\mathbf{E}^2 + \mathbf{B}^2) = \frac{1}{2} \int d^3x (\mathbf{E}_T^2 + \mathbf{B}^2) + \frac{1}{2} \int d^3x \mathbf{E}_L^2. \quad (12.81)$$

Using (12.73), we see that the longitudinal field is simply given by

$$\begin{aligned} \mathbf{E}_L(x) &= -\frac{1}{4\pi} \nabla \int d^3x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} e\psi^\dagger(\mathbf{x}', t)\psi(\mathbf{x}', t) \\ &= \nabla \left[\frac{1}{\nabla^2} e\psi^\dagger(x)\psi(x) \right]. \end{aligned} \quad (12.82)$$

It is the Coulomb field caused by the charge density of the electron $e\psi^\dagger(x)\psi(x)$. The field energy carried by $E_L^i(x)$ is

$$\begin{aligned} \frac{1}{2} \int d^3x \mathbf{E}_L^2(x) &= \frac{e^2}{2} \int d^3x \left\{ \nabla \left[\frac{1}{\nabla^2} \psi^\dagger(x)\psi(x) \right] \right\}^2 \\ &= -\frac{e^2}{2} \int d^3x \psi^\dagger(x)\psi(x) \frac{1}{\nabla^2} \psi^\dagger(x)\psi(x) \\ &= \frac{e^2}{8\pi} \int d^3x d^3x' \psi^\dagger(\mathbf{x}, t)\psi(\mathbf{x}, t) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \psi^\dagger(\mathbf{x}', t)\psi(\mathbf{x}', t). \end{aligned} \quad (12.83)$$

This coincides precisely with the classical Coulomb energy associated with the charge density (12.52). The term $\frac{1}{2} \int d^3x (\mathbf{E}_T^2 + \mathbf{B}^2)$ in Eq. (12.81), on the other hand, is an operator and contains the energy of the field quanta.

In order to develop a perturbation theory for QED in this quantization, we must specify the free and interacting parts of the action. Since A^0 and $\nabla \cdot \mathbf{A}$ are unquantized and appear only quadratically in the action, they may be eliminated in the action in the same way as in the energy, so that the action becomes

$$\mathcal{A} = \int d^4x \left\{ \bar{\psi}(x)(i\cancel{\partial} - M)\psi(x) + \frac{1}{2} [\mathbf{E}_T^2(x) - \mathbf{B}^2(x)] \right\} + \mathcal{A}^{\text{int}}. \quad (12.84)$$

The first two terms are the actions of the Dirac field ψ and transverse electromagnetic fields $\mathbf{A}_T$, and $\mathcal{A}^{\text{int}}$ denotes the interaction

$$\mathcal{A}^{\text{int}} = -\frac{e^2}{8\pi} \int dt \int d^3x d^3x' \psi^\dagger(\mathbf{x}, t) \psi(\mathbf{x}, t) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \psi(\mathbf{x}', t) \psi(\mathbf{x}', t) + \int d^4x \frac{1}{c} \mathbf{j} \cdot \mathbf{A}_T. \quad (12.85)$$

The interaction contains two completely different terms: The first is an instantaneous Coulomb interaction at a distance, which takes place without retardation and involves the charge density. It is a nontrivial field-theoretic exercise to show that the absence of retardation in the first term is compensated by current-current interaction resulting from the second term, so that it does not cause any conflicts with relativity. This will be done at the end of Section 14.16.

The special role of the Coulomb interaction is avoided from the beginning in the Gupta-Bleuler quantization procedure that was discussed in Subsection 7.5.2. There the free action was

$$\mathcal{A} = \int d^4x \left[\bar{\psi}(i\cancel{\partial} - m)\psi - \frac{1}{4} F^{\mu\nu} F_{\mu\nu} - D\partial^\mu A_\mu + D^2/2 \right], \quad (12.86)$$

and the interaction had the manifestly covariant form

$$\mathcal{A}^{\text{int}} = - \int d^4x j^\mu A_\mu. \quad (12.87)$$

12.4 Perturbation Theory

Let us now set up the rules for building the Feynman diagrams to calculate the effect of the interaction. In this context, we shall from now on attach, to the free propagator, a subscript 0. The propagator of the free photon depends on the gauge. It is most simple in the Gupta-Bleuler quantization scheme, where [see (7.510)]

$$G_0^{\mu\nu}(x, x') = -g^{\mu\nu} G_0(x, x') = -g^{\mu\nu} \int \frac{d^4q}{(2\pi)^4} \frac{i}{q^2 + i\eta} e^{-ik(x-x')}. \quad (12.88)$$

Since we want to calculate the effect of interactions, we shall from now on attach to the free propagator a subscript 0.

The free-particle propagator of the electrons was given in (7.289):

$$S_0(x - x') = \int \frac{d^4 p}{(2\pi)^4} \frac{i}{\not{p} - M + i\eta} e^{-ip(x-x')}. \quad (12.89)$$

In a Wick expansion of $e^{i\mathcal{A}^{\text{int}}}$, each contraction is represented by one of these two propagators:

$$\overbrace{A^\mu(x) A^\nu(x')} = G_0^{\mu\nu}(x - x'), \quad (12.90)$$

$$\overbrace{\psi(x) \bar{\psi}(x')} = S_0(x - x'). \quad (12.91)$$

In the Feynman diagrams, they are pictured by the lines

$$\text{wavy line } q = -g^{\mu\nu} \frac{i}{q^2 + i\epsilon}, \quad (12.92)$$

$$\text{solid line } p = \frac{i}{\not{p} - m}. \quad (12.93)$$

The interaction Lagrangian

$$\mathcal{L}^{\text{int}} = -e\bar{\psi}\gamma^\mu A_\mu(x) \quad (12.94)$$

is pictured by the vertex

$$\begin{array}{c} \text{wavy line } q = p' - p \\ \uparrow \\ \text{solid line } p' \text{ and } p \end{array} = -e\gamma^\mu. \quad (12.95)$$

With these graphical elements we must form all Feynman diagrams which can contribute to a given physical process.

In the transverse quantization scheme, the Feynman diagrams are much more complicated. Recalling the propagator (7.361), the photon line stands now for

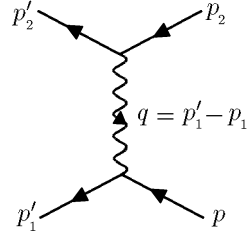
$$\text{wavy line } q = P_{\text{phys}}^{\mu\nu}(q) \frac{i}{q^2 + i\epsilon}, \quad (12.96)$$

with the physical off-shell polarization sum [compare (12.7)]

$$P_{\text{phys}}^{\mu\nu}(q) = -g^{\mu\nu} - \frac{q_\mu q_\nu}{(q\eta)^2 - q^2} + q\eta \frac{q_\mu \eta_\nu + q_\nu \eta_\mu}{(q\eta)^2 - q^2} - \eta_\mu \eta_\nu \frac{q^2}{(q\eta)^2 - q^2}. \quad (12.97)$$

The photon propagator is very complicated due to the appearance of the frame-dependent auxiliary vector $\eta = (1, 0, 0, 0)$. As a further complication, there are

diagrams from the four-fermion Coulomb interactions in (12.85). These can be pictured by a photon exchange diagram

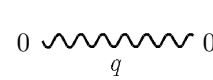


$$= \frac{i}{\mathbf{q}^2} \gamma^0 \times \gamma^0. \quad (12.98)$$

They may be derived from an auxiliary interaction

$$\mathcal{A}^{\text{int}} = - \int d^4x j^0 A_0, \quad (12.99)$$

assuming the A_0 -field to have the propagator



$$= \frac{i}{\mathbf{q}^2}. \quad (12.100)$$

If this propagator is added to the physical one, it cancels precisely the last term in the off-shell polarization sum (12.97), which becomes effectively

$$P_{\text{phys,eff}}^{\mu\nu}(\mathbf{k}) = -g^{\mu\nu} - \frac{q_\mu q_\nu}{(q\eta)^2 - q^2} + q\eta \frac{q_\mu \eta_\nu + q_\nu \eta_\mu}{(q\eta)^2 - q^2}. \quad (12.101)$$

Of course, the final physical results cannot depend on the frame in which the theory is quantized. Thus it must be possible to drop all η -dependent terms. We shall now prove this in three steps:

First, a photon may be absorbed (or emitted) by an electron which is on their mass shell before and after the process. The photon propagator is contracted with an electron current as follows

$$\bar{u}(\mathbf{p}', s'_3) \gamma_\mu u(\mathbf{p}, s'_3) P_{\text{phys,eff}}^{\mu\nu}(q). \quad q = p' - p. \quad (12.102)$$

Since the spinors on the right and left-hand side satisfy the Dirac equation, the current is conserved and satisfies

$$\bar{u}(\mathbf{p}', s'_3) \gamma_\mu u(\mathbf{p}, s'_3) q^\mu = 0. \quad (12.103)$$

This condition eliminates the terms containing the vector q^μ in the polarization sum (12.101). Only the reduced polarization sum

$$P_{\text{red}}^{\mu\nu}(q) = -g^{\mu\nu} \quad (12.104)$$

survives, which is the polarization tensor of the Gupta-Bleuler propagator (12.88).

The same cancellation occurs if a photon is absorbed by an internal line, although due to a slightly more involved mechanism. An internal line may arise in two ways.

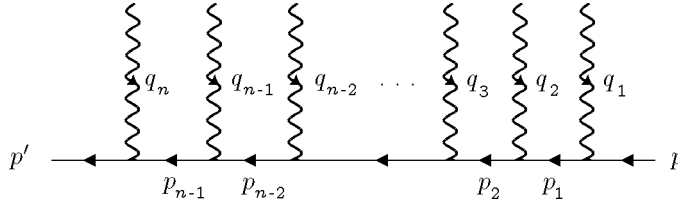


FIGURE 12.1 An electron on the mass shell absorbing several photons.

An electron may enter a Feynman diagram on the mass shell, absorb a number of photons, say n of them, and leave again on the mass shell as shown in Fig. 12.1. The associated off-shell amplitude is

$$a(p', p, q_i) = \frac{1}{\not{p}' - M} \not{q}_n \frac{1}{\not{p}_{n-1} - M} \not{q}_{n-1} \not{q}_{n-1} \cdots \not{q}_3 \frac{1}{\not{p}_2 - M} \not{q}_2 \frac{1}{\not{p}_1 - M} \not{q}_1. \quad (12.105)$$

It has to be amputated and evaluated between the initial and final spinors, which amounts to multiplying it from the left and right with $\bar{u}(\mathbf{p}', s'_3)(\not{p}' - M)$ and with $(\not{p} - M)u(\mathbf{p}, s_3)$, respectively. If an additional photon is absorbed, it must be inserted as shown in Fig. 12.2. At each vertex, there is no current conservation since the

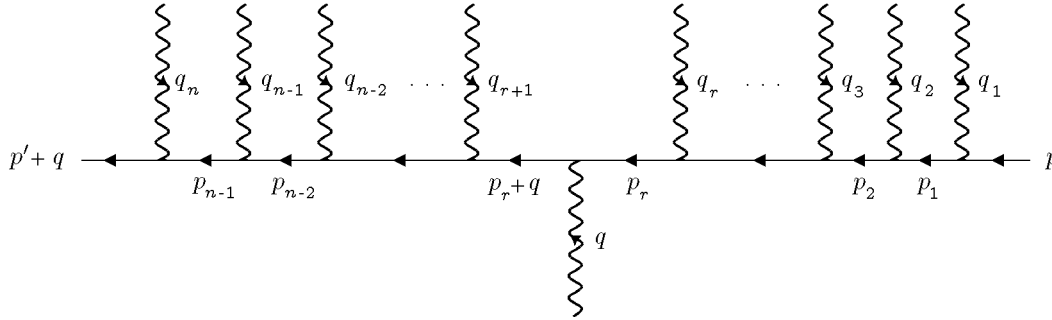


FIGURE 12.2 An electron on the mass shell absorbing several photons, plus one additional photon.

photon lines are not on their mass shell. Nevertheless, the sum of all $n + 2$ diagrams does have a conserved current.

To prove this we observe the following *Ward-Takahashi identity* for free particles [2, 3]:

$$\frac{1}{\not{p}_r + \not{q} - M} \not{q} \frac{1}{\not{p}_r - M} = \frac{1}{\not{p}_r - M} - \frac{1}{\not{p}_r + \not{q} - M}. \quad (12.106)$$

More details on this important identity will be given in the next section.

The sum of all off-shell absorption diagrams can be written as

$$a(p', p, q_i; q) = \frac{1}{\not{p}' + \not{q} - M} \not{q}_n \frac{1}{\not{p}_{n-1} + \not{q} - M} \not{q}_{n-1} \cdots$$

$$\cdots \frac{1}{\not{p}_r + \not{q} - M} \not{q} \frac{1}{\not{p}_r - M} \cdots \not{q}_2 \frac{1}{\not{p}_1 - M} \not{q}_1 u(\mathbf{p}, s_3), \quad (12.107)$$

to be evaluated between $\bar{u}(\mathbf{p}' + \mathbf{q}, s'_3)(\not{p}' + \not{q} - M)$ and $(\not{p} - M)u(\mathbf{p}, s_3)$. With the help of the Ward-Takahashi identity we can now remove the $\not{q}$ recursively from $a(p', p, q_i; q)$ and remain with the difference

$$a(p', p, q_i; q) = a(p', p, q_i) - a(p' + q, p + q, q_i). \quad (12.108)$$

When evaluating the right-hand side between the above spinors, we see that the first term in the difference vanishes since the left-hand spinor satisfies the Dirac equation. The same thing holds for the second term and the right-hand spinor. Thus the polarization sum in the photon propagator can again be replaced by the reduced expression (12.104).

Finally, the electron line can be closed to a loop as shown in Fig. 12.3. Here the

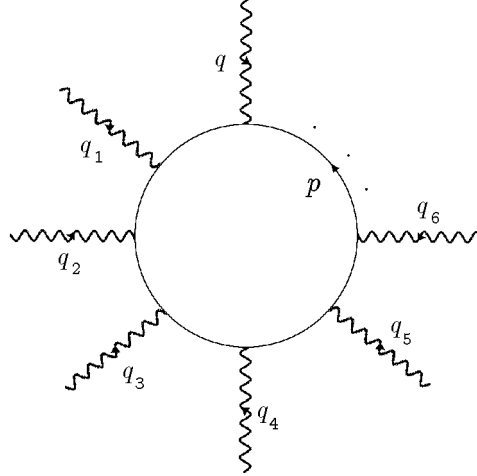


FIGURE 12.3 An internal electron loop absorbing several photons, plus an additional photon, and leaving again on the mass shell.

amplitude (12.108) appears in a loop integral with an additional photon vertex:

$$\int \frac{d^4 p}{(2\pi)^4} \text{tr}[\not{q} a(p', p, q_i; q)] = \int \frac{d^4 p}{(2\pi)^4} \text{tr}\{\not{q} [a(p', p, q_i) - a(p' + q, p + q, q_i)]\}. \quad (12.109)$$

If the divergence of the integral is made finite by a dimensional regularization, the loop integral is translationally invariant in momentum space and the amplitude difference vanishes. Hence, also in this case, the polarization sum can be replaced by the reduced expression (12.104).

Thus we have shown that due to current conservation and the Ward-Takahashi identity, the photon propagator in all Feynman diagrams can be replaced by

$$(12.110)$$

$$\text{wavy line with } q \text{ below it} = G^{\mu\nu}(q) = \frac{-ig^{\mu\nu}}{q^2 + i\eta}.$$

As a matter of fact, for the same reason, any propagator

$$\text{wavy line with } q \text{ below it} = G^{\mu\nu}(q) = -\frac{i}{q^2} \left[g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} (1 - \alpha) \right] \quad (12.111)$$

can be used just as well, and the parameter α is arbitrary. Indeed, this is the propagator arising when adding to the gauge-invariant Lagrangian in (12.84) the gauge-fixing expression

$$\mathcal{L}_{\text{GF}} = \frac{\alpha}{2} D^2 - D\partial^\mu A_\mu. \quad (12.112)$$

For the value $\alpha = 1$ favored by Feynman, the propagator (12.4) reduces to (12.110).

12.5 Ward-Takahashi Identity

From the application of Eq. (12.106), it is apparent that the Ward-Takahashi identity plays an important role in ensuring the gauge invariance of loop diagrams. In fact, the renormalizability of quantum electrodynamics was completed only after making use of the diagonal part of it, which was the original *Ward identity*. For free particles, we observe that the Ward-Takahashi identity (12.106) can be written in terms of the electron propagator (12.90), and the free vertex function $\Gamma_0^\mu(p', p) = \gamma^\mu$, as

$$S_0^{-1}(p') - S_0^{-1}(p) = i(p - q)_\mu \Gamma_0^\mu(p', p). \quad (12.113)$$

The original Ward identity is obtained from this by forming the limit $p' \rightarrow p$:

$$\frac{\partial}{\partial p_\mu} S_0^{-1}(p) = i\Gamma_0^\mu(p, p). \quad (12.114)$$

The important contribution of Ward and Takahashi was to prove that their identity is valid for the *interacting* propagators and vertex functions, order by order in perturbation theory. Thus we may drop the subscripts zero in Eq. (12.113) and write

$$S^{-1}(p') - S^{-1}(p) = i(p' - p)_\mu \Gamma^\mu(p', p). \quad (12.115)$$

This identity is a general consequence of gauge invariance, as was first conjectured by Rohrlich [4].

For the general proof of (12.115), the key observation is that the operator version of the fully interacting electromagnetic current $j^\mu(x) = e\bar{\psi}(x)\gamma^\mu\psi(x)$ satisfies, at equal times, the commutation rules with the interacting electron and photon fields

$$[j^0(x), \psi(y)]\delta(x^0 - y^0) = -e\gamma^0\psi(x)\delta(x^0 - y^0), \quad (12.116)$$

$$[j^0(x), \bar{\psi}(y)]\delta(x^0 - y^0) = e\bar{\psi}(x)\gamma^0\delta(x^0 - y^0), \quad (12.117)$$

$$[j^0(x), \bar{A}^\mu(y)]\delta(x^0 - y^0) = 0. \quad (12.118)$$

This follows directly from the canonical equal-time anticommutation rules of the electrons written in the form

$$\{\psi(x), \psi^\dagger(y)\} \delta(x^0 - y^0) = \delta^{(4)}(x - y). \quad (12.119)$$

As a consequence of (12.116)–(12.118), we find for any local operator $O(x)$:

$$\partial_\mu (\hat{T} j^\mu(x) O(y)) = (j^0(x) O(y)) \delta(x^0 - y^0) + \hat{T} (\partial_\mu j^\mu(x) O(y)). \quad (12.120)$$

The first term on the right-hand side arises when the derivative is applied to the Heaviside functions in the definition (2.232) of the time-ordered product. The generalization to many local operators reads:

$$\begin{aligned} \partial_\mu (\hat{T} j^\mu(x) O(y_1) \cdots O(y_i) \cdots O(y_n)) = & \sum_{i=1}^n \hat{T} O(y_1) \cdots [j^0(x), O(y_i)] \cdots O(y_n) \delta(x^0 - y_i^0) \\ & + \hat{T} (\partial_\mu j^\mu(x) O(y_1) \cdots O(y_i) \cdots O(y_n)). \end{aligned} \quad (12.121)$$

Since the electromagnetic current is conserved, the last term vanishes.

A particular case of (12.121) for a conserved current is the relation

$$\partial_\mu (\hat{T} j^\mu(x) \bar{\psi}(y_1) \psi(y_2)) = e \hat{T} (\bar{\psi}(y_1) \psi(y_2)) [\delta(x - y_1) - \delta(x - y_2)]. \quad (12.122)$$

Taking this between single-particle states and going to momentum space yields an identity that is valid to all orders in perturbation theory [5]

$$-i(p' - p)_\mu S(p') \Gamma^\mu(p', p) S(p) = S(p') - S(p). \quad (12.123)$$

This is precisely the Ward-Takahashi identity (12.113).

12.6 Magnetic Moment of Electron

For dimensional reasons, the magnetic moment of the electron is proportional to the Bohr magnetic moment

$$\mu_B = \frac{e\hbar}{2Mc}. \quad (12.124)$$

Since it is caused by the spin of the particle, it is proportional to it and can be written as

$$\boldsymbol{\mu} = g \mu_B \frac{\mathbf{S}}{\hbar}. \quad (12.125)$$

The proportionality factor g is called the *gyromagnetic ratio*. If the spin is polarized in the z -direction, the z -component of $\boldsymbol{\mu}$ is

$$\mu = g \mu_B \frac{1}{2} = g \frac{e\hbar}{2Mc} \frac{1}{2}. \quad (12.126)$$

We have discussed in Subsec. 4.15 that, as a result of the *Thomas precession*, an explanation of the experimental fine structure will make the g -factor of the electron

magnetic moment to have a value near 2. This is twice as large as that of a charged rotating sphere of angular momentum L , whose magnetic moment is

$$\boldsymbol{\mu} = \frac{e\hbar}{2Mc} \frac{\mathbf{L}}{\hbar}, \quad (12.127)$$

i.e., whose g -value is unity. The result $g = 2$ has been found also in Eq. (6.119) by bringing the Dirac equation in an electromagnetic field to the second-order Pauli form (6.110).

Let us convince ourselves that a Dirac particle possesses the correct gyromagnetic ratio $g = 2$. Consider an electron of momentum $\mathbf{p}$ in a electromagnetic field which changes the momentum to $\mathbf{p}'$ (see Fig. 12.95). The interaction Hamiltonian is given by the matrix element

$$H^{\text{int}} = \int d^3x A_\mu(\mathbf{x}) \langle \mathbf{p}' | j^\mu(x) | \mathbf{p} \rangle, \quad (12.128)$$

where in Dirac's theory:

$$\langle \mathbf{p}', s'_3 | j^\mu(x) | \mathbf{p}, s_3 \rangle = e \langle 0 | a(\mathbf{p}', s'_3) \bar{\psi}(x) \gamma^\mu \psi(x) a^\dagger(\mathbf{p}, s_3) | 0 \rangle. \quad (12.129)$$

Inserting the field expansion (7.224) in terms of creation and annihilation operators

$$\psi(x) = \sum_{\mathbf{p}, s_3} \frac{1}{\sqrt{V E_{\mathbf{p}}/M}} \left[e^{-ipx} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ipx} v(\mathbf{p}, s_3) b^\dagger(\mathbf{p}, s_3) \right], \quad (12.130)$$

and using the anticommutators (7.228) and (7.229), we obtain

$$\langle \mathbf{p}', s'_3 | j^\mu(x) | \mathbf{p}, s_3 \rangle = e \bar{u}(\mathbf{p}', s'_3) \gamma^\mu u(\mathbf{p}, s_3) \frac{e^{i(p'-p)x}}{\sqrt{V E_{\mathbf{p}'}/M} \sqrt{V E_{\mathbf{p}}/M}}. \quad (12.131)$$

The difference between final and initial four-momenta

$$q' \equiv p' - p \quad (12.132)$$

is the momentum transfer caused by the incoming photon.

In order to find the size of the magnetic moment we set up a constant magnetic field in the third space direction by assuming the second component of the vector potential to be the linear function $A_2(x) = x^1 B_3$. Then we put the final electron to rest, i.e., $p'^\mu = (M, \mathbf{0})$, and let the initial electron move slowly in the 1-direction. We create an associated spinor $u(\mathbf{p}, s_3)$ by applying a small Lorentz-boost $e^{-i\zeta^1(i\gamma^0\gamma^1)/2}$ to the rest spinors (4.676), and expanding the matrix element (12.131) up to the first order in $\mathbf{p}$. In zeroth order, we see that

$$\bar{u}(\mathbf{0}, s'_3) \gamma^\mu u(\mathbf{0}, s_3) = \chi^\dagger(s'_3) \chi(s_3) \delta^\mu_0, \quad (12.133)$$

showing that the charge is unity. The linear term in q^1 gives rise to a 2-component:

$$\langle \mathbf{p}', s'_3 | j^2(x) | \mathbf{p}, s_3 \rangle = e \bar{u}(\mathbf{0}, s'_3) \gamma^2 e^{-i\zeta^1(i\gamma^0\gamma^1)/2} u(\mathbf{0}, s_3) \frac{e^{iq^1 x^1}}{V}. \quad (12.134)$$

The two normalization factors on the right-hand side of (12.131) differ only by second-order terms in q^1 . Now, since $\bar{u}(\mathbf{0}, s_3)\gamma^2 u(\mathbf{0}, s_3) = 0$ and $i\gamma^1\gamma^2/2 = S_3$, the spinors on the right-hand side reduce to

$$-ie\zeta^1 u^\dagger(\mathbf{0}, s_3)S_3 u(\mathbf{0}, s_3) = -ie\zeta^1 s_3. \quad (12.135)$$

Momentum conservation enforces $\zeta^1 = -q^1/M$, so that we find

$$\langle \mathbf{p}', s'_3 | j^2(x) | \mathbf{p}, s_3 \rangle = ie \frac{q^1}{M} s_3 \frac{e^{iq^1 x^1}}{V}. \quad (12.136)$$

Inserting this into the interaction Hamiltonian (12.128), we obtain

$$\begin{aligned} E^{\text{int}} &= \lim_{q^1 \rightarrow 0} \int d^3x A_2(\mathbf{x}) i q^1 e^{iq^1 x^1} \frac{e}{M} s_3 \frac{1}{V} = \lim_{q^1 \rightarrow 0} \int d^3x A_2(\mathbf{x}) \partial_1 e^{iq^1 x^1} \frac{e}{M} s_3 \frac{1}{V} \\ &= - \int d^3x \partial_1 A_2(\mathbf{x}) \frac{e}{M} s_3 \frac{1}{V}. \end{aligned} \quad (12.137)$$

Inserting here the above vector potential $A_2(x) = x^1 B_3$, we obtain the magnetic interaction Hamiltonian

$$H^{\text{int}} = -B_3 \frac{e}{M} s_3. \quad (12.138)$$

Since a magnetic moment μ interacts, in general, with a magnetic field via the energy $-\boldsymbol{\mu} \cdot \mathbf{B}$, we identify the magnetic moment as being (12.126), implying a gyromagnetic ratio $g = 2$.

Note that the magnetic field caused by the orbital motion of an electron leads to a coupling of the orbital angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ with a g -factor $g = 1$. In order to see this relative factor 2 most clearly, consider the interaction Hamiltonian

$$H^{\text{int}} = - \int d^3x \mathbf{A}(x) \langle \mathbf{p}', s'_3 | \mathbf{j}(x) | \mathbf{p}, s_3 \rangle, \quad (12.139)$$

and insert the Dirac current (12.131). For slow electrons we may neglect quantities of second order in the momenta, so that the normalization factors E/M are unity, and we obtain

$$H^{\text{int}} = -e \int d^3x \mathbf{A}(x) \bar{u}(\mathbf{p}', s_3) \boldsymbol{\gamma} u(\mathbf{p}, s_3) e^{-i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}}. \quad (12.140)$$

At this place we make use of the so-called *Gordon decomposition formula*

$$\bar{u}(\mathbf{p}', s'_3) \gamma^\mu u(\mathbf{p}, s_3) = \bar{u}(\mathbf{p}', s'_3) \left[\frac{1}{2M} (p'^\mu + p^\mu) + \frac{i}{2M} \sigma^{\mu\nu} q_\nu \right] u(\mathbf{p}, s_3), \quad (12.141)$$

where $q \equiv p' - p$ is the momentum transfer. This formula follows directly from the anticommutation rules of the γ -matrices and the Dirac equation.

An alternative decomposition is

$$\langle \mathbf{p}' | j^\mu | \mathbf{p} \rangle = e \bar{u}(\mathbf{p}') \left[\frac{1}{2M} (p'^\mu + p^\mu) F_1(q^2) + \frac{i}{2M} \sigma^{\mu\nu} q_\nu F_2(q^2) \right] u(\mathbf{p}), \quad (12.142)$$

with the form factors $F_1(q^2)$, $F_2(q^2)$ related to $F(q^2)$, $G(q^2)$ via (12.141) by

$$F(q^2) = F_1(q^2), \quad G(q^2) = F_1(q^2) + F_2(q^2). \quad (12.143)$$

Then we rewrite the interaction Hamiltonian as

$$H^{\text{int}} = -\frac{e}{M} \int d^3x \mathbf{A}(x) \bar{u}(\mathbf{p}', s_3) (\mathbf{p} + \mathbf{q} - i\mathbf{q} \times \mathbf{S}) u(\mathbf{p}, s_3) e^{-i\mathbf{q}\mathbf{x}}, \quad (12.144)$$

where we have used the relations (4.518) and (4.515). We now replace $\mathbf{q}$ by the derivatives $i\partial_{\mathbf{x}}$ in front of the exponential $e^{-i\mathbf{q}\mathbf{x}}$, and perform an integration by parts to make the derivatives act on the vector potential $\mathbf{A}(x)$, with the opposite sign. In the transverse gauge, the term $\mathbf{A}(x) \cdot \mathbf{q}$ gives zero while $-i\mathbf{A}(x) \cdot (\mathbf{q} \times \mathbf{S})$ becomes $\mathbf{B} \cdot \mathbf{S}$. For equal incoming and outgoing momenta, this leads to the interaction Hamiltonian

$$H^{\text{int}} = -\frac{e}{M} \int d^3x [\mathbf{A}(x) \cdot \mathbf{p} + \mathbf{B}(x) \cdot \mathbf{S}]. \quad (12.145)$$

We now express the vector potential in terms of the magnetic field as

$$\mathbf{A}(x) = \frac{1}{2} \mathbf{B} \times \mathbf{x}, \quad (12.146)$$

and rewrite (12.145) in the final form

$$H^{\text{int}} = -\frac{e}{2M} \mathbf{B} \cdot (\mathbf{L} + 2\mathbf{S}), \quad (12.147)$$

where $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ is the orbital angular momentum. The relative factor 2 discovered by Alfred Landé in 1921 between orbital and spin angular momentum gives rise to a characteristic splitting of atomic energy levels in an external magnetic field. If the field is weak, both orbital and spin angular momenta will precess around the direction of the total angular momentum. Their averages will be, for example,

$$\bar{\mathbf{L}} = \mathbf{J} \frac{\mathbf{J} \cdot \mathbf{L}}{\mathbf{J}^2}, \quad \bar{\mathbf{S}} = \mathbf{J} \frac{\mathbf{J} \cdot \mathbf{S}}{\mathbf{J}^2}. \quad (12.148)$$

By rewriting

$$\mathbf{J} \cdot \mathbf{L} = \frac{1}{2} (\mathbf{J}^2 + \mathbf{L}^2 - \mathbf{S}^2), \quad \mathbf{J} \cdot \mathbf{S} = \frac{1}{2} (\mathbf{J}^2 - \mathbf{L}^2 + \mathbf{S}^2), \quad (12.149)$$

we see that

$$\bar{\mathbf{L}} = f_{LJ} \mathbf{J}, \quad \bar{\mathbf{S}} = f_{SJ} \mathbf{J} \quad (12.150)$$

with the factors

$$f_{LJ} = [J(J+1) + L(L+1) - S(S+1)] / 2J(J+1), \quad (12.151)$$

$$f_{SJ} = [J(J+1) - L(L+1) + S(S+1)] / 2J(J+1). \quad (12.152)$$

Inserting this into (12.147), we obtain the interaction energies of an atomic state $|JM\rangle$:

$$H^{\text{int}} = -g_{LS} \frac{e}{2M} BM, \quad (12.153)$$

where

$$g_{LS} = f_{LJ} + 2f_{SJ} = 1 + [J(J+1) - L(L+1) + S(S+1)] / 2J(J+1) \quad (12.154)$$

is the *gyromagnetic ratio* of the coupled system. This has been measured in many experiments as *Zeeman effect*, if the external field is small, and as *anomalous Zeeman effect* or *Paschen-Back effect*, if the external field strength exceeds the typical field strength caused by the electron orbit. Then orbital and spin angular momenta decouple and precess independently around the direction of the external magnetic field.

12.7 Decay of Atomic State

The first important result of quantum electrodynamics is the explanation of the decay of an atom. In quantum mechanics, this decay can only be studied by means of the correspondence principle.

Consider an electron in an atomic state undergoing a transition from a state n with energy E_n to a lower state n' with energy $E_{n'}$, whereby a photon is emitted with a frequency $\omega = (E_n - E_{n'})/\hbar$ (see Fig. 12.4). According to the correspondence

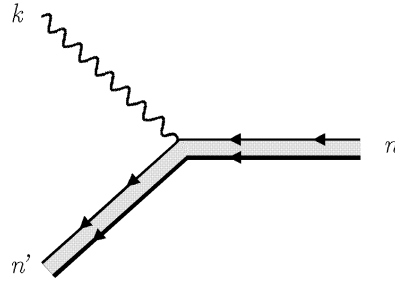


FIGURE 12.4 Transition of an atomic state from a state n with energy E_n to a lower state n' with energy $E_{n'}$, thereby emitting a photon with a frequency $\omega = (E_n - E_{n'})/\hbar$.

principle, this is the frequency with which the center of charge of the electronic cloud oscillates back and forth along the direction $\hat{\epsilon}$ with an amplitude:

$$\mathbf{x}_0 = \langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle = \boldsymbol{\epsilon} \langle n' | \hat{\epsilon} \cdot \mathbf{x} | n \rangle. \quad (12.155)$$

The oscillating charge emits antenna radiation. The classical theory of this process has been recapitulated in Section 5.1, where we have given in Eq. (5.37) the radiated power per solid angle. Its directional integral led to the Larmor formula (5.38), and reduced to (5.38) for a harmonic oscillator.

Quantum mechanically, the antenna radiation formula (5.37) can be applied to an atom that decays from level n to n' , if we replace $|\mathbf{x}_0|^2$ by the absolute square of the quantum mechanical matrix element (12.155):

$$|\mathbf{x}_0|^2 \rightarrow |\langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle|^2. \quad (12.156)$$

Then formula (5.37) yields the radiated power per unit solid angle

$$\frac{d\dot{\mathcal{E}}_{n'n}}{d\Omega} = \frac{e^2}{8\pi^2} \frac{\omega^4}{c^3} |\langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle|^2 \sin^2 \theta. \quad (12.157)$$

Integrating over all $d\Omega$ gives the total radiated power, and if we divide this by the energy per photon $\hbar\omega$, we obtain the decay rate

$$\dot{\Gamma}_{n'n} = \frac{4}{3} \frac{e^2}{4\pi} \frac{\omega^3}{\hbar c^3} |\langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle|^2 = \frac{4}{3} \alpha \omega |\mathbf{k}|^2 |\langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle|^2. \quad (12.158)$$

Let us now confirm this result by a proper calculation within quantum electrodynamics. Consider a single nonrelativistic electron in a hydrogen-like atom with central charge Ze . For an electron of mass M moving in a Coulomb potential

$$V_C(\mathbf{x}) \equiv -\frac{Z\alpha}{|\mathbf{x}|}, \quad (12.159)$$

the Hamiltonian reads in the transverse gauge with $\nabla \mathbf{A}(x) = 0$,

$$H = \frac{\mathbf{p}^2}{2M} - \frac{1}{M} \mathbf{A}(\mathbf{x}, t) \cdot \mathbf{p} + \frac{e^2}{2M} \mathbf{A}^2(\mathbf{x}, t) + V_C(\mathbf{x}) + eA^0(\mathbf{x}, t) = H_C + H^{\text{int}}. \quad (12.160)$$

where

$$H_C = \frac{\mathbf{p}^2}{2M} + V_C(\mathbf{x}) \quad (12.161)$$

is the Hamiltonian of the hydrogen-like atom by itself, and H^{int} contains the interaction of the electron with the vector potential $A^\mu(\mathbf{x}, t) = 0$. Its magnitude is determined by the electronic charge distribution via the Coulomb law as shown in Eq. (12.73). The radiation field $\mathbf{A}(\mathbf{x}, t)$, has an expansion in terms of photon creation and annihilation operators given in Eq. (7.350):

$$\mathbf{A}(\mathbf{x}, t) = \sum_{\mathbf{k}, h} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[e^{-ikx} \boldsymbol{\epsilon}(\mathbf{k}, h) a_{\mathbf{k}, h} + \text{h.c.} \right]. \quad (12.162)$$

Let $|n\rangle$ be an excited initial state of an atom with an electron orbit having the principal quantum number n , and suppose that it decays into lower state $a^\dagger(\mathbf{k}, h)|n'\rangle$ with a principal quantum number n' . In addition to the electron, the lower atomic state contains a photon with wave vector $\mathbf{k}$, energy $\omega = ck$, and helicity h . According to Eq. (9.235), the decay probability of the initial state per unit time is given by Fermi's golden rule (in the remainder of this section we use physical units):

$$\frac{dP_{n'n}}{dt} = \int \frac{d^3kV}{(2\pi)^3} 2\pi\hbar\delta(E_n + \hbar\omega - E_{n'}) \left| \frac{1}{\hbar} \langle n' | a(\mathbf{k}, h) T | n \rangle \right|^2, \quad (12.163)$$

where T is the T -matrix which coincides, in lowest order perturbation theory, with the matrix $H_{\text{int}} \int d^3x \mathcal{H}_{\text{int}}(\mathbf{x})$ [see (9.132) and (9.288)]. The matrix element is obviously

$$\langle n' | a(\mathbf{k}, h) H^{\text{int}} | n \rangle = \frac{c}{\sqrt{2V\omega}} \frac{e}{Mc} \langle n' | e^{-i\mathbf{k}\mathbf{x}} \boldsymbol{\epsilon}^*(\mathbf{k}, h) \cdot \mathbf{p} | n \rangle. \quad (12.164)$$

Performing the integral over the photon momentum (neglecting recoil) we find from (12.163) the differential decay rate [compare (9.338)]

$$\frac{d\Gamma_{n'n}}{d\Omega} = \frac{e^2}{8\pi^2\hbar} \frac{\omega}{M^2c^3} |\langle n' | e^{-i\mathbf{k}\cdot\mathbf{x}} \boldsymbol{\epsilon}^*(\mathbf{k}, h) \cdot \mathbf{p} | n \rangle|^2. \quad (12.165)$$

Further calculations are simplified by the observation that the wavelength of the emitted photons is the inverse of their energy (in massless units), and thus of the order of $\hbar/Z\alpha^2Mc$, about 100 times larger than the atomic diameter which is of the order of the Bohr radius $a_B = \hbar/Z\alpha Mc$ for an atom of charge Z . The exponential $e^{-i\mathbf{k}\cdot\mathbf{x}}$ is therefore almost unity and can be dropped. This yields the *dipole approximation* to the atomic decay rate:

$$\frac{d\Gamma_{n'n}}{d\Omega} \approx \frac{e^2}{8\pi^2\hbar} \frac{\omega}{M^2c^3} |\boldsymbol{\epsilon}^*(\mathbf{k}, h) \cdot \langle n' | \mathbf{p} | n \rangle|^2. \quad (12.166)$$

Another way of writing this result is

$$\frac{d\Gamma_{n'n}}{d\Omega} \approx \alpha \frac{\omega}{2\pi\hbar} \frac{\omega^2}{c^2} |\boldsymbol{\epsilon}^*(\mathbf{k}, h) \cdot \langle n' | \mathbf{x} | n \rangle|^2. \quad (12.167)$$

The momentum operator $\mathbf{p}$ can be replaced by $M\dot{\mathbf{x}} = i[\hat{H}, \mathbf{x}]/\hbar$, and thus, in the matrix element $\langle n' | \mathbf{p} | n \rangle^2$, by $iM(E_{n'} - E_n)\mathbf{x}/\hbar = -iM\omega\mathbf{x}$. Multiplying the decay rate by the energy of the photon $\hbar\omega$ to get the rate of radiated energy, the result (12.167) coincides with the classical result (12.158).

It is customary to introduce the so-called *oscillator strength* for an oscillator in the direction ϵ :

$$f_{n'n}^\epsilon \approx \frac{2M\omega}{\hbar} \left| \sum_\nu \langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle \right|^2 = 2 \frac{|\mathbf{k}|}{\lambda_e} \left| \sum_\nu \langle n' | \boldsymbol{\epsilon} \cdot \mathbf{x} | n \rangle \right|^2. \quad (12.168)$$

This quantity fulfills the *Thomas-Reiche-Kuhn sum rule*:

$$\sum_{n'} f_{n'n}^\epsilon = 1. \quad (12.169)$$

For an atom with Z electrons, the right-hand side is equal to Z .

To derive this sum rule (and a bit more) we define the operator

$$\hat{E}^\epsilon \equiv \frac{1}{|\mathbf{k}|} e^{-i|\mathbf{k}|\boldsymbol{\epsilon}\cdot\mathbf{x}}, \quad (12.170)$$

whose time derivative is

$$\dot{\hat{E}}^\epsilon = \frac{i}{\hbar} [\hat{H}, \hat{E}^\epsilon] = \frac{\hbar}{2M} \left(e^{-i|\mathbf{k}|\boldsymbol{\epsilon}\cdot\mathbf{x}} \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} + \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} e^{-i|\mathbf{k}|\boldsymbol{\epsilon}\cdot\mathbf{x}} \right). \quad (12.171)$$

According to the canonical commutator $[\hat{p}_i, \hat{x}_j] = -i\hbar\delta_{ij}$, the Hermitian-conjugate of $\dot{\hat{E}}^\epsilon$ commutes with $\hat{E}^\epsilon$ like

$$[\dot{\hat{E}}^{\epsilon\dagger}, \hat{E}^\epsilon] = -i\frac{\hbar}{M}. \quad (12.172)$$

Taking this commutator between states $\langle n|$ and $|n\rangle$, and inserting a completeness relation $\sum_{n'} |n'\rangle\langle n'| = 1$ in the middle, we may go to small $\mathbf{k}$, to find indeed the sum rule (12.169).

Let us calculate the angular properties of the radiation in more detail. The decomposition of the hydrogen wave functions into radial and angular parts is

$$\langle \mathbf{x}|nlm\rangle = R_{nl}(r)Y_{lm}(\theta, \varphi). \quad (12.173)$$

Then the matrix elements of $\mathbf{x}$ factorize:

$$\langle n'l'm'|\mathbf{x}|nlm\rangle = r_{n'l';nl} \times \langle l'm'|\hat{\mathbf{x}}|lm\rangle. \quad (12.174)$$

The matrix elements of r ,

$$r_{n'l';nl} \equiv \int_0^\infty dr r^2 R_{n'l'}(r) r R_{nl}(r), \quad (12.175)$$

have been calculated by Gordon [25]:

$$\begin{aligned} r_{n'l';nl} = & \frac{(-1)^{n'-l}}{4(2l-1)!} \sqrt{\frac{(n+l)!(n'+l-1)!}{(n'-l)!(n-l-1)!}} (4nn')^{l+1} \frac{(n-n')^{n+n'-2l-2}}{(n+n')^{n+n'}} \\ & \times \left\{ F\left(-n'_r, 2l, -\frac{4nn'}{(n-n')^2}\right) - \left(\frac{n-n'}{n+n'}\right)^2 F\left(-n_r-2, -n'_r, 2l, -\frac{4nn'}{(n-n')^2}\right) \right\}, \end{aligned} \quad (12.176)$$

with $F(a, b, c; z)$ being hypergeometric functions. The angular matrix elements of the unit vector in (12.174),

$$\langle l'm'|\hat{\mathbf{x}}|lm\rangle \equiv \int d\hat{\mathbf{x}} Y_{l'm'}^*(\theta, \varphi) \hat{\mathbf{x}} Y_{lm}(\theta, \varphi), \quad (12.177)$$

are easily calculated since $\hat{x}_3 = \cos \theta$, and the spherical harmonics satisfy the recursion relation

$$\cos \theta Y_{lm}(\theta, \varphi) = \sqrt{\frac{(l+1)^2 - m^2}{(2l+2)(2l+1)}} Y_{l+1,m}(\theta, \varphi) + \sqrt{\frac{l^2 - m^2}{(2l+1)(2l-1)}} Y_{l-1,m}(\theta, \varphi). \quad (12.178)$$

On account of the orthonormality relation [recall (4F.3)]

$$\int d\hat{\mathbf{x}} Y_{l'm'}^*(\theta, \varphi) Y_{lm}(\theta, \varphi) = \delta_{l'l} \delta_{m'm}, \quad (12.179)$$

we obtain immediately the angular matrix elements of $\hat{x}_3$:

$$\langle l+1 \ m|\hat{x}_3|lm\rangle = \sqrt{\frac{(l+1)^2 - m^2}{(2l+2)(2l+1)}}, \quad \langle l-1 \ m'|\hat{x}_3|lm\rangle = \sqrt{\frac{l^2 - m^2}{(2l+1)(2l-1)}}, \quad (12.180)$$

with all others vanishing. The matrix elements of $\hat{x}_1$ and $\hat{x}_2$ are found with the help of the commutation rule

$$[\hat{L}_i, \hat{x}_j] = i\epsilon_{ijk} \hat{x}_k, \quad (12.181)$$

which states that $\hat{x}_i$ is a *vector operator*. As a consequence, the matrix elements satisfy the Wigner-Eckart theorem,

$$\langle l'm' \pm 1 | \hat{x}^M | lm \rangle = \langle l'm' | 1M; lm \rangle \hat{x}_{\nu l}, \quad (12.182)$$

where $\langle l'm' | 1m''; lm \rangle$ are Clebsch-Gordan coefficients (see Appendix 4E) and $\hat{x}^{m''}$ are the spherical components of $\hat{\mathbf{x}}$ [recall the definition in Eq. (4.893)]:

$$\hat{x}^3 = \cos \theta, \quad \hat{x}^{\pm} = \mp(\hat{x}^2 \pm \hat{x}^2)/\sqrt{2} = \sin \theta e^{\pm i\varphi}/\sqrt{2}. \quad (12.183)$$

Explicitly:

$$\begin{aligned} \langle l+1 \ m \pm 1 | \hat{x}^{\pm} | lm \rangle &= \sqrt{\frac{(l \pm m + 2)(l \pm m + 1)}{2(2l+3)(2l+1)}}, \\ \langle l-1 \ m \pm 1 | \hat{x}^{\pm} | lm \rangle &= \sqrt{\frac{(l \mp m)(l \mp m - 1)}{2(2l+1)(2l-1)}}. \end{aligned} \quad (12.184)$$

12.8 Rutherford Scattering

The scattering of electrons on the Coulomb potential of nuclei of charge Ze ,

$$V_C(r) = -\frac{ZE^2}{4\pi r} = -\frac{Z\alpha}{r}, \quad (12.185)$$

was the first atomic collision observed experimentally by Rutherford.

The associated scattering cross section can easily be calculated in an estimated classical approximation.

12.8.1 Classical Cross Section

In a Coulomb potential the electronic orbits are hyperbola. If an incoming electron runs along the z -direction and is deflected by a scattering angle θ towards the x direction (see Fig. 12.5), the nucleus has the coordinates

$$(x_F, z_F) = (b, -a), \quad (12.186)$$

where

$$\frac{a}{b} = \tan \frac{\theta}{2}, \quad \frac{b}{d} = \cos \frac{\theta}{2}. \quad (12.187)$$

The parameter d is equal to $a\epsilon$, where $\epsilon > 1$ is the excentricity of the hyperbola. The distance of closest approach to the nucleus is

$$r_c = d - a. \quad (12.188)$$

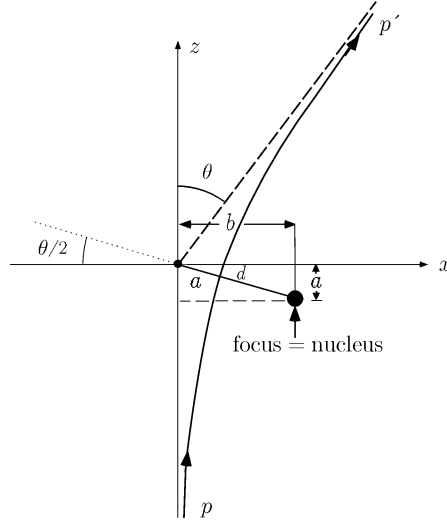


FIGURE 12.5 Kinematics of Rutherford scattering.

It is determined by the conservation of the nonrelativistic energy:

$$E^{\text{nr}} = \frac{p^2}{2M} = \frac{p'^2}{2M} = \frac{p_c^2}{2M} - \frac{Z\alpha}{r_c}, \quad (12.189)$$

where p_c is the momentum at the point of closest approach. This momentum is determined by the conservation of orbital angular momentum:

$$l = pb = p'b = p_cr_c. \quad (12.190)$$

From these equations we find

$$b = \frac{Z\alpha}{2E \tan(\theta/2)}. \quad (12.191)$$

The quantity b is called the *impact parameter* of the scattering process. It is the closest distance which an particle would have from the nucleus if it were not deflected at all. Particles which would pass through a thin annular ring with the radii b and $b + db$ are, in fact, scattered into a solid angle $d\Omega$ given by

$$db = -\frac{1}{4\pi} \frac{Z\alpha}{4E} \frac{1}{\sin^3(\theta/2) \cos(\theta/2)} d\Omega. \quad (12.192)$$

The current density of a single randomly incoming electron is $j = v/V$. It would pass through the annular ring, with a probability per unit time

$$d\dot{P} = j 2\pi b db. \quad (12.193)$$

With this probability it winds up in the solid angle $d\Omega$. Inserting Eq. (12.192), we find the differential cross section [recall the definition Eq. (9.242)]

$$\frac{d\sigma}{d\Omega} = \frac{d\dot{P}}{d\Omega} = 2\pi b \frac{db}{d\Omega} = \frac{1}{4 \sin^4(\theta/2)} \left(\frac{Z\alpha}{2E} \right)^2. \quad (12.194)$$

12.8.2 Quantum-Mechanical Born Approximation

Somewhat surprisingly, the same result is obtained in quantum mechanics within the Born approximation. According to Eqs. (9.147) and (9.248), the differential cross section is

$$\frac{d\sigma}{d\Omega} \approx \frac{M^2 V^2}{(2\pi)^2} |V_{\mathbf{p}'\mathbf{p}}|^2, \quad (12.195)$$

where

$$V_{\mathbf{p}'\mathbf{p}} = -\frac{1}{V} \int d^3x e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}} \frac{Z\alpha}{r} = -\frac{4\pi}{V} \frac{Z\alpha}{|\mathbf{q}|^2}. \quad (12.196)$$

The quantity

$$\mathbf{q}^2 \equiv |\mathbf{p}' - \mathbf{p}|^2 = 2p^2(1 - \cos\theta) = 4p^2 \sin^2(\theta/2) = 8EM \sin^2(\theta/2) \quad (12.197)$$

is the momentum transfer of the process. Inserting this into (12.196), the differential cross section (12.195) coincides indeed with the classical expression (12.194).

12.8.3 Relativistic Born Approximation: Mott Formula

Let us now see how the above cross section formula is modified in a relativistic calculation involving Dirac electrons. The scattering amplitude is, according to Eq. (10.142),

$$S_{\text{fi}} = -ie \langle \mathbf{p}', s'_3 | \int d^4x \bar{\psi}(x) \gamma^\mu \psi(x) | \mathbf{p}, s_3 \rangle A_\mu(x), \quad (12.198)$$

where $A_\mu(x)$ has only the time-like component

$$A^0(x) = -\frac{Ze}{4\pi r} = -\int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{x}} \frac{Ze}{|\mathbf{q}|^2}. \quad (12.199)$$

The time-ordering operator has been dropped in (12.198) since there are no operators at different times to be ordered in first-order perturbation theory. By evaluating the matrix element of the current in (12.198), and performing the spacetime integral we obtain

$$S_{\text{fi}} = i2\pi\delta(E' - E) \sqrt{\frac{M^2}{V^2 E' E}} \bar{u}(\mathbf{p}', s'_3) \gamma^0 u(\mathbf{p}, s_3) \frac{Ze^2}{|\mathbf{q}|^2}, \quad (12.200)$$

where E and E' are the initial and final energies of the electron, which are in fact equal in this elastic scattering process.

Comparing this with (9.130) we identify the T -matrix elements

$$T_{\mathbf{p}'\mathbf{p}} = \frac{M}{VE} \bar{u}(\mathbf{p}', s'_3) \gamma^0 u(\mathbf{p}, s_3) \frac{Ze^2}{|\mathbf{q}|^2}, \quad (12.201)$$

In the nonrelativistic limit this is equal to

$$T_{\mathbf{p}'\mathbf{p}} = -\frac{1}{V} \frac{Ze^2}{|\mathbf{q}|^2}. \quad (12.202)$$

Its relativistic extension contains a correction factor

$$C = \frac{M}{E} \bar{u}(\mathbf{p}', s_3) \gamma^0 u(\mathbf{p}, s_3). \quad (12.203)$$

Its absolute square multiplies the nonrelativistic differential cross section (12.194). Apart from this, the relativistic cross section contains an extra kinematic factor E^2/M^2 accounting for the different phase space of a relativistic electron with respect to the nonrelativistic one [the ratio between (9.247) and (9.244)]. The differential cross section (12.194) receives therefore a total relativistic correction factor

$$\frac{E^2}{M^2} |C|^2 = |\bar{u}(\mathbf{p}', s'_3) \gamma^0 u(\mathbf{p}, s_3)|^2. \quad (12.204)$$

If we consider the scattering of unpolarized electrons and do not observe the final spin polarizations, this factor has to be summed over s'_3 and averaged over s_3 , and the correction factor is

$$\frac{E^2}{M^2} |C|^2 = \frac{1}{2} \sum_{s'_3, s_3} \bar{u}(\mathbf{p}', s'_3) \gamma^0 u(\mathbf{p}, s_3) \bar{u}(\mathbf{p}, s_3) \gamma^0 \bar{u}(\mathbf{p}', s'_3). \quad (12.205)$$

To write the absolute square in this form we have used the general identity in the spinor space, valid for any 4×4 spinor matrix M :

$$(\bar{u}' M u)^* = \bar{u} \bar{M} u', \quad (12.206)$$

where the operation *bar* is defined for a spinor matrix in complete analogy to the corresponding operation for a spinor:

$$\bar{M} \equiv \gamma^0 M^\dagger \gamma^{0-1}. \quad (12.207)$$

The Dirac matrices themselves satisfy

$$\bar{\gamma}^\mu = \gamma^\mu. \quad (12.208)$$

The “bar” operation has the typical property of an “adjoining” operation. If it is applied to a product of matrices, the order is reversed:

$$\overline{M_1 \cdots M_n} = \bar{M}_n \cdots \bar{M}_1. \quad (12.209)$$

We use now the semi-completeness relation (4.702) for the u -spinors and rewrite (12.205) as

$$\frac{E^2}{M^2} |C|^2 = \frac{1}{2} \text{tr} \left(\gamma^0 \frac{\not{p}' + M}{2M} \gamma^0 \frac{\not{p} + M}{2M} \right). \quad (12.210)$$

The trace over product of gamma matrices occurring in this expression is typical for quantum electrodynamic calculations. Its evaluation is somewhat tedious, but follows a few quite simple algebraic rules.

The first rule states that a trace containing an odd number of gamma matrices vanishes. This is a simple consequence of the fact that γ^μ and any product of an odd number of gamma matrices change sign under the similarity transformation $\gamma_5 \gamma^\mu \gamma_5 = -\gamma^\mu$, while the trace is invariant under *any* similarity transformation.

The second rule governs the evaluation of a trace containing an even number of gamma matrices. It is a recursive rule which makes essential use of the invariance of the trace under cyclic permutations

$$\text{tr}(\gamma^{\mu_1} \gamma^{\mu_2} \gamma^{\mu_3} \dots \gamma^{\mu_{n-1}} \gamma^{\mu_n}) = \text{tr}(\gamma^{\mu_2} \gamma^{\mu_3} \dots \gamma^{\mu_{n-1}} \gamma^{\mu_n} \gamma^{\mu_1}). \quad (12.211)$$

This leads to an explicit formula that is a close analog of Wick's expansion formula for time-ordered products of fermion field operators. To find this, we define a pair contraction between $\not{a}$ and $\not{b}$ as

$$\overline{\not{a}\not{b}} \equiv \frac{1}{4} \text{tr}(\not{a}\not{b}) = ab. \quad (12.212)$$

Then we consider a more general trace

$$\frac{1}{4} \text{tr}(\not{a}_1 \dots \not{a}_n) \quad (12.213)$$

and move the first gamma matrix step by step to the end, using the anticommutation rules between gamma matrices (4.566), which imply that

$$\not{a}_1 \not{a}_i = -\not{a}_i \not{a}_1 + 2a_1 a_i = -\not{a}_i \not{a}_1 + 2 \overline{\not{a}_1 \not{a}_i}. \quad (12.214)$$

Having arrived at the end, it can be taken back to the front, using the cyclic invariance of the trace. This produces once more the initial trace, except for a minus sign, thus doubling the initial trace on the left-hand side of the equation if n is even. In this way, we find the recursion relation

$$\begin{aligned} \frac{1}{4} \text{tr}(\not{a}_1 \not{a}_2 \not{a}_3 \dots \not{a}_{n-1} \not{a}_n) &= \frac{1}{4} \text{tr}(\overline{\not{a}_1 \not{a}_2}) + \frac{1}{4} \text{tr}(\overline{\not{a}_1 \not{a}_2 \not{a}_3} \dots \not{a}_{n-1} \not{a}_n) \\ &+ \dots + \frac{1}{4} \text{tr}(\overline{\not{a}_1 \not{a}_2 \not{a}_3 \dots \not{a}_{n-1}} \not{a}_n) + \dots + \frac{1}{4} \text{tr}(\overline{\not{a}_1 \not{a}_2 \not{a}_3 \dots \not{a}_{n-1} \not{a}_n}). \end{aligned} \quad (12.215)$$

The contractions within the traces are defined as in (12.212), but with a minus sign for each permutation necessary to bring the Dirac matrices to adjacent positions. Performing these operations, the result of (12.215) is

$$\begin{aligned} \frac{1}{4} \text{tr}(\not{a}_1 \not{a}_2 \not{a}_3 \dots \not{a}_{n-1} \not{a}_n) &= (a_1 a_2) \frac{1}{4} \text{tr}(\not{a}_3 \not{a}_4 \dots \not{a}_{n-1} \not{a}_n) + (a_1 a_3) \frac{1}{4} \text{tr}(\not{a}_2 \not{a}_4 \dots \not{a}_{n-1} \not{a}_n) \\ &+ \dots + (a_1 a_{n-1}) \frac{1}{4} \text{tr}(\not{a}_2 \not{a}_3 \dots \not{a}_{n-2} \not{a}_n) + (a_1 a_n) \frac{1}{4} \text{tr}(\not{a}_2 \not{a}_3 \dots \not{a}_{n-1} \not{a}_n). \end{aligned} \quad (12.216)$$

By applying this formula iteratively, we arrive at the expansion rule of the Wick type:

$$\frac{1}{4} \text{tr}(\not{a}_1 \dots \not{a}_n) = \sum_{\text{pair contractions}} (-)^P (a_{p(1)} a_{p(2)}) (a_{p(3)} a_{p(4)}) \dots (a_{p(n-1)} a_{p(n)}), \quad (12.217)$$

where P is the number of permutations to adjacent positions.

The derivation of the rule is completely parallel to that of the thermodynamic version of Wick's rule in Section 4.14, whose Eqs. (7.857) and (7.858) can directly be translated into anticommutation rules between gamma matrices and the cyclic invariance of their traces, respectively.

Another set of useful rules following from (12.214) and needed later is

$$\gamma^\mu \not{a} \gamma^\nu = \not{a} + 2a^\mu \gamma^\nu, \quad (12.218)$$

$$\gamma^\mu \gamma_\mu = 4, \quad (12.219)$$

$$\gamma^\mu \not{a} \gamma_\mu = -2\not{a}, \quad (12.220)$$

$$\gamma^\mu \not{a} \not{b} \gamma_\mu = -2\not{a} \not{b}, \quad (12.221)$$

$$\gamma^\mu \not{a} \not{b} \not{c} \gamma_\mu = -2\not{c} \not{b} \not{a}. \quad (12.222)$$

Following the Wick rule (12.253) for γ -matrices, we now calculate the expression (12.210) as

$$\begin{aligned} \frac{E^2}{M^2} |C|^2 &= \frac{1}{2M^2} \left[\frac{1}{4} \text{tr}(\gamma^0 \not{p} \gamma^0 \not{p}') + M^2 \text{tr}(\gamma^{02}) \right] \\ &= \frac{1}{2M^2} (2p^0 p'^0 - pp' + M^2). \end{aligned} \quad (12.223)$$

Inserting $p^0 = p'^0 = E$ and, in the center-of-mass frame,

$$pp' = E^2 - |\mathbf{p}|^2 \cos \theta = M^2 + 2|\mathbf{p}|^2 \sin^2 \frac{\theta}{2}, \quad (12.224)$$

the total cross section in the center-of-mass frame becomes

$$\frac{d\sigma}{d\Omega_{\text{CM}}} = \frac{Z^2 \alpha^2 M^2}{4|\mathbf{p}|^4 \sin^4(\theta/2)} \times \frac{E^2}{M^2} |C|^2. \quad (12.225)$$

This relativistic version of Rutherford's formula is known as *Mott's formula*.

In terms of the incident electron velocity, the total modification factor reads

$$\frac{E^2}{M^2} |C|^2 = \frac{1}{1 - (v/c)^2} \left[1 - \left(\frac{v}{c} \right)^2 \sin^2 \frac{\theta}{2} \right]. \quad (12.226)$$

It is easy to verify that the same differential cross section is valid for positrons. In the nonrelativistic case, this follows directly from the invariance of (12.195) under $e \rightarrow -e$. But also the relativistic correction factor remains the same under the interchange of electrons and positrons, where (12.205) becomes

$$\frac{E^2}{M^2} |C|^2 = \frac{1}{2} \sum_{s'_3, s_3} \bar{v}(\mathbf{p}', s'_3) \gamma^0 v(\mathbf{p}, s_3) \bar{v}(\mathbf{p}, s_3) \gamma^0 \bar{v}(\mathbf{p}', s'_3). \quad (12.227)$$

Inserting the semi-completeness relation (4.703) for the spinors $v(\mathbf{p}, s_3)$, this becomes

$$\frac{E^2}{M^2} |C|^2 = \frac{1}{2} \text{tr} \left(\gamma^0 \frac{\not{p} - M}{2M} \gamma^0 \frac{\not{p}' - M}{2M} \right), \quad (12.228)$$

which is the same as (12.205), since only traces of an even number of gamma matrices contribute.

12.9 Compton Scattering

A simple scattering process, whose cross section can be calculated to a good accuracy by means of the above diagrammatic rules, is photon-electron scattering, also referred to as *Compton scattering*. It gives an important contribution to the blue color of the sky.¹

Consider now a beam of photons with four-momentum k_i and polarization λ_i impinging upon an electron target of four-momentum p_i and spin orientation σ_i . The two particles leave the scattering regime with four-momenta k_f and p_f , and spin indices λ_f, σ_f , respectively. Adapting formula (10.103) for the scattering amplitude to this situation we have

$$\begin{aligned} S_{fi} &= S(\mathbf{p}', s'_3; \mathbf{k}', h' | \mathbf{k}, h; \mathbf{p}, s_3) \\ &\equiv \frac{\langle 0 | a(\mathbf{p}', s'_3) a(\mathbf{k}', h') \hat{T} e^{-i \int_{-\infty}^{\infty} dt V_I(t)} a^\dagger(\mathbf{k}, h) a^\dagger(\mathbf{p}, s_3) | 0 \rangle}{\langle 0 | e^{-i \int_{-\infty}^{\infty} dt V_I(t)} | 0 \rangle} \\ &\equiv S_N(\mathbf{p}', s'_3; \mathbf{k}', h' | \mathbf{k}, h; \mathbf{p}, s_3) / Z[0], \end{aligned} \quad (12.229)$$

with

$$e^{-i \int_{-\infty}^{\infty} dt V_I(t)} = e^{-ie \int d^4x \bar{\psi}(x) \gamma^\mu \psi(x) A^\mu(x)}. \quad (12.230)$$

Expanding the exponential in powers of e , we see that the lowest-order contribution to the scattering amplitude comes from the second-order term which gives rise to the two Feynman diagrams shown in Fig. 12.6. In the first, the electron s_1 of momentum p absorbs a photon of momentum k , and emits a second photon of momentum k' , to arrive in the final state of momentum p' . In the second diagram, the acts of emission and absorption have the reversed order. Before we calculate the scattering cross section associated with these Feynman diagrams, let us first recall the classical result.

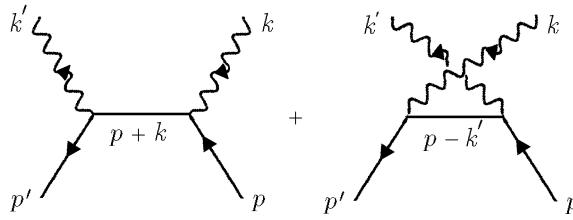


FIGURE 12.6 Lowest-order Feynman diagrams contributing to Compton Scattering and giving rise to the Klein-Nishina formula.

¹The blue color is usually attributed to *Rayleigh scattering*. This arises from generalizing Thomson's formula (12.233) for the scattering of light of wavelength λ on electrons to that on droplets of diameter d with refractive index n . That yields $\sigma_{\text{Rayleigh}} = 2\pi^5 d^6 [(n^2 - 1)/(n^2 + 2)]^2 / 3\lambda^4$.

12.9.1 Classical Result

Classically, the above process is described as follows. A target electron is shaken by an incoming electromagnetic field. The acceleration of the electron causes an emission of antenna radiation. For a weak and slowly oscillating electromagnetic field of amplitude, the electron is shaken nonrelativistically and moves with an instantaneous acceleration

$$\ddot{\mathbf{x}} = \frac{e}{M} \mathbf{E} = \frac{e}{M} \boldsymbol{\epsilon} E_0 e^{-i\omega t + i\mathbf{k} \cdot \mathbf{x}}, \quad (12.231)$$

where ω is the frequency and E_0 the amplitude of the incoming field.

The acceleration of the charge gives rise to antenna radiation following Larmor's formula. Inserting (12.231) into (5.37), and averaging over the temporal oscillations, the radiated power per unit solid angle is

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{1}{2} \left(\frac{e^2}{4\pi M} \right)^2 E_0^2 \sin^2 \beta, \quad (12.232)$$

where β is the angle between the direction of polarization of the incident light and the direction of the emitted light.

For a later comparison with quantum electrodynamic calculations we associate this emitted power with a differential cross section of the electron with respect to light. According to the definition in Chapter 6, a cross section is obtained by dividing the radiated power per unit solid angle by the incident power flux density $c\mathbf{E}_0^2/2$. This yields

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi M c^2} \right)^2 \sin^2 \beta = r_e^2 \sin^2 \beta, \quad (12.233)$$

where

$$r_e = \frac{e^2}{4\pi M c^2} = \frac{\hbar \alpha}{M c} \approx 2.82 \times 10^{-13} \text{ cm} \quad (12.234)$$

is the *classical electron radius*. Formula (12.233) describes the so-called *Thomson scattering cross section*. It is applicable to linearly polarized incident waves. For unpolarized waves, we have to form the average between the cross section (12.233) and another one in which the plane of polarization is rotated by 90%. Suppose the incident light runs along the z -axis, and the emitted light along the direction $\hat{\mathbf{k}} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. For a polarization direction $\boldsymbol{\epsilon} = \hat{\mathbf{x}}$ along the x -axis, the angle β is found from

$$\sin^2 \beta = (\hat{\mathbf{k}} \times \boldsymbol{\epsilon})^2 = \cos^2 \theta + \sin^2 \theta \sin^2 \phi. \quad (12.235)$$

For a polarization direction $\boldsymbol{\epsilon} = \hat{\mathbf{y}}$ along the y -axis, it is

$$\sin^2 \beta = (\hat{\mathbf{k}} \times \boldsymbol{\epsilon})^2 = \cos^2 \theta + \sin^2 \theta \cos^2 \phi. \quad (12.236)$$

The average is

$$\overline{\sin^2 \beta} = \cos^2 \theta + \frac{1}{2} \sin^2 \theta = \frac{1}{2} (1 + \cos^2 \theta). \quad (12.237)$$

Integrating this over all solid angles yields the Thomson cross section for unpolarized light

$$\sigma_{\text{tot}} = \frac{8\pi}{3} r_e^2. \quad (12.238)$$

12.9.2 Klein-Nishina Formula

The scattering amplitude corresponding to the two Feynman diagrams in Fig. 12.6 is obtained by expanding formula (10.103) up to second order in e :

$$S_{\text{fi}} = -e^2 \int d^4x d^4y \langle 0 | a_{\mathbf{p}', s'_3} \hat{T} \bar{\psi}(y) \not{\epsilon}' \psi(y) \bar{\psi}(x) \not{\epsilon} \psi(x) a_{\mathbf{p}, s_3}^\dagger | 0 \rangle, \quad (12.239)$$

and by performing the Wick contractions of Section 7.8:

$$\begin{aligned} \langle 0 | a_{\mathbf{p}', s'_3} \hat{T} \bar{\psi}(y) \not{\epsilon}' \psi(y) \bar{\psi}(x) \not{\epsilon} \psi(x) a_{\mathbf{p}, s_3}^\dagger | 0 \rangle &= \langle 0 | \hat{T} \overbrace{a_{\mathbf{p}', s'_3} \bar{\psi}(y) \not{\epsilon}' \psi(y) \bar{\psi}(x) \not{\epsilon} \psi(x)}^{\text{Wick contractions}} a_{\mathbf{p}, s_3}^\dagger | 0 \rangle \\ &+ \langle 0 | \hat{T} \overbrace{a_{\mathbf{p}', s'_3} \bar{\psi}(y) \not{\epsilon}' \psi(y) \bar{\psi}(x) \not{\epsilon} \psi(x)}^{\text{Wick contractions}} a_{\mathbf{p}, s_3}^\dagger | 0 \rangle | 0 \rangle. \end{aligned} \quad (12.240)$$

After Fourier-expanding the intermediate electron propagator,

$$G_0(y, x) = \int \frac{d^4p^i}{(2\pi)^4} e^{-ip^i(y-x)} \frac{i}{\not{p}^i - M}, \quad (12.241)$$

we find

$$\begin{aligned} S_{\text{fi}} &= -e^2 \int d^4x d^4y e^{k'y - kx} \int \frac{d^4p^i}{(2\pi)^4} \frac{M}{\sqrt{V^2 E E' 2\omega 2\omega'}} \\ &\times \left[e^{i(p' - p^i)y - (p - p^i)x} \bar{u}(\mathbf{p}', s'_3) \not{\epsilon}'^* \frac{i}{\not{p}^i - M} \not{\epsilon} u(\mathbf{p}, s_3) \right. \\ &\quad \left. + e^{i(p' - p^i)x - (p - p^i)y} \bar{u}(\mathbf{p}', s'_3) \not{\epsilon} \frac{i}{\not{p}^i - M} \not{\epsilon}'^* u(\mathbf{p}, s_3) \right]. \end{aligned} \quad (12.242)$$

One of the spatial integrals fixes the intermediate momentum in accordance with energy-momentum conservation, the other yields a $\delta^{(4)}$ -function for overall energy-momentum conservation. The result is

$$S_{\text{fi}} = -i(2\pi)^4 \delta^{(4)}(p' + k' - p - k) e^2 \frac{M}{\sqrt{V^2 E E' 2\omega 2\omega'}} \bar{u}(\mathbf{p}', s'_3) H u(\mathbf{p}, s_3), \quad (12.243)$$

where H is the 4×4 -matrix in spinor space

$$H \equiv \not{\epsilon}'^* \frac{(\not{p} + \not{k}) + M}{(p + k)^2 - M^2} \not{\epsilon} + \not{\epsilon} \frac{(\not{p} - \not{k}') + M}{(p - k')^2 - M^2} \not{\epsilon}'^*. \quad (12.244)$$

We have written $\epsilon(\mathbf{k}, h)$, $\omega_{\mathbf{k}}$ as ϵ, ω , and $\epsilon(\mathbf{k}', h')$, $\omega_{\mathbf{k}'}$ as ϵ', ω' , respectively, with a similar simplification for E and E' . The second term of the matrix H arises from the first by the *crossing symmetry*

$$\epsilon \leftrightarrow \epsilon', \quad k \leftrightarrow -k'. \quad (12.245)$$

Simplifications arise from the properties (12.246). It can, moreover, be simplified by recalling that external electrons and photons are on their mass shell, so that

$$p^2 = p'^2 = M^2, \quad k^2 = k'^2 = 0, \quad (12.246)$$

$$k \epsilon = k' \epsilon' = 0. \quad (12.247)$$

A further simplification arises by working in the laboratory frame in which the initial electron is at rest, $p = (M, 0, 0, 0)$. Also, we choose a gauge in which the polarization vectors have only spatial components. Then

$$p \epsilon = p' \epsilon' = 0, \quad (12.248)$$

since p has only a temporal component and ϵ only space components. We also use the fact that H stands between spinors which satisfy the Dirac equation $(\not{p} - M)u(\mathbf{p}, s_3) = 0$, $\bar{u}(\mathbf{p}, s_3)(\not{p} - M) = 0$. Further we use the commutation rules (4.566) for the gamma matrices to write [as in (12.214)]

$$\not{\epsilon} \not{p} = -\not{p} \not{\epsilon} + 2p\epsilon. \quad (12.249)$$

The second term vanishes by virtue of Eq. (12.248). Similarly, we see that $\not{p}$ anti-commutes with $\not{\epsilon}'$. Using these results, we may eliminate the terms $\not{p} + M$ occurring in M . Finally, using Eq. (12.247), we obtain

$$\bar{u}(\mathbf{p}', s'_3)Hu(\mathbf{p}, s_3) = \bar{u}(\mathbf{p}', s'_3) \left\{ \epsilon'^* \frac{\not{k}}{2pk} \not{\epsilon} + \not{\epsilon} \frac{\not{k}'}{2pk'} \epsilon'^* \right\} u(\mathbf{p}, s_3). \quad (12.250)$$

To obtain the transition probability, we must take the absolute square of this. If we do not observe initial and final spins, we may average over the initial spin and sum over the final spin directions. This produces a factor 1/2 times the sum over both spin directions, which is equal to

$$F = \sum_{s'_3, s_3} |\bar{u}(\mathbf{p}', s'_3)Hu(\mathbf{p}, s_3)|^2 = \sum_{s'_3, s_3} \bar{u}(\mathbf{p}', s'_3)Hu(\mathbf{p}, s_3)\bar{u}(\mathbf{p}, s_3)Hu(\mathbf{p}', s'_3). \quad (12.251)$$

Here we apply the semi-completeness relation (4.702) for the spinors to find

$$F = \frac{1}{4M^2} \text{tr} [(\not{p}' + M)H(\not{p} + M)H]. \quad (12.252)$$

The trace over the product of gamma matrices can be evaluated according to the Wick-type of rules explained on p. 830.

$$\frac{1}{4} \text{tr}(\not{\epsilon}_1 \cdots \not{\epsilon}_n) = \sum_{\text{pair contractions}} (-)^P \not{\epsilon}_1 \cdots \not{\epsilon}_n. \quad (12.253)$$

After some lengthy algebra (see Appendix 9A), we find

$$F = \frac{1}{2M^2} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - 2 + 4|\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}|^2 \right]. \quad (12.254)$$

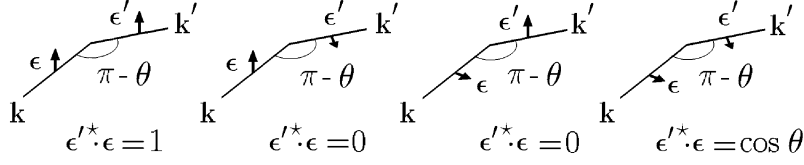


FIGURE 12.7 Illustration of the photon polarization sum $\sum_{h,h'} |\epsilon'^* \epsilon|^2 = 1 + \cos^2 \theta$ in Compton scattering in the laboratory frame. Incoming and outgoing photon momenta with scattering angle θ are shown in the scattering plane, together with their transverse polarization vectors.

This holds for specific polarizations of the incoming and outgoing photons. If we sum over all final polarizations and average over all initial ones, we find (see Fig. 12.7)

$$\frac{1}{2} \sum_{h,h'} |\epsilon'^* \epsilon|^2 = \frac{1}{2} (1 + \cos^2 \theta), \quad (12.255)$$

This can also be found more formally using the transverse completeness relation (4.334) of the polarization vectors:

$$\begin{aligned} \frac{1}{2} \sum_{h,h'} |\epsilon'^* \epsilon|^2 &= \frac{1}{2} \sum_{h,h'} \epsilon'^{i*}(\mathbf{k}', h') \epsilon^i(\mathbf{k}, h) \epsilon^{*j}(\mathbf{k}, h) \epsilon'^j(\mathbf{k}', h') \\ &= \frac{1}{2} \left(\delta^{ij} - \frac{k^i k^j}{\mathbf{k}^2} \right) \left(\delta^{ji} - \frac{k'^j k'^i}{\mathbf{k}'^2} \right) = \frac{1}{2} \left[1 + \frac{(\mathbf{k} \cdot \mathbf{k}')^2}{\mathbf{k}^2 \mathbf{k}'^2} \right] = \frac{1}{2} (1 + \cos^2 \theta). \end{aligned} \quad (12.256)$$

The average value of F is therefore

$$\bar{F} = \frac{1}{2} \sum_{h,h'} \frac{1}{2M^2} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - 2 + 4|\epsilon'^* \cdot \epsilon|^2 \right] = \frac{1}{M^2} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \sin^2 \theta \right]. \quad (12.257)$$

We are now ready to calculate the transition rate, for which we obtain from Eq. (9.298):

$$\frac{dP}{dt} = V(2\pi)^4 \int \frac{d^3 p' V}{(2\pi)^3} \int \frac{d^3 k' V}{(2\pi)^3} \delta^{(4)}(p' - p) |t_{fi}|^2, \quad (12.258)$$

with the squared t -matrix elements

$$|t_{fi}|^2 = e^4 \frac{1}{V^4} \frac{M^2}{E E' 2\omega 2\omega'} \frac{1}{2} F. \quad (12.259)$$

The spatial part of the δ -function removes the momentum integral over $\mathbf{p}'$. The temporal part of the δ -function enforces energy conservation. This is incorporated into the momentum integral over $\mathbf{k}'$ as follows. We set $E_f = p'_0 + k'_0$, and write

$$d^3 k' = k'^2 dk' d\Omega = \omega'^2 \frac{d\omega'}{dE_f} d\Omega dE_f, \quad (12.260)$$

where Ω is the solid angle into which the photon has been scattered. Then (12.258) becomes

$$\frac{dP}{dt d\Omega} = V e^4 (2\pi)^4 \frac{V^2}{(2\pi)^6} \left(\frac{\omega'}{\omega} \right) \left. \frac{d\omega'}{dE_f} \right|_{E_f=E_i} \frac{1}{4V^4} \frac{M^2}{EE'} \frac{1}{2} F. \quad (12.261)$$

For an explicit derivative $d\omega'/dE_f$, we go to the laboratory frame and express the final energy as

$$E_f = \omega' + \sqrt{\mathbf{p}'^2 + M^2} = \omega' + \sqrt{(\mathbf{k} - \mathbf{p}')^2 + M^2} = \omega' + \sqrt{\omega^2 - 2\omega\omega' \cos \theta + \omega'^2 + M^2}, \quad (12.262)$$

where θ is the scattering angle in the laboratory. This yields the derivative

$$\frac{dE_f}{d\omega'} = 1 + \frac{\omega' - \omega \cos \theta}{E'}. \quad (12.263)$$

By equating $E_i = M + \omega$ with E_f , we derive the *Compton relation*

$$\omega\omega'(1 - \cos \theta) = M(\omega - \omega'), \quad (12.264)$$

or

$$\omega' = \frac{\omega}{1 + \omega(1 - \cos \theta)/M}, \quad (12.265)$$

and therefore

$$\frac{dE_f}{d\omega'} = 1 + \frac{\omega' - \omega \cos \theta}{E'} = \frac{E' + \omega' - \omega \cos \theta}{E'} = \frac{M + \omega - \omega \cos \theta}{E'} = \frac{M}{E'} \frac{\omega}{\omega'}. \quad (12.266)$$

Since $E = M$ in the laboratory frame, Eq. (12.261) yields the differential probability rate

$$\frac{dP}{dt d\Omega} = V e^4 (2\pi)^4 \frac{V^2}{(2\pi)^6} V \left(\frac{\omega'}{\omega} \right)^2 \frac{1}{4V^4} \frac{1}{2} F. \quad (12.267)$$

To find the differential cross section, this has to be divided by the incoming particle current density. According to Eq. (9.315), this is given by

$$j = \frac{v}{V}, \quad (12.268)$$

where v is the velocity of the incoming particles. The incoming photons move with light velocity, so that (in natural units with $c = 1$)

$$j = \frac{1}{V}. \quad (12.269)$$

This leaves us with the Klein-Nishina formula for the differential cross section

$$\frac{d\sigma}{d\Omega} = \alpha^2 \left(\frac{\omega'}{\omega} \right)^2 \frac{1}{2} F. \quad (12.270)$$

In the nonrelativistic limit where $\omega \ll M$, the Compton relation (12.265) shows that $\omega' \approx \omega$, and Eq. (12.257) reduces to

$$F \rightarrow \frac{1}{M^2}(1 + \cos^2 \theta). \quad (12.271)$$

Expressed in terms of the classical electron radius $r_0 = \alpha/M$, the differential scattering cross section becomes, expressed in terms of the classical electron radius $r_0 \equiv \alpha/M$,

$$\frac{d\sigma}{d\Omega} \approx r_0^2 \frac{1}{2}(1 + \cos^2 \theta). \quad (12.272)$$

This is the Thomson formula for the scattering of low energy radiation by a static charge. To find the total Thomson cross section, we must integrate (12.272) over all solid angles and obtain:

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} \approx 2\pi \int_{-1}^1 d\cos\theta \, r_0^2 \frac{1}{2}(1 + \cos^2 \theta). \quad (12.273)$$

In the low-energy limit we identify

$$\sigma_{\text{Thomson}} \equiv r_0^2 \frac{8\pi}{3}. \quad (12.274)$$

Let us also calculate the total cross section for relativistic scattering, integrating (12.270) over all solid angles:

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 2\pi \int_{-1}^1 d\cos\theta \, \frac{\alpha^2}{2M^2} \left(\frac{\omega'}{\omega} \right)^2 \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \sin^2 \theta \right]. \quad (12.275)$$

Inserting

$$\omega' = \frac{\omega}{1 + \omega(1 - \cos\theta)/M}, \quad (12.276)$$

which follows from (12.265), the angular integral yields

$$\sigma = \sigma_{\text{Thomson}} f(\omega), \quad (12.277)$$

where $f(\omega)$ contains the relativistic corrections to Thomson's cross section:

$$f(\omega) = \frac{3}{8\omega^3} \left\{ \frac{2\omega[\omega(\omega+1)(\omega+8)+2]}{(2\omega+1)^2} - (2+2\omega-\omega^2) \log(1+2\omega) \right\} \quad (12.278)$$

For small ω , $f(\omega)$ starts out like (see Fig. 12.8a):

$$f(\omega) = 1 - 2\omega + \mathcal{O}(\omega^2). \quad (12.279)$$

For large ω , $\omega f(\omega)$ increases like (see Fig. 12.8b):

$$\omega f(\omega) = \frac{3}{8\omega} \log 2\omega + \mathcal{O}(1/\log \omega). \quad (12.280)$$

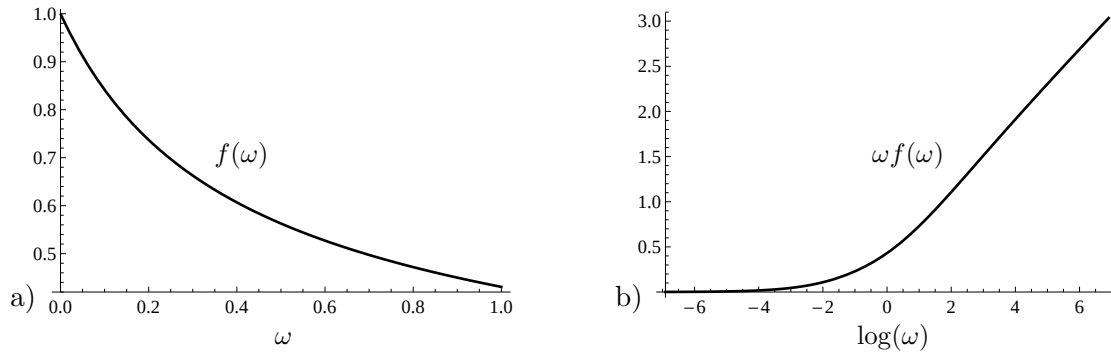


FIGURE 12.8 Ratio between total relativistic Compton cross section and nonrelativistic Thomson cross section.

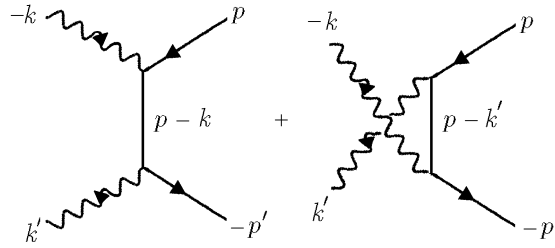


FIGURE 12.9 Lowest-order Feynman diagrams contributing to electron-positron annihilation. It arises from the Compton diagram by the crossing operation $p' \rightarrow -p'$, $k \rightarrow -k$, $\epsilon \rightarrow \epsilon^*$.

12.10 Electron-Positron Annihilation

The Feynman diagrams in Fig. 12.6 can also be read from bottom to top in which case they describe annihilation processes. In order to see this, we use as much as possible previous results and reinterpret the Feynman diagrams as shown in Fig. 12.9. Instead of an outgoing electron with momentum p' , we let a negative-energy electron go out with momentum $-p'$. Instead of an incoming photon with momentum k we let a negative-energy photon go out with momentum $-k$. The former are represented by spinors $\bar{v}(\mathbf{p}', s_3)$, which are negative energy solutions of the Dirac equation with inverted momenta and spin directions. The S -matrix element to lowest order is found from a slightly modified (12.239):

$$S_{\text{fi}} = -e^2 \int d^4x d^4y \langle 0 | \hat{T} \bar{\psi}(y) \not{\epsilon}' \psi(y) \bar{\psi}(x) \not{\epsilon} \psi(x) b_{\mathbf{p}', s'_3}^\dagger a_{\mathbf{p}, s_3} | 0 \rangle. \quad (12.281)$$

Performing the Wick contractions as in (12.240) we obtain

$$\begin{aligned} S_{\text{fi}} = & -e^2 \int d^4x d^4y e^{k'y + kx} \int \frac{d^4p^i}{(2\pi)^4} \frac{M}{\sqrt{V^2 E E' 2\omega 2\omega'}} \\ & \times \left[e^{i(-p' - p^i)y - (p - p^i)x} \bar{v}(\mathbf{p}', s'_3) \not{\epsilon}'^* \frac{i}{\not{p}^i - M} \not{\epsilon}^* u(\mathbf{p}, s_3) \right] \end{aligned}$$

$$+ e^{i(-p'-p)x-(p-p')y} \bar{v}(\mathbf{p}', s'_3) \not{\epsilon}^* \frac{i}{\not{p}' - M} \not{\epsilon}' u(\mathbf{p}, s_3) \Big]. \quad (12.282)$$

Note that this arises from the Compton expression (12.242) by the crossing operation

$$p' \rightarrow -p', \quad \bar{u}(\mathbf{p}, s_3) \rightarrow \bar{v}(\mathbf{p}, s_3), \quad k \rightarrow -k, \quad \epsilon(k, h) \rightarrow \epsilon^*(k, h). \quad (12.283)$$

As before, one of the spatial integrals fixes the intermediate momentum in accordance with energy-momentum conservation, the other yields a $\delta^{(4)}$ -function for overall energy-momentum conservation. The result is

$$S_{\text{fi}} = -i(2\pi)^4 \delta^{(4)}(k + k' - p - p') e^2 \frac{M}{\sqrt{V^2 E E' 2\omega 2\omega'}} \bar{v}(\mathbf{p}', s'_3) H u(\mathbf{p}, s_3), \quad (12.284)$$

where H is the 4×4 -matrix in spinor space

$$H \equiv \not{\epsilon}'^* \frac{(\not{p}' - \not{k}) + M}{(p - k)^2 - M^2} \not{\epsilon}^* + \not{\epsilon}^* \frac{(\not{p}' - \not{k}') + M}{(p - k')^2 - M^2} \not{\epsilon}'^*. \quad (12.285)$$

As before, we have written $\epsilon(\mathbf{k}, h)$, $\omega_{\mathbf{k}}$ as ϵ, ω , and $\epsilon(\mathbf{k}', h')$, $\omega_{\mathbf{k}'}$ as ϵ', ω' , respectively, with a similar simplification for E and E' . The second term of the matrix H arises from the first by the *Bose symmetry*

$$\epsilon \leftrightarrow \epsilon', \quad k \leftrightarrow k'. \quad (12.286)$$

Simplifications arise from the mass shell properties (12.246), the gauge conditions (12.247), and the other relations (12.248), (12.249). We also work again in the laboratory frame in which the initial electron is at rest, $p = (M, 0, 0, 0)$ and the positron comes in with momentum $\mathbf{p}'$ and energy $E' = \sqrt{\mathbf{p}'^2 + M^2}$. This leads to

$$\bar{v}(\mathbf{p}', s'_3) H u(\mathbf{p}, s_3) = \bar{v}(\mathbf{p}', s'_3) \left\{ \epsilon'^* \frac{\not{k}}{2pk} \not{\epsilon}^* + \not{\epsilon}^* \frac{\not{k}'}{2pk'} \not{\epsilon}'^* \right\} u(\mathbf{p}, s_3). \quad (12.287)$$

To obtain the transition probability, we must take the absolute square of this. If we do not observe initial spins, we may average over the initial spin components which gives a factor 1/4 times the spin sum

$$F = \sum_{s'_3, s_3} |\bar{v}(\mathbf{p}', s'_3) H u(\mathbf{p}, s_3)|^2 = \sum_{s'_3, s_3} \bar{v}(\mathbf{p}', s'_3) H u(\mathbf{p}, s_3) \bar{u}(\mathbf{p}, s_3) H u(\mathbf{p}', s'_3). \quad (12.288)$$

Now we use the semi-completeness relations (4.702) and (4.703) for the spinors to rewrite (12.288) as

$$F = -\frac{1}{4M^2} \text{tr} [(-\not{p}' + M) H (\not{p} + M) H]. \quad (12.289)$$

The trace over a product of gamma matrices is now evaluated as before and we obtain, for specific polarizations of the two outgoing photons, almost the same expression as before in Eq. (12.257) (see Appendix 12A):

$$F = \frac{1}{2M^2} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} + 2 - 4|\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}^*|^2 \right]. \quad (12.290)$$

This result can be deduced directly from the previous polarization sum (12.254) by the crossing operation (12.283), apart from an overall minus sign, whose origin is the negative sign in front of (12.289).

We are now ready to calculate the transition rate, for which we obtain from Eq. (9.298)

$$\frac{dP}{dt} = V(2\pi)^4 \int \frac{d^3k'V}{(2\pi)^3} \int \frac{d^3kV}{(2\pi)^3} \delta^{(4)}(p' - p) |t_{fi}|^2, \quad (12.291)$$

with the squared t -matrix elements

$$|t_{fi}|^2 = e^4 \frac{1}{V^4} \frac{M^2}{EE'2\omega2\omega'} \frac{1}{4} F. \quad (12.292)$$

The spatial part of the δ -function removes the momentum integral over $\mathbf{k}'$. The temporal part of the δ -function enforces energy conservation. This is incorporated into the momentum integral over $\mathbf{k}$ as follows. We set $E_f = \omega + \omega'$, and write

$$d^3k = k^2 dk d\Omega = \omega^2 \frac{d\omega}{dE_f} d\Omega dE_f, \quad (12.293)$$

where Ω is the solid angle into which the photon with momentum k emerges. Then (12.291) becomes

$$\frac{dP}{dt d\Omega} = V e^4 (2\pi)^4 \frac{V^2}{(2\pi)^6} \left(\frac{\omega}{\omega'} \right) \frac{d\omega}{dE_f} \bigg|_{E_f=E_i} \frac{1}{4V^4} \frac{M^2}{EE'} \frac{1}{4} F. \quad (12.294)$$

To calculate $d\omega/dE_f$ explicitly, we express the final energy in the laboratory frame as

$$E_f = \omega + \sqrt{\mathbf{k}'^2} = \omega + \sqrt{(\mathbf{p}' - \mathbf{k})^2} = \omega + \sqrt{\mathbf{p}'^2 - 2\omega|\mathbf{p}'| \cos \theta + \omega^2}, \quad (12.295)$$

where θ is the scattering angle in the laboratory. Hence:

$$\begin{aligned} \frac{dE_f}{d\omega} &= 1 + \frac{1}{2\omega'} \frac{d}{d\omega} (\mathbf{p}'^2 - 2\omega|\mathbf{p}'| \cos \theta + \omega^2) = \frac{1}{\omega\omega'} (\omega\omega' - 2\omega|\mathbf{p}'| \cos \theta + \omega^2) \\ &= \frac{1}{\omega\omega'} \left[\omega (M + \sqrt{\mathbf{p}'^2 + M^2}) - 2\omega|\mathbf{p}'| \cos \theta \right] = \frac{k(p + p')}{\omega\omega'} = \frac{M(M + E')}{\omega\omega'}. \end{aligned} \quad (12.296)$$

We must now divide (12.294) by the incoming positron current density $j = |\mathbf{p}'|/E'V$ [recall (9.315)], and find the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{|\mathbf{p}'|(M + E')} \left(\frac{\omega}{M} \right)^2 \frac{1}{4} M^2 F, \quad (12.297)$$

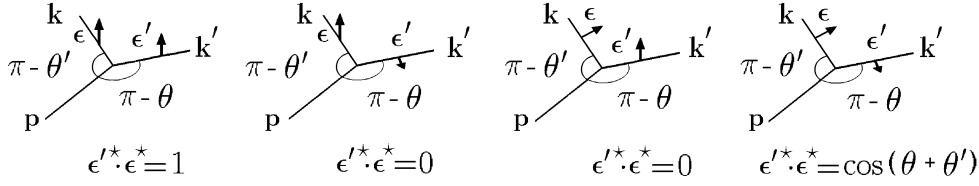


FIGURE 12.10 Illustration of the photon polarization sum $\sum_{h,h'} |\epsilon'^* \epsilon|^2$ in electron-positron annihilation in the laboratory frame. Incoming positron and outgoing photon momenta with scattering angles θ and θ' are shown in the scattering plane, together with their transverse polarization vectors.

where

$$\frac{M}{\omega} = \frac{M + E' - |\mathbf{p}'| \cos \theta}{M + E'}, \quad (12.298)$$

as follows from equating the right-hand sides of

$$k k' = \frac{1}{2}(k + k')^2 = \frac{1}{2}(p + p')^2 = M(M + E'), \quad (12.299)$$

and

$$k k' = k(p + p' - k) = \omega(M + E' - |\mathbf{p}'| \cos \theta). \quad (12.300)$$

If the incoming positron is very slow, then $\omega \approx \omega' \approx M$, and the two photons share equally the rest energies of the electron and the positron. We can now substitute in F of Eq. (12.290):

$$\frac{\omega'}{\omega} = \frac{E' - |\mathbf{p}'| \cos \theta}{M}, \quad (12.301)$$

and sum over all photon polarizations to obtain [see Fig. 12.10 and Eq. (12.257)]

$$\sum_{h,h'} |\epsilon'^* \epsilon|^2 = 1 + \frac{(\mathbf{k} \cdot \mathbf{k}')^2}{k^2 k'^2} = 1 + \cos^2(\theta + \theta') = \left(1 - \frac{M}{\omega} - \frac{M}{\omega'}\right)^2. \quad (12.302)$$

The last expression is found by observing that

$$k k' = \omega \omega' [1 - \cos(\theta + \theta')], \quad (12.303)$$

so that we can express

$$\cos(\theta + \theta') = 1 - \frac{k k'}{\omega \omega'} = 1 - \frac{1}{2} \frac{(k + k')^2}{\omega \omega'} = 1 - \frac{1}{2} \frac{(p + p')^2}{\omega \omega'} = 1 - \frac{M(M + E')}{\omega \omega'}.$$

Energy conservation leads to

$$\cos(\theta + \theta') = 1 - \frac{k k'}{\omega \omega'} = 1 - \frac{M(\omega + \omega')}{\omega \omega'}, \quad (12.304)$$

thus obtaining the right-hand side of (12.302). Note that from (12.303) and (12.304) we find a relation

$$k k' = M(\omega + \omega'). \quad (12.305)$$

We now introduce the relativistic factor of the incoming positron $\gamma \equiv E'/M$ and write the relation (12.298) as

$$\frac{M}{\omega} = 1 - \sqrt{\frac{\gamma-1}{\gamma+1}} \cos \theta, \quad \frac{M}{\omega'} = \frac{1 - \sqrt{\frac{\gamma-1}{\gamma+1}} \cos \theta}{\gamma - \sqrt{\gamma^2 - 1} \cos \theta}. \quad (12.306)$$

The result is integrated over all solid angles, and divided by 2 to account for Bose statistics of the two final photons. This yields the cross section expressed in terms of the classical electron radius $r_0 = \alpha/M$:

$$\sigma(\gamma) = \frac{1}{2} \int d\Omega \frac{d\sigma}{d\Omega} = \frac{\pi r_0^2}{1+\gamma} \left[\frac{\gamma^2 + 4\gamma + 1}{\gamma^2 - 1} \log \left(\gamma + \sqrt{\gamma^2 - 1} \right) - \frac{\gamma + 3}{\sqrt{\gamma^2 - 1}} \right]. \quad (12.307)$$

For small incoming positron energy, the cross section diverges like

$$\sigma(\gamma) \xrightarrow[\text{small } \mathbf{p}]{} \sigma_{\text{low-energy}}(\gamma) \equiv \frac{\pi r_0^2 \gamma}{\sqrt{\gamma^2 - 1}} \approx \frac{\pi r_0^2 c}{v}, \quad (12.308)$$

whereas in the high-energy limit it behaves like

$$\sigma \xrightarrow[|\mathbf{p}| \rightarrow \infty]{} \frac{\pi r_0^2}{\gamma} [\log(2\gamma) - 1]. \quad (12.309)$$

The detailed behavior is shown in Fig. 12.11.

The above result can be used to estimate the lifetime of a positron moving through matter. We simply have to multiply the cross section σ by the incident current density $j = |\mathbf{p}|/EV$ of a single positron and by the number N of target electrons, which is Z per atom. For slow positrons we may use Eq. (12.308) to find the decay rate

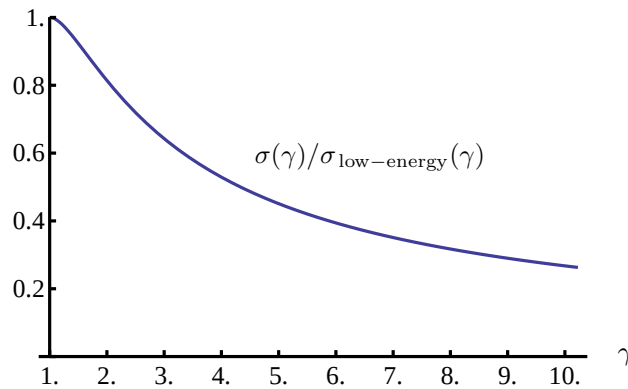


FIGURE 12.11 Electron-positron annihilation cross section divided by its low-energy limiting expression (12.308) as a function of $\gamma = 1/\sqrt{1 - v^2/c^2}$ of the incoming positron in the laboratory frame.

$$\dot{P} = \pi r_0^2 v Z \frac{N}{V}. \quad (12.310)$$

For lead, this yields a lifetime $\tau = 1/\dot{P} \approx 10^{-10}$ s.

The formula (12.313) is actually not very precise, since the incoming positron wave is strongly distorted towards the electron by the Coulomb attraction. This is the so-called initial-state interaction. It is closely related to the problem to be discussed in the next section.

12.11 Positronium Decay

The previous result can be used to calculate the lifetime of positronium. Since the momenta in positronium are nonrelativistic, the annihilation cross section (12.308) is relevant. The wave function of positronium at rest in an s-wave is approximately given by [recall (7.311)]

$$|\psi^{S,S_3}\rangle = \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(\mathbf{p}) a_{\mathbf{p},s_3}^\dagger b_{-\mathbf{p},s'_3}^\dagger |0\rangle \langle S, S_3 | s, s_3; s, s'_3 \rangle, \quad \tilde{\psi}(\mathbf{p}) = \frac{8\sqrt{\pi}a^3}{(1+a^2|\mathbf{p}|^2)^2}, \quad (12.311)$$

where $S = 1$ for ortho-positronium and $S = 0$ for para-positronium, and a is the Bohr radius of positronium, which is twice the Bohr radius of hydrogen: $a = 2a_H = 2/\alpha M$, the factor 2 being due to the reduced mass μ being half the electron mass [recall the general formula (6.132)]. This amplitude can be pictured by the Feynman diagrams shown in Fig. 12.12.

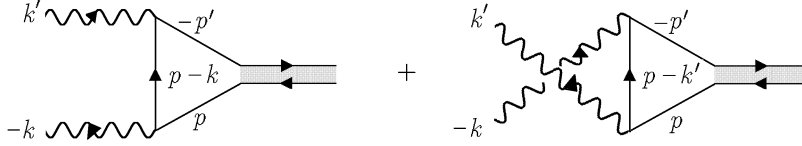


FIGURE 12.12 Lowest-order Feynman diagrams contributing to the decay of the spin singlet para-positronium, i.e., the ground state.

In Eq. (7.310) we have calculated the charge conjugation parity η_C of these states to be ∓ 1 , respectively. Since a photon is odd under charge conjugation [recall (7.550)], ortho-positronium can only decay into three photons (one is forbidden by energy-momentum conservation). Thus only para-positronium decays into two photons and the cross section calculated in the last section arises only from the spin singlet contribution of the initial state. Since it was obtained from the average of a total of four states, three of which do not decay at all, the decay rate of the singlet state is four times as big as calculated previously from (12.308). The integral over all momenta in the amplitude (12.281) can be factored out since the low-energy decay rate is approximately independent of v and hence of $\mathbf{p}$. Thus we obtain directly the decay rate [15]

$$\Gamma_{\text{para} \rightarrow 2\gamma} \equiv \dot{P}_{\text{para}} = 4\pi r_0^2 c \left| \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(\mathbf{p}) \right|^2 = 4\pi r_0^2 c |\psi(\mathbf{0})|^2 = 4\pi r_0^2 c \frac{1}{\pi a^3}$$

$$= \frac{Mc^2}{\hbar} \frac{\alpha^5}{2}. \quad (12.312)$$

Using the electron energy $Mc^2 \approx 0.510$ MeV and the Planck constant $\hbar \approx 6.682 \times 10^{-16}$ eVs, the ratio $\hbar/Mc^2$ is equal to 1.288×10^{-22} s. Together with the factor $2/\alpha^5$, this leads to a lifetime $\tau = 1/\Gamma \approx 0.13 \times 10^{-9}$ s.

The decay of the spin triplet ortho-positronium state proceeds at a roughly thousand times slower rate

$$\Gamma_{\text{orth} \rightarrow 3\gamma} \equiv \dot{P}_{\text{orth}} = \frac{Mc^2}{\hbar} \frac{\alpha^6}{2} \frac{4(\pi^2 - 9)}{9\pi}, \quad (12.313)$$

with a lifetime of 140×10^{-9} s.

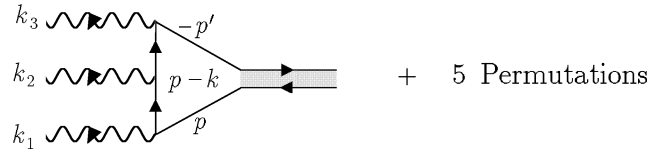


FIGURE 12.13 Lowest-order Feynman diagrams contributing to decay of the spin-triplet ortho-positronium, the first excited state which lies 203.5 GHz above the ground state.

Decays into 4 and 5 photons have also been calculated and measured experimentally. The theoretical rates are [14, 15]:

$$\Gamma_{\text{para} \rightarrow 4\gamma} \approx 0.0138957 \frac{Mc^2}{\hbar} \alpha^7 \left[1 - 14.5 \frac{\alpha}{\pi} + \mathcal{O}(\alpha^2) \right] \approx 1.43 \times 10^{-6} \times \Gamma_{\text{para} \rightarrow 2\gamma}. \quad (12.314)$$

$$\Gamma_{\text{orth} \rightarrow 5\gamma} \approx 0.0189 \alpha^2 \times \Gamma_{\text{orth} \rightarrow 3\gamma} \approx 0.959 \times 10^{-6} \times \Gamma_{\text{orth} \rightarrow 3\gamma}. \quad (12.315)$$

Experimentally, the branching ratios are $1.14(33) \times 10^{-6}$ and $1.67(99) \times 10^{-6}$, in reasonable agreement with the theoretical numbers. The validity of C -invariance has also been tested by looking for the forbidden decays of para-positronium into an odd and ortho-positronium into an even number of photons. So far, there is no indication of C -violation.

12.12 Bremsstrahlung

If a charged particle is accelerated or slowed down, it emits an electromagnetic radiation called *Bremsstrahlung*. This is a well-known process in classical electrodynamics and we would like to find the quantum field theoretic generalization of it. First, however, we shall recapitulate the classical case.

12.12.1 Classical Bremsstrahlung

Consider a trajectory in which a particle changes its momentum abruptly from p to p' [see Fig. 12.14].

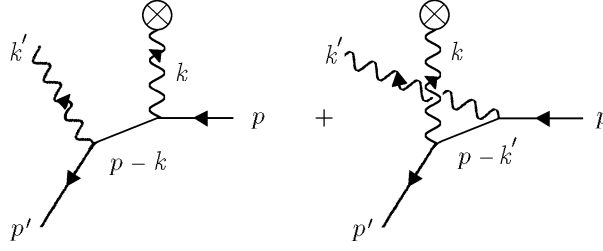


FIGURE 12.14 Trajectories in the simplest classical Bremsstrahlung process: An electron changing abruptly its momentum.

The trajectory may be parametrized as:

$$x^\mu(\tau) = \begin{cases} \tau p/M & \text{for } \tau < 0, \\ \tau p'/M & \text{for } \tau > 0, \end{cases} \quad (12.316)$$

where τ is the proper time. The electromagnetic current associated with this trajectory is

$$\begin{aligned} j^\mu(x) &= e \int d\tau \frac{dx^\mu(\tau)}{d\tau} \delta^{(4)}(x - x(\tau)) \\ &= \frac{e}{M} \int d\tau \left[\Theta(\tau) p^\mu \delta^{(4)}(x - \tau p/M) + \theta(-\tau) p'^\mu \delta^{(4)}(x - \tau p'/M) \right]. \end{aligned} \quad (12.317)$$

After a Fourier decomposition of the δ -functions, this can be written as

$$j^\mu(x) = \int \frac{d^4 k}{(2\pi)^4} e^{-ikx} j^\mu(k), \quad (12.318)$$

with the Fourier components

$$j^\mu(k) = -ie \left(\frac{p^\mu}{pk} - \frac{p'^\mu}{p'k} \right). \quad (12.319)$$

The vector potential associated with this current is found by solving the Maxwell equation Eq. (12.50). Under the initial condition that at large negative time, the vector potential describes the retarded Coulomb potential of the incident particle, we obtain

$$A^\mu(x) = i \int dx' G_R(x - x') j^\mu(x'), \quad (12.320)$$

where $G_R(x - x')$ is the retarded Green function defined in Eq. (7.162). At very large times the particle has again a Coulomb field associated with it which can be found by using the advanced Green function of Eq. (7.168):

$$A_{\text{out}}^\mu(x) = i \int dx' G_A(x - x') j^\mu(x'). \quad (12.321)$$

As the acceleration takes place, the particle emits radiation which is found from the difference between the two fields,

$$A_{\text{rad}}^\mu = \frac{1}{i} \int dx' [G_R(x, x') - G_A(x, x')] j^\mu(x'). \quad (12.322)$$

Remembering the list (7.212) of Fourier transforms of the various Green functions, we see that the Fourier components of the radiation field are given by

$$A_{\text{rad}}^{\mu}(k) = -i2\pi\epsilon(k^0)\delta(k^2)j^{\mu}(k). \quad (12.323)$$

The energy of the electromagnetic field is, by Eq. (7.427):

$$H = \int d^3x \frac{1}{2} (-\dot{A}^{\mu} \dot{A}_{\mu} - \nabla A^{\mu} \nabla A_{\mu}). \quad (12.324)$$

A classical field which solves the field equations can be Fourier decomposed into positive- and negative-frequency components as in (7.390),

$$A^{\mu}(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left(e^{-ikx} a_{\mathbf{k}}^{\mu} + e^{ikx} a_{\mathbf{k}}^{\mu\dagger} \right), \quad (12.325)$$

where

$$a_{\mathbf{k}}^{\mu} \equiv \sum_{\lambda=0}^3 \epsilon^{\mu}(\mathbf{k}, \lambda) a_{\mathbf{k}, \lambda} \quad (12.326)$$

are classical Fourier components. Then the combination of time and space derivatives in (12.324) eliminates all terms of the form $a_{\mathbf{k}} a_{\mathbf{k}}$ and $a_{\mathbf{k}}^* a_{\mathbf{k}}^*$, and we find

$$H = \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2} (-a_{\mathbf{k}}^{\mu*} a_{\mathbf{k}}^{\nu} - a_{\mathbf{k}}^{\mu} a_{\mathbf{k}}^{\nu*}) g_{\mu\nu}, \quad (12.327)$$

just as in the calculation of the energy in (7.428). The radiation field (12.323) corresponds to

$$a_{\mathbf{k}}^{\mu} = -ij^{\mu}(k)|_{k^0=|\mathbf{k}|}. \quad (12.328)$$

Inserting everything into (12.327) we derive, for large t , an emitted energy

$$\mathcal{E} = - \int \frac{d^3k}{2k^0(2\pi)^3} k^0 \sum_{h=1,2} j_{\mu}^*(k) j^{\mu}(k). \quad (12.329)$$

Inserting (12.319) we obtain the energy emitted into a momentum space element d^3k :

$$d\mathcal{E} = \frac{1}{2} \frac{d^3k}{(2\pi)^3} e^2 \left[\frac{2pp'}{(pk)(p'k)} - \frac{M^2}{(pk)^2} - \frac{M^2}{(p'k)^2} \right], \quad (12.330)$$

where polarization vectors have vanishing zeroth components. Dividing out the energy per photon k^0 , this can be interpreted as the probability of emitting a photon into d^3k :

$$dP = \frac{d^3k}{2k^0(2\pi)^3} e^2 \left[\frac{2pp'}{(pk)(p'k)} - \frac{M^2}{(pk)^2} - \frac{M^2}{(p'k)^2} \right]. \quad (12.331)$$

If we are interested in the polarization of the radiated electromagnetic field, we make use of the local current conservation law $\partial_{\mu} j^{\mu}$ which reads, in momentum space,

$$\mathbf{k} \cdot \mathbf{j} = k^0 j^0. \quad (12.332)$$

This allows us to rewrite

$$j_\mu^*(k)j^\mu(k) = |j^0(k)|^2 - |\mathbf{j}(k)|^2 = \frac{1}{\mathbf{k}^2} |\mathbf{k} \cdot \mathbf{j}(k)|^2 - |\mathbf{j}(k)|^2 = -|\mathbf{j}_T(\mathbf{k})|^2, \quad (12.333)$$

where

$$j_T^i(k) \equiv \left(\delta^{ij} - \frac{k^i k^j}{\mathbf{k}^2} \right) j^j(k) \quad (12.334)$$

is the transverse part of the current. In the second-quantized description of the energy, the transverse projection is associated with a sum over the two outgoing photon polarization vectors [recall (4.334)]:

$$\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} = \sum_{h=1,2} \epsilon_i^*(\mathbf{k}, h) \epsilon_j(\mathbf{k}, h). \quad (12.335)$$

The emitted energy (12.329) can therefore be resolved with respect to the polarization vectors as

$$\mathcal{E} = \int \frac{d^3 k}{2k^0 (2\pi)^3} k^0 \sum_{h=1,2} |\boldsymbol{\epsilon}(\mathbf{k}, h) \cdot \mathbf{j}(k)|^2. \quad (12.336)$$

This leads to an energy emitted into a momentum space element $d^3 k$:

$$d\mathcal{E} = \frac{d^3 k}{2(2\pi)^3} e^2 \sum_{h=1,2} \left| \frac{p\epsilon}{pk} - \frac{p'\epsilon}{p'k} \right|^2, \quad (12.337)$$

and a corresponding probability of omitting a photon into $d^3 k$, by analogy with (12.331).

Let us calculate the angular distribution of the emitted energy in Eq. (12.330). Denote the direction of $\mathbf{k}$ by $\mathbf{n}$:

$$\mathbf{n} \equiv \frac{\mathbf{k}}{|\mathbf{k}|}. \quad (12.338)$$

Then we can write pk as

$$pk = E|\mathbf{k}|(1 - \mathbf{v} \cdot \mathbf{n}) \quad (12.339)$$

and find

$$d\mathcal{E} = \frac{d^3 k}{(2\pi)^3 2} \frac{e^2}{|\mathbf{k}|^2} \left[\frac{2(1 - \mathbf{v} \cdot \mathbf{v}')}{(1 - \mathbf{v} \cdot \mathbf{n})(1 - \mathbf{v}' \cdot \mathbf{n})} - \frac{M^2}{E^2(1 - \mathbf{v} \cdot \mathbf{n})^2} - \frac{M'^2}{E'^2(1 - \mathbf{v}' \cdot \mathbf{n})^2} \right]. \quad (12.340)$$

The radiation is peaked around the directions of the incoming and outgoing particles.

12.12.2 Bremsstrahlung in Mott Scattering

We now turn to the more realistic problem of an electron scattering on a nucleus. Here the electron changes its momentum within a finite period of time rather than abruptly. Still, the Bremsstrahlung will be very similar to the previous one. Let us consider immediately a Dirac electron, i.e., we study the Bremsstrahlung emitted

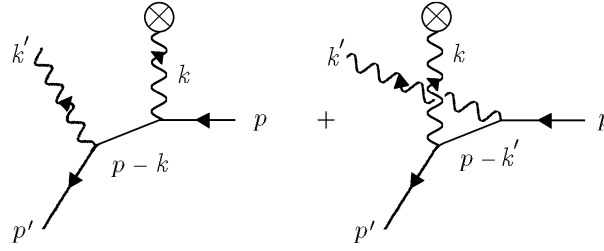


FIGURE 12.15 Lowest-order Feynman diagrams contributing to Bremsstrahlung. The vertical photon line indicates the nuclear Coulomb potential.

in Mott scattering. The lowest-order Feynman diagrams governing this process are shown in Fig. 12.15. The vertical photon line indicates the nuclear Coulomb potential

$$V_C(\mathbf{x}) = -\frac{Z\alpha}{4\pi r}. \quad (12.341)$$

The scattering amplitude is found from the Compton amplitude by simply interchanging the incoming photon field

$$eA^\mu(x) = \epsilon_{k,\lambda}^\mu e^{-ikx} \sqrt{2V k_0}$$

with the static vector potential

$$\delta^\mu_0 V_C(r) = -\delta^\mu_0 Z\alpha \int \frac{d^4 q}{(2\pi)^4} 2\pi \delta(q^0) e^{-iqx} \frac{1}{|\mathbf{q}|^2}. \quad (12.342)$$

The scattering amplitude is therefore

$$S_{\text{fi}} = i \frac{4\pi Z\alpha e}{|\mathbf{q}|^2} 2\pi \delta(p'^0 + k'^0 - p^0) \frac{M}{\sqrt{V^2 E' E}} \frac{1}{\sqrt{2V k_0}} \\ \times \bar{u}(\mathbf{p}', s'_3) \left[\not{\epsilon}'^* \frac{1}{\not{p}' + \not{k}' - M} \gamma^0 - \gamma^0 \frac{1}{\not{p}' - \not{k}' - M} \not{\epsilon}' \right] u(\mathbf{p}, s_3), \quad (12.343)$$

where

$$\mathbf{q} = \mathbf{p}' + \mathbf{k}' - \mathbf{p} \quad (12.344)$$

is the spatial momentum transfer. The amplitude conserves only energy, not spatial momentum. The latter is transferred from the nucleus to the electron without any restriction. The unpolarized cross section following from S_{fi} is

$$d\sigma = M^2 Z^2 (4\pi\alpha)^3 \frac{1}{2k'^0 E' E} \frac{1}{\mathbf{v}} \int \frac{d^3 p' d^3 k'}{(2\pi)^6} 2\pi \delta(p'^0 + k'^0 - p^0) \frac{F}{|\mathbf{q}|^2}, \quad (12.345)$$

where we have used the incoming particle current density $\mathbf{v}/V = \mathbf{p}/EMV$ and set

$$F \equiv \frac{1}{2} \sum_h \text{tr} \left[\left(\not{\epsilon}'^* \frac{\not{p}' + \not{k}' + M}{2p'k'} \gamma^0 - \gamma^0 \frac{\not{p}' - \not{k}' + M}{2pk} \not{\epsilon}' \right) \frac{\not{p}' + M}{2M} \right. \\ \left. \left(\gamma^0 \frac{\not{p}' + \not{k}' + M}{2p'k} \not{\epsilon}' - \not{\epsilon}' \frac{\not{p}' - \not{k}' + M}{2pk} \gamma^0 \right) \frac{\not{p}' + M}{2M} \right]. \quad (12.346)$$

Let $d\Omega_e$ and $d\Omega_\gamma$ be the solid angles of outgoing electrons and photons $d\Omega_e$ and $d\Omega_\gamma$, respectively. If we drop the prime on the emitted photon variables, so that ϵ' and k' are written as ϵ and k , and write for the energy k^0 of the outgoing photon the variable ω , the differential cross section becomes

$$\frac{d\sigma}{d\Omega_e d\Omega_\gamma d\omega} = \frac{Z^2 \alpha^3}{\pi^2} \frac{M^2}{|\mathbf{q}|^4} \frac{|\mathbf{p}'|}{|\mathbf{p}|} \omega F. \quad (12.347)$$

The calculation of F is as tedious as that of the trace (12.289) in the Klein-Nishina cross section. It can be done again with the help of the formulas in Appendix 12A. Let us introduce the angles θ and θ' between the outgoing photon momentum and the initial and final electron momenta p and p' , respectively (see Fig. 12.16). Then

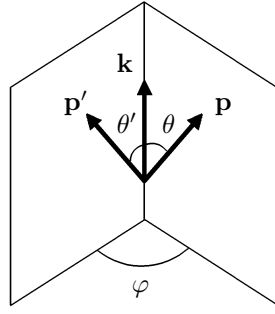


FIGURE 12.16 The angles θ' , θ , φ in the Bethe-Heitler cross section formula.

we calculate the polarization sums

$$\begin{aligned} \sum_h (\epsilon \cdot \mathbf{p}')^2 &= |\mathbf{p}'|^2 \sin^2 \theta', \\ \sum_h (\epsilon \cdot \mathbf{p})^2 &= |\mathbf{p}|^2 \sin^2 \theta, \end{aligned} \quad (12.348)$$

$$\sum_h (\epsilon \cdot \mathbf{p}')(\epsilon \cdot \mathbf{p}) = |\mathbf{p}'||\mathbf{p}| \sin \theta' \sin \theta \cos \varphi, \quad (12.349)$$

and obtain

$$\begin{aligned} F &= \frac{1}{4\omega^2} \left[\frac{p'^2 \sin^2 \theta'}{(E' - p' \cos \theta')^2} (4E^2 - q^2) + \frac{p^2 \sin^2 \theta}{(E - p \cos \theta)^2} (4E'^2 - q^2) \right. \\ &\quad + 2\omega^2 \frac{p^2 \sin^2 \theta + p'^2 \sin^2 \theta'}{(E' - p' \cos \theta')(E - p \cos \theta)} \\ &\quad \left. - 2 \frac{p' p \sin \theta' \sin \theta \cos \varphi}{(E' - p' \cos \theta')(E - p \cos \theta)} (4E' E - q^2 + 2\omega^2) \right]. \end{aligned} \quad (12.350)$$

With this form of the function F , Eq. (12.347) is known as the *Bethe-Heitler cross section* formula. For soft photon emission, $\omega \rightarrow 0$, the cross section becomes:

$$\frac{d\sigma}{d\Omega_e} \approx \frac{d\sigma}{d\Omega_e} \Big|_{\text{elastic}} \times e^2 \frac{d^3 k}{2\omega(2\pi)^3} \left| \frac{\epsilon p'}{k p'} - \frac{\epsilon p}{k p} \right|^2. \quad (12.351)$$

It consists of the elastic cross section that is multiplied by the cross section of the classical Bremsstrahlung.

12.13 Electron-Electron Scattering

The leading Feynman diagrams are shown in Fig. 12.17. The associated scattering

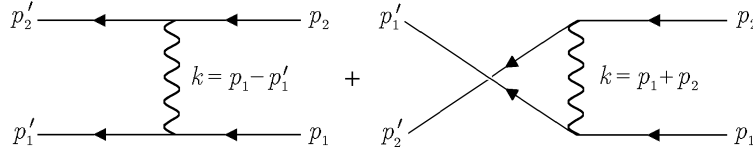


FIGURE 12.17 Lowest-order Feynman diagrams contributing to electron-electron scattering.

amplitude is given by

$$S_{fi} = (2\omega)^4 \delta^4(p_1' + p_2' - p_1 - p_2) (-ie)^2 \quad (12.352)$$

$$\times \left[-\bar{u}(p_1', \varepsilon_1') \gamma^\nu u(p_1, \varepsilon_1) \frac{-ig_{\nu\rho}}{(p_1 - p_1')^2} \bar{u}(p_2', \varepsilon_2') \gamma^\rho u(p_2, \varepsilon_2) \right. \\ \left. + \bar{u}(p_2', \varepsilon_2') \gamma^\nu u(p_1, \varepsilon_1) \frac{-ig_{\nu\rho}}{(p_1 - p_2')^2} \bar{u}(p_1', \varepsilon_1') \gamma^\rho u(p_2, \varepsilon_2) \right].$$

For the scattering amplitude t_{fi} defined by

$$S_{fi} \equiv -ie^2 (2\pi)^4 \delta^4(p_1' + p_2' - p_1 - p_2) t_{fi}, \quad (12.353)$$

we find

$$t_{fi} = \frac{\bar{u}(p_1', \varepsilon_1') u(p_1, \varepsilon_1) \bar{u}(p_2', \varepsilon_2') \gamma_\nu u(p_2, \varepsilon_2)}{(p_1 - p_1')^2} - \frac{\bar{u}(p_2', \varepsilon_2') \gamma^\nu u(p_1, \varepsilon_1) \bar{u}(p_1', \varepsilon_1') \gamma_\nu u(p_2, \varepsilon_2)}{(p_1 - p_2')^2}. \quad (12.354)$$

There is a manifest antisymmetry of the initial or final states accounting for the Pauli principle. Due to the identity of the electrons, the total cross section is obtained by integrating over only half of the final phase space.

Let us compute the differential cross section for unpolarized initial beams, when the final polarizations are not observed. The kinematics of the reaction in the center of mass frame is represented in Fig. 12.18, where θ is the scattering angle in this frame. The energy E is conserved, and we denote $|\mathbf{p}| = |\mathbf{p}'| = p = \sqrt{E^2 - m^2}$. Using the general formula (9.311) with the covariant fermion normalization $V \rightarrow 1/E$, we obtain

$$\frac{d\sigma}{d\Omega_{\text{CM}}} = \frac{M^2 e^4}{4E^2 (2\pi)^2} \overline{|t_{fi}|^2}. \quad (12.355)$$

The bar on the right-hand side indicates an average over the initial polarizations and a sum over the final polarizations. More explicitly, we must evaluate the traces¹

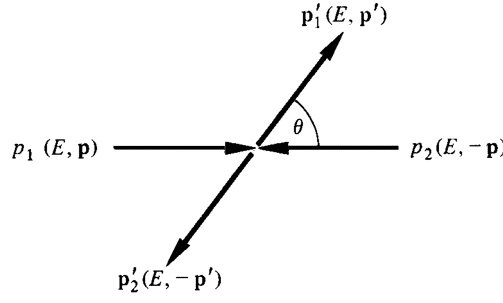


FIGURE 12.18 Kinematics of electron-electron scattering in the center of mass frame.

$$\begin{aligned}
 \overline{|t_{fi}|^2} &= \frac{1}{4} \sum_{\varepsilon_1 \varepsilon_2 \varepsilon'_1 \varepsilon'_2} |t_{fi}|^2 \\
 &= \frac{1}{4} \left\{ \text{tr} \left(\gamma_\nu \frac{\not{p}_1 + M}{2M} \gamma_\rho \frac{\not{p}'_1 + M}{2M} \right) \text{tr} \left(\gamma^\nu \frac{\not{p} + M}{2M} \gamma^\rho \frac{\not{p}' + M}{2M} \right) \frac{1}{[(p'_1 - p_1)^2]^2} \right. \\
 &\quad \left. - \text{tr} \left(\gamma_\nu \frac{\not{p} + M}{2M} \gamma_\rho \frac{\not{p}' + M}{2M} \gamma^\nu \frac{\not{p}_1 + M}{2M} \gamma^\rho \frac{\not{p}'_1 + M}{2M} \right) \frac{1}{(p'_1 - p_1)^2 (p'_2 - p_1)^2} \right. \\
 &\quad \left. + (p'_1 \leftrightarrow p'_2) \right\}. \tag{12.356}
 \end{aligned}$$

This is done using the formulas

$$\begin{aligned}
 \text{tr} [\gamma_\nu (\not{p}_1 + M) \gamma_\rho (\not{p}'_1 + M)] &= 4(p_{1\nu} p'_{1\rho} - g_{\nu\rho} p_1 \cdot p'_1 + p_{1\rho} p'_{1\nu} + M^2 g_{\nu\rho}), \\
 \text{tr} [\gamma_\nu (\not{p}_1 + M) \gamma_\pi (\not{p}'_1 + M)] \times \text{tr} [\gamma^\nu (\not{p}_2 + M) \gamma^\rho (\not{p}'_2 + M)] \\
 &= 32[(p_1 \cdot p_2)^2 + (p_1 \cdot p'_2)^2 + 2M^2(p_1 \cdot p'_2 - p_1 \cdot p_2)], \tag{12.357}
 \end{aligned}$$

and further

$$\gamma_\nu (\not{p}_1 + M) \gamma_\rho (\not{p}'_2 + M) \gamma^\nu = -2 \not{p}'_2 \gamma_\rho \not{p}_1 + 4M(p'_{2\rho} + p_{1\rho}) - 2M^2 \gamma_\rho, \tag{12.358}$$

leading to

$$\text{tr} [\gamma_\nu (\not{p}_1 + M) \gamma_\rho (\not{p}'_2 + M) \gamma^\nu (\not{p}_2 + M) \gamma^\rho (\not{p}'_1 + M)] = -32(p_1 p_2)^2 - 2M^2 p_1 p_2,$$

and thus to

$$\begin{aligned}
 \overline{|t_{fi}|^2} &= \frac{1}{2M^4} \left\{ \frac{(p_1 p_2)^2 + (p_1 p'_2)^2 + 2M(p_1 p'_2 - p_1 p_2)}{[(p'_1 - p_1)^2]^2} \right. \\
 &\quad \left. + \frac{(p_1 p_2)^2 + (p_1 p'_1)^2 + 2M^2(p_1 p'_1 - p_1 p_2)}{[(p'_2 - p_1)^2]^2} \right. \\
 &\quad \left. + 2 \frac{(p_1 p_2)^2 - 2M^2 p_1 p_2}{(p'_1 - p_1)^2 (p'_2 - p_1)^2} \right\}. \tag{12.359}
 \end{aligned}$$

This can be expressed in terms of the Mandelstam variables s, t, u whose properties were discussed in Eqs. (9.318)–(9.331), yielding

$$\begin{aligned}
 \overline{|t_{fi}|^2} &= \frac{1}{2M^4} \left\{ \frac{1}{t^2} \left[\frac{s^2 + u^2}{4} + 2m^2(t - m^2) \right] + \frac{1}{u^2} \left[\frac{s^2 + t^2}{4} + 2m^2(u - m^2) \right] \right. \\
 &\quad \left. + \frac{1}{tu} \left[\left(\frac{s}{2} - m^2 \right) \left(\frac{s}{2} - 3m^2 \right) \right] \right\}. \tag{12.360}
 \end{aligned}$$

We may now easily express all invariants in terms of the center-of-mass energy E_{CM} and the scattering angle θ :

$$\begin{aligned} p_1 p_2 &= 2E_{\text{CM}}^2 - M^2, \\ p_1 p'_1 &= E_{\text{CM}}^2(1 - \cos \theta) + M^2 \cos \theta, \\ p_1 p'_2 &= E_{\text{CM}}^2(1 - \cos \theta) - M^2 \cos \theta. \end{aligned} \quad (12.361)$$

This leads to the *Møller formula* (1932):

$$\frac{d\sigma}{d\Omega_{\text{CM}}} = \frac{\alpha^2(2E_{\text{CM}}^2 - M^2)^2}{4E_{\text{CM}}^2(E_{\text{CM}}^2 - M^2)^2} \left[\frac{4}{\sin^4 \theta} - \frac{3}{\sin^2 \theta} + \frac{(E_{\text{CM}}^2 - M^2)^2}{(2E_{\text{CM}}^2 - M^2)^2} \left(1 + \frac{4}{\sin^2 \theta} \right) \right]. \quad (12.362)$$

In the ultrarelativistic limit of high incident energies $M/E_{\text{CM}} \rightarrow 0$, we have

$$\left. \frac{d\sigma}{d\Omega_{\text{CM}}} \right|_{\text{ur}} \approx \frac{\alpha^2}{E_{\text{CM}}^2} \left(\frac{4}{\sin^4 \theta} - \frac{2}{\sin^2 \theta} + \frac{1}{4} \right) = \frac{\alpha^2}{4E_{\text{CM}}^2} \left(\frac{1}{\sin^4 \theta/2} + \frac{1}{\cos^4 \theta/2} + 1 \right). \quad (12.363)$$

For small energies where $E_{\text{CM}}^2 \simeq M^2$, $v^2 = (p^2 - M^2)/E_{\text{CM}}^2$, we obtain the nonrelativistic formula

$$\begin{aligned} \left. \frac{d\sigma}{d\Omega_{\text{CM}}} \right|_{\text{nr}} &= \left(\frac{\alpha}{M} \right)^2 \frac{1}{4v^4} \left(\frac{4}{\sin^4 \theta} - \frac{3}{\sin^2 \theta} \right) \\ &= \left(\frac{\alpha}{M} \right)^2 \frac{1}{16v^4} \left(\frac{1}{\sin^4 \theta/2} + \frac{1}{\cos^4 \theta/2} - \frac{1}{\sin^2 \theta/2 \cos^2 \theta/2} \right), \end{aligned} \quad (12.364)$$

that was first derived by Mott in 1930.

Comparing (12.364) with the classical Rutherford formula for Coulomb scattering in Eq. (12.194), we see that the forward peak is the same for both if we set $Z = 1$ and replace M by the reduced mass $M/2$. The particle identity yields, in addition, the backward peak.

12.14 Electron-Positron Scattering

Let us now consider electron-positron scattering. The kinematics and lowest-order diagrams are depicted in Figs. 12.19 and 12.20. Polarization indices are omitted

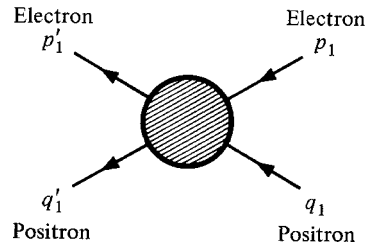


FIGURE 12.19 General form of diagrams contributing to electron-positron scattering.

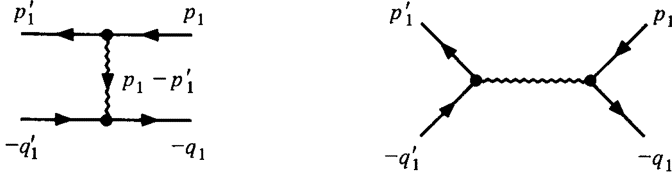


FIGURE 12.20 Lowest-order contributions to electron-positron scattering.

and in Fig. 12.20 four-momenta are oriented according to the charge flow. The scattering amplitude may then be obtained from (12.354) by substituting

$$\begin{aligned} p_2 &\rightarrow q_1', & u(p_2) &\rightarrow v(q_1'), \\ p_2' &\rightarrow -q_1', & u(p_2') &\rightarrow v(q_1'), \end{aligned}$$

and by changing the sign of the amplitude. The center of mass cross section is then given by the formula

$$\frac{d\sigma}{d\Omega} = \frac{M^4 e^4}{4E_{\text{CM}}^2 (2\pi)^2} \overline{|t_{fi}|^2} \quad (12.365)$$

with

$$\begin{aligned} \overline{|t_{fi}|^2} = \frac{1}{2M^4} &\left\{ \frac{(p_1 q_1')^2 + (p_1 q_1)^2 - 2M^2(p_1 q_1 - p_1 q_1')}{[(p_1' + p_1)^2]^2} \right. \\ &+ \frac{(p_1 q_1')^2 + (p_1 p_1')^2 + 2M^2(p_1 p_1' + p_1 q_1')}{[(p_1 + q_1)^2]^2} \\ &\left. + 2 \frac{(p_1 q_1')^2 + 2M^2 p_1 q_1'}{(p_1 - p_1')^2 (p_1 + q_1)^2} \right\}. \end{aligned} \quad (12.366)$$

This can be expressed in terms of the Mandelstam variables s, t, u whose properties were discussed in Eqs. (9.318)–(9.331) as follows:

$$\begin{aligned} \overline{|t_{fi}|^2} = \frac{1}{2M^4} &\left\{ \frac{1}{t^2} \left[\frac{u^2 + s^2}{4} + 2m^2(t - m^2) \right] + \frac{1}{s^2} \left[\frac{u^2 + t^2}{4} + 2m^2(s - m^2) \right] \right. \\ &\left. + \frac{1}{st} \left[\left(\frac{u}{2} - m^2 \right) \left(\frac{u}{2} - 3m^2 \right) \right] \right\}. \end{aligned} \quad (12.367)$$

It is then straightforward to derive the cross section formula first obtained by Bhabha (1936):

$$\begin{aligned} \frac{d\sigma^{e^-e^+}}{d\Omega} = \frac{\alpha}{2E_{\text{CM}}^2} &\left[\frac{5}{4} - \frac{8E_{\text{CM}}^4 - M^4}{E_{\text{CM}}^2(E_{\text{CM}}^2 - M^2)(1 - \cos\theta)} + \frac{(2E_{\text{CM}}^2 - M^2)^2}{2(E_{\text{CM}}^2 - M^2)^2(1 - \cos\theta)^2} \right. \\ &\left. + \frac{2E_{\text{CM}}^4(-1 + 2\cos\theta + \cos^2\theta) + 4E_{\text{CM}}^2 M^2(1 - \cos\theta)(2 + \cos\theta) + 2M^4 \cos^2\theta}{16E_{\text{CM}}^4} \right]. \end{aligned} \quad (12.368)$$

In the ultrarelativistic limit, this becomes

$$\frac{d\sigma^{e^-e^+}}{d\Omega} \stackrel{\text{ur}}{=} \frac{\alpha^2}{8E_{\text{CM}}^2} \left[\frac{1 + \cos^4 \theta/2}{\sin^4 \theta/2} + \frac{1}{2}(1 + \cos^2 \theta) - 2 \frac{\cos^4 \theta/2}{\sin^2 \theta/2} \right]. \quad (12.369)$$

The nonrelativistic limit is simply

$$\frac{d\sigma^{e^-e^+}}{d\Omega} \stackrel{\text{nr}}{=} \left(\frac{\alpha}{M} \right)^2 \frac{1}{16v^4 \sin^4 \theta/2}. \quad (12.370)$$

This agrees again with the classical Rutherford cross section (12.194). The annihilation diagram does not contribute in this limit,

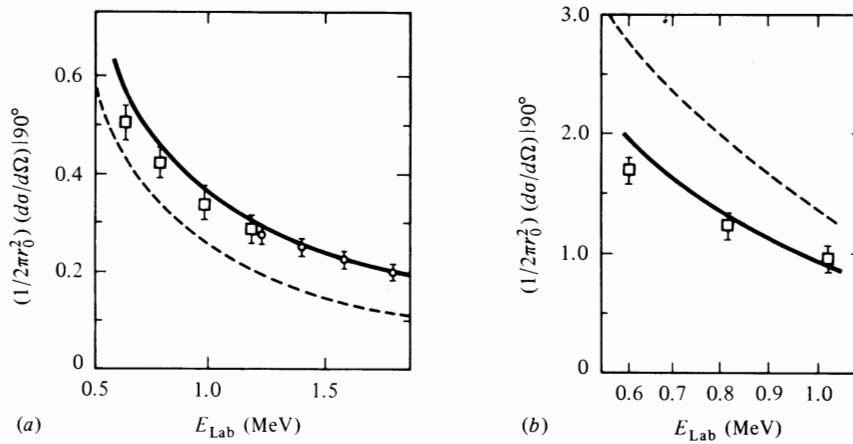


FIGURE 12.21 Experimental data for electron-electron and electron-positron scattering at $\theta = 90^\circ$ as a function of the incident electron energy in the laboratory frame. (a) Electron-electron scattering. The solid line represents the Møller formula, the broken one the Møller formula when the spin terms are omitted. (b) Electron-positron scattering. The solid line follows the Bhabha formula, the broken one the prediction when annihilation terms are deleted. Data are from A. Ashkin, L.A. Page, and W.M. Woodward, *Phys. Rev.* *94*, 357, (1974).

The results of Eqs. (12.362) and (12.368) may be compared with experimental data. At low energies we show in Fig. 12.21 some experimental data for electron-electron scattering at 90 degrees [7]. Møller's formula (12.362) is in good agreement with the data. The agreement confirms the fact that the spin of the electron is really $1/2$. If it was zero, the agreement would have been bad (see the dashed curve in Fig. 12.21).

Electron-positron scattering data are fitted well by Bhabha's cross section, and the annihilation term is essential for the agreement. The energy of the incident particle in the laboratory frame plotted on the abscissa is chosen in the intermediate range where neither the nonrelativistic nor the ultrarelativistic approximation is valid. The numerical values show a significant departure from the ratio 2:1 between e^-e^- and e^-e^+ cross sections, expected on the basis of a naive argument of indistinguishability of the two electrons.

12.15 Anomalous Magnetic Moment of Electron and Muon

The most directly observable effect of loop diagrams is a change in the magnetic moment of the electron. Recall the precession equation (6.74).

As a consequence of loop diagrams in quantum electrodynamics, the gyromagnetic ratio g in the relation (12.125) receives a correction and becomes $g = 2(1 + a)$. The number

$$a = (g - 2)/2 > 0 \quad (12.371)$$

is called the *anomalous magnetic moment* of the electron. It has been measured experimentally with great accuracy [16]:

$$a = 1\,159\,652\,188.4(4.3) \times 10^{-12}. \quad (12.372)$$

The numbers in parentheses indicate the error estimate in the last two digits. For the positron, the result is

$$\bar{a} = 1\,159\,652\,187.9(4.3) \times 10^{-12}. \quad (12.373)$$

Quantum electrodynamics has been able to explain these numbers up to the last digits – a triumph of quantum field theory.

To lowest order in α , the anomalous magnetic moment can easily be calculated. Interestingly enough, it is found to be a *finite* quantity; no divergent integrals occur in its calculation. The Feynman diagram responsible for it is the vertex correction shown in Fig. 12.23. This diagram changes the electromagnetic current of an electron from

$$\langle \mathbf{p}', s'_3 | j^\mu | \mathbf{p}, s_3 \rangle = e \bar{u}(\mathbf{p}') \gamma^\mu u(\mathbf{p}) \quad (12.374)$$

to

$$\langle \mathbf{p}', s'_3 | j^\mu | \mathbf{p}, s_3 \rangle = e \bar{u}(\mathbf{p}') [\gamma^\mu + \Lambda^\mu(p', p)] u(\mathbf{p}), \quad (12.375)$$

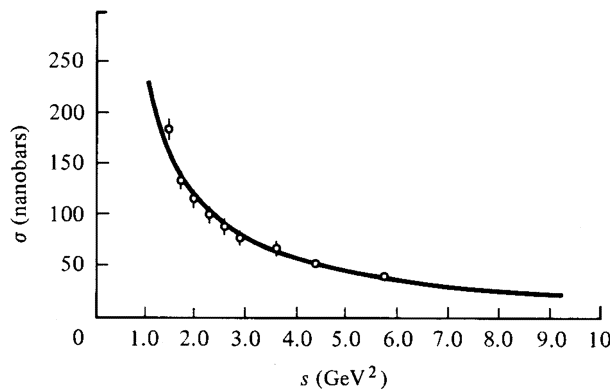


FIGURE 12.22 Cross section for Bhabha scattering at high energy, for scattering angle $45^\circ < \theta < 135^\circ$ as a function of total energy-momentum square s . The solid line is calculated from quantum electrodynamics with first-order radiative corrections [8].

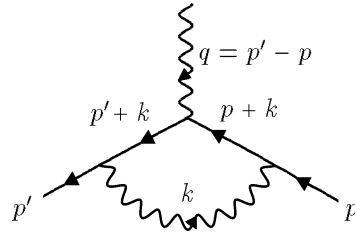


FIGURE 12.23 Vertex correction responsible for the anomalous magnetic moment.

where the vertex correction $\Lambda^\mu(p', p)$ is given by the Feynman integral

$$\Lambda^\mu(p', p) = -i4\pi\alpha \int \frac{d^4k}{(2\pi)^4} \gamma^\nu \frac{1}{\not{p}' + \not{k} - M} \gamma^\mu \frac{1}{\not{p} + \not{k} - M} \gamma_\nu \frac{1}{k^2}. \quad (12.376)$$

This integral is logarithmically divergent at large momenta k_μ . It can be regularized by cutting the integration off at some large but finite momentum Λ which is later removed by a renormalization of the charge in the Lagrangian. There is also an infrared divergence which is kept finite by cutting off the k -integration at a small mass value $k^2 = \mu^2$, much smaller than the electron mass, i.e., $\mu^2 \ll M^2$.

To do the integral, we rewrite the integrand as

$$\gamma^\nu \frac{\not{p}' + \not{k} + M}{(p' + k)^2 - M^2} \gamma^\mu \frac{\not{p} + \not{k} + M}{(p + k)^2 - M^2} \gamma_\nu \frac{1}{k^2 - \mu^2}, \quad (12.377)$$

where we have introduced a small photon mass μ to avoid infrared divergencies at small momenta. We now collect the product of denominators into a single denominator with the help of Feynman's formula (11.158) for three denominators

$$\frac{1}{ABC} = 2 \int_0^1 dx \int_0^x dy [Ay + B(x - y) + C(1 - x)]^{-3}, \quad (12.378)$$

so that

$$\begin{aligned} & \frac{1}{(p' + k)^2 - M^2} \frac{1}{(p + k)^2 - M^2} \frac{1}{k^2} \\ &= 2 \int_0^1 dx \int_0^x dy \left\{ [(p' + k)^2 - M^2] y + [(p + k)^2 - M^2] (x - y) + (k^2 - \mu^2)(1 - x) \right\}^{-3}. \end{aligned} \quad (12.379)$$

This can be simplified to

$$2 \int_0^1 dx \int_0^x dy \left\{ [k - p'y - p(x - y)]^2 - \mu^2(1 - x) - M^2x^2 + q^2y(x - y) \right\}^{-3}. \quad (12.380)$$

After performing a shift of the integration variable

$$k \rightarrow k + p'y + p(x - y),$$

the vertex correction (12.376) takes the form

$$\Lambda^\mu(p', p) = -i4\pi\alpha \, 2 \int_0^1 dx \int_0^x dy \int \frac{d^4k}{(2\pi)^4} \quad (12.381)$$

$$\times \gamma^\nu \frac{[\not{p}'(1-y) - \not{k} - \not{p}(x-y) + M] \gamma^\mu [\not{p}(1-x-y) - \not{k} - \not{p}'y + M]}{[k^2 - \mu^2(1-x) - M^2x^2 + q^2y(x-y)]^3} \gamma_\nu.$$

Instead of calculating this general expression, we shall restrict ourselves to matrix elements of the current between electron states and evaluate $\bar{u}(\mathbf{p}', s'_3) \Lambda^\mu(p', p) u(\mathbf{p}, s_3)$. Then we can use the mass shell conditions $p^2 = p'^2 = M^2$ and the Dirac equations $\not{p}u(\mathbf{p}, s_3) = Mu(\mathbf{p}, s_3)$ and $\bar{u}(\mathbf{p}', s'_3) \not{p}' = M\bar{u}(\mathbf{p}', s'_3)$. We now employ appropriately the anticommutation rules of the gamma matrices using the formulas (12.220)–(12.222), perform a Wick rotation $k^0 \rightarrow ik^4$, and integrate over the Euclidean four-momenta $d^4k_E = 2\pi^2 dk^3$, setting $p^2 = -p_E^2$, $p'^2 = -p_E'^2$. Cutting off the k -integral at $k_E = \Lambda$, we arrive at the triple integral

$$\bar{u}(\mathbf{p}', s'_3) \Lambda^\mu(p', p) u(\mathbf{p}, s_3) = \alpha \int_0^1 dx \int_0^x dy \int_0^\Lambda dk_E k_E^3 \frac{k_E^3}{[k_E^2 + \mu^2(1-x) + M^2x^2 + q_E^2y(x-y)]^3} \quad (12.382)$$

$$\times \bar{u}(\mathbf{p}', s'_3) \left\{ \gamma^\mu [k_E^2 - 2M^2(x^2 - 4x + 2) + 2q^2(y(x-y) + 1 - x)] \right. \\ \left. - 4Mp'^\mu(y - x + xy) - 4Mp^\mu(x^2 - xy - y) \right\} u(\mathbf{p}, s_3).$$

The denominator is symmetric under the exchange $y \rightarrow x - y$. Under this operation, the coefficients of p^μ and p'^μ are interchanged, showing that the vertex function is symmetric in p^μ and p'^μ . We can therefore replace each of these coefficients by the common average

$$\left\{ \frac{y - x + xy}{x^2 - xy - y} \right\} \rightarrow \frac{1}{2}[(y - x + xy) + (x^2 - xy - y)] = -\frac{1}{2x(1-x)},$$

and rewrite (12.382) as

$$\bar{u}(\mathbf{p}', s'_3) \Lambda^\mu(p', p) u(\mathbf{p}, s_3) = \alpha \int_0^1 dx \int_0^x dy \int_\mu^\Lambda dk_E k_E^3 \frac{k_E^3}{[k_E^2 + \mu^2(1-x) + M^2x^2 - q^2y(x-y)]^3} \quad (12.383)$$

$$\times \bar{u}(\mathbf{p}', s'_3) \left\{ \gamma^\mu [k_E^2 - 2M^2(x^2 - 4x + 2) + 2q^2(y(x-y) + 1 - x)] \right. \\ \left. - 2M(p'^\mu + p^\mu)x(1-x) \right\} u(\mathbf{p}, s_3).$$

This expression may be decomposed as follows:

$$\bar{u}(\mathbf{p}', s'_3) \Lambda^\mu(p', p) u(\mathbf{p}, s_3) = \bar{u}(\mathbf{p}', s'_3) \left[\gamma^\mu H(q^2) - \frac{1}{2M}(p'^\mu + p^\mu)G(q^2) \right] u(\mathbf{p}, s_3), \quad (12.384)$$

with the invariant functions

$$H(q^2) = \frac{\alpha}{\pi} \int_0^1 dx \int_0^x dy \int_\mu^\Lambda dk_E k_E^3 \frac{k_E^2 - 2M^2(x^2 - 4x + 2) + 2q^2[y(x-y) + 1 - x]}{[k_E^2 + \mu^2(1-x) + M^2x^2 - q^2y(x-y)]^3} \quad (12.385)$$

and

$$G(q^2) = \frac{\alpha}{\pi} M^2 \int_0^1 dx \int_0^x dy \int_\mu^\Lambda dk_E k_E^3 \frac{4M^2 x(1-x)}{[k_E^2 + \mu^2(1-x) + M^2 x^2 - q^2 y(x-y)]^3}. \quad (12.386)$$

The momentum integral in the second invariant function $G(q^2)$ is convergent at small and large momenta, such that we can set the photon mass μ to zero and ultraviolet to infinity. Using the integral formula

$$\int_0^\infty dk_E^2 k_E^2 \frac{1}{(k_E^2 + M_1^2)^3} = \frac{1}{2M_1^2}, \quad (12.387)$$

we obtain

$$G(q^2) = \frac{\alpha}{\pi} M^2 \int_0^1 dx \int_0^x dy \frac{x(1-x)}{M^2 x^2 - q^2 y(x-y)}. \quad (12.388)$$

The integral over y yields

$$G(q^2) = \frac{\alpha}{\pi} M^2 \int_0^1 dx 4(1-x) \frac{1}{\sqrt{q^2(4M^2 - q^2)}} \arctan \sqrt{\frac{q^2}{4M^2 - q^2}}, \quad (12.389)$$

leading to

$$G(q^2) = \frac{\alpha}{\pi} \frac{2M^2}{\sqrt{q^2(4M^2 - q^2)}} \arctan \sqrt{\frac{q^2}{4M^2 - q^2}}, \quad (12.390)$$

which can be rewritten as

$$G(q^2) = \frac{\alpha}{2\pi} \frac{2\theta}{\sin 2\theta}, \quad \text{with} \quad \sin^2 \theta \equiv \frac{q^2}{4M^2}. \quad (12.391)$$

For small q^2 , it has the expansion

$$G(q^2) = \frac{\alpha}{2\pi} \left(1 + \frac{q^2}{6M^2} + \dots \right). \quad (12.392)$$

In the first invariant function $H(q^2)$, both the cutoff and the photon mass are necessary to obtain a finite result. The divergence can be isolated by a subtraction of the integrand, separating

$$H(q^2) = H(0) + \Delta H(q^2), \quad (12.393)$$

with a divergent integral

$$H(0) = \frac{\alpha}{\pi} \int_0^1 dx \int_0^x dy \int_0^\infty dk_E k_E^3 \frac{k_E^2 - 2M^2(x^2 - 4x + 2)}{[k_E^2 + \mu^2(1-x) + M^2 x^2]^3} \quad (12.394)$$

and a convergent one at large momenta

$$\Delta H(q^2) = \frac{\alpha}{\pi} \int_0^1 dx \int_0^x dy \int_0^\infty dk_E k_E^3 \left\{ \frac{k_E^2 - 2M^2(x^2 - 4x + 2) + 2q^2[y(x-y) + 1 - x]}{[k_E^2 + \mu^2(1-x) + M^2x^2 - q^2y(x-y)]^3} - \frac{k_E^2 - 2M^2(x^2 - 4x + 2)}{[k_E^2 + \mu^2(1-x) + M^2x^2]^3} \right\}. \quad (12.395)$$

The divergent momentum integral in (12.394) must be performed with the help of some regularization scheme, for which we choose the Pauli-Villars regularization, replacing the photon propagator as follows:

$$\frac{1}{k^2 - \mu^2} \rightarrow \frac{1}{k^2 - \mu^2} - \frac{1}{k^2 - \Lambda^2}, \quad (12.396)$$

where Λ is a large cutoff mass. Then we may use the formula

$$\begin{aligned} \int_0^\infty dk_E^2 k_E^2 & \left\{ \left[\frac{k_E^2 + M_2^2}{(k_E^2 + \mu^2(1-x) + M_1^2)^3} \right] - [\mu^2 \rightarrow \Lambda^2] \right\} \\ & = -\log \frac{\mu^2(1-x) + M_1^2}{\Lambda^2(1-x)} + \frac{1}{2} \frac{M_2^2}{\mu^2(1-x) + M_1^2}. \end{aligned} \quad (12.397)$$

With this, the convergent momentum integral (12.395) yields

$$\begin{aligned} \Delta H(q^2) &= \frac{\alpha}{2\pi} \int_0^1 dx \int_0^x dy \left\{ -\frac{M^2(x^2 - 4x + 2) - q^2[y(x-y) + 1 - x]}{\mu^2(1-x) + M^2x^2 - q^2y(x-y)} \right. \\ & \quad \left. + \frac{M^2(x^2 - 4x + 2)}{\mu^2(1-x) + M^2x^2} - \log \left[\frac{\mu^2(1-x) + M^2x^2 - q^2y(x-y)}{\mu^2(1-x) + M^2x^2} \right] \right\}. \end{aligned} \quad (12.398)$$

If the photon mass is set equal to zero, the integral is divergent at $x = 0$. The physical meaning of this infrared divergence will be explained later.

Let us first understand $\Delta H(q^2)$ for small q^2 by expanding $\Delta H(q^2) = \Delta H'(0)q^2 + \mathcal{O}(q^4)$. Then $\Delta H'(0)$ is given by the integral

$$\begin{aligned} \Delta H'(0) &= \frac{\alpha}{2\pi} \int_0^1 dx \int_0^x dy \left\{ \frac{y(x-y) + 1 - x}{\mu^2(1-x) + M^2x^2} \right. \\ & \quad \left. - \frac{M^2(x^2 - 4x + 2)y(x-y)}{[\mu^2(1-x) + M^2x^2]^2} + \frac{y(x-y)}{\mu^2(1-x) + M^2x^2} \right\} \\ &= \frac{\alpha}{2\pi} \left(\frac{1}{3} \log \frac{M^2}{\mu^2} - \frac{1}{12} \right), \end{aligned} \quad (12.399)$$

where we have discarded all terms which go to zero for $\mu \rightarrow 0$.

The full result is

$$\begin{aligned} H(q^2) &= H(0) + \frac{\alpha}{2\pi} \left[\left(\log \frac{M^2}{\mu^2} - 2 \right) \left(1 - \frac{2\theta}{\tan 2\theta} \right) \right. \\ & \quad \left. + \theta \tan \theta + \frac{4}{\tan 2\theta} \int_0^\theta dx x \tan x + \frac{2\theta}{\sin 2\theta} \right], \end{aligned} \quad (12.400)$$

which has precisely the first Taylor coefficient (12.399).

12.15.1 Form Factors

We now introduce the customary Lorentz-invariant decompositions of the matrix elements of the current (12.375) of a spin-1/2 particle as follows:

$$\langle \mathbf{p}' | j^\mu | \mathbf{p} \rangle = e \bar{u}(\mathbf{p}') \left[\gamma^\mu F(q^2) + \frac{i}{2M} \sigma^{\mu\nu} q_\nu G(q^2) \right] u(\mathbf{p}). \quad (12.401)$$

The invariant functions $F(q^2)$ and $G(q^2)$ are the standard *form factors* of the electron. The relation between this and (12.384) follows directly from Gordon's decomposition formula (12.141), showing that $G(q^2)$ in (12.386) coincides with $G(q^2)$ in (12.401), whereas

$$F(q^2) = 1 + H(q^2) - G(q^2). \quad (12.402)$$

The *charge form factor* $F(q^2)$ at $q^2 = 0$ specifies the charge of the electron. Inserting (12.400), we obtain

$$\begin{aligned} F(q^2) = F(0) + \frac{\alpha}{2\pi} & \left[\left(\log \frac{M^2}{\mu^2} - 2 \right) \left(1 - \frac{2\theta}{\tan 2\theta} \right) \right. \\ & \left. + \theta \tan \theta + \frac{4}{\tan 2\theta} \int_0^\theta dx x \tan x \right], \end{aligned} \quad (12.403)$$

where

$$F(0) \equiv 1 + \frac{\alpha}{2\pi} \left(\log \frac{\Lambda}{M} + \frac{9}{4} - \log \frac{M^2}{\mu^2} \right). \quad (12.404)$$

The value $F(0)$ contains both the ultraviolet and the infrared cutoff. The subtracted function $\Delta F(q^2) \equiv F(q^2) - F(0)$ has only an infrared divergence. In writing down the expressions (12.403) and (12.404), we have ignored all contributions which vanish for $\mu \rightarrow 0$ and $\Lambda \rightarrow \infty$.

Due to the loop integral, the charge is changed to the new value

$$e_1 = e F(0) = e \left[1 + \frac{\alpha}{2\pi} \left(\log \frac{\Lambda}{M} + \frac{9}{4} - 2 \log \frac{M}{\mu} \right) \right]. \quad (12.405)$$

The factor is commonly denoted as the renormalization constant Z_1^{-1} . To order α , it is

$$Z_1 \equiv F^{-1}(0) = 1 - \frac{\alpha}{2\pi} \left(\log \frac{\Lambda}{M} + \frac{9}{4} - 2 \log \frac{M}{\mu} \right). \quad (12.406)$$

According to the theory of renormalization, this has to be equated with the experimentally observed charge. After this we can replace, in Eq. (12.403), the number $F(0)$ by 1, and the bare fine-structure constant α by the physical one (keeping the notation, for simplicity). The latter substitution is also done in $G(q)$.

12.15.2 Charge Radius

For small momentum transfers q^2 , the renormalized charge form factor has the Taylor series expansion

$$F_R(q^2) = 1 + q^2 \frac{\alpha}{3\pi M^2} \left(\log \frac{M}{\mu} - \frac{3}{8} \right) + \mathcal{O}(q^4). \quad (12.407)$$

The form factor of the anomalous magnetic moment is, for small q ,

$$G_R(q^2) = q^2 \frac{\alpha}{3\pi M^2} \frac{1}{4} + \mathcal{O}(q^4). \quad (12.408)$$

Due to the emission and absorption of virtual photons, the electron is shaken over a finite range. It is customary to define here a charge radius R_e of the electron by the first term in the expansion of the charge form factor²

$$F(q^2) = 1 - q^2 \frac{R_e^2}{6} + \dots \quad (12.409)$$

The factor $1/6$ is due to the fact that for a uniformly charged shell of radius R_e , the Fourier transform of the charge density has the expansion

$$\begin{aligned} F(q^2) &= \int d^3x e^{i\mathbf{q}\mathbf{x}} \rho(\mathbf{x}) = \int d^3x \left[1 + i\mathbf{q}\mathbf{x} - \frac{1}{2}(\mathbf{q}\mathbf{x})^2 + \dots \right] \rho(\mathbf{x}) \\ &= 1 - \frac{1}{6} \mathbf{q}^2 \int d^3x r^2 \rho(\mathbf{x}) = 1 - \mathbf{q}^2 \frac{R_e^2}{6} + \dots \end{aligned} \quad (12.410)$$

Setting $q^0 = 0$ in Eq. (12.407), we find that due to the vertex correction, the charge radius R_e^{vc} of the electron is given by

$$R_e^{\text{vc}} = \frac{\alpha}{\pi} \frac{2}{M^2} \left(\log \frac{M}{\mu} - \frac{3}{8} \right). \quad (12.411)$$

If the zeroth component of the current (12.401) couples to a static electric potential $A_0(\mathbf{x})$, the q^2 -term in (12.407) yields a correction factor

$$\left[1 + \frac{R_e^2}{6} \nabla^2 \right] A_0(\mathbf{x}). \quad (12.412)$$

The fluctuations of the electron position leads to an extra term proportional to the harmonic average of the potential. Since the potential obeys Gauss' law, this is nonzero only where there are charges. In an atom of nuclear charge Ze at the origin, the potential is

$$eA_0(\mathbf{x}) = V_C(\mathbf{x}) = -\frac{Z\alpha}{r} \quad (12.413)$$

²Note the difference of this quantity with respect to the classical electron radius (12.234).

and the harmonic average produces an additional δ -function at the origin:

$$e \nabla^2 A_0(\mathbf{x}) = 4\pi Z\alpha \delta^{(3)}(\mathbf{x}). \quad (12.414)$$

Thus the correction factor changes the Coulomb potential into an effective potential

$$V_C^{\text{eff}} = -\frac{Z\alpha}{r} + \frac{R_e^{2\text{vc}}}{6} Z\alpha 4\pi \delta^{(3)}(\mathbf{x}). \quad (12.415)$$

The prediction of this additional term is the origin of one of the early triumphs of QED. The δ -function leads to an energy shift of s -wave orbits with respect to those of nonzero orbital angular momentum, called the *Lamb shift*. It removes the degeneracy between the $2S_{1/2}$ and the $2P_{1/2}$ predicted by Dirac's equation in an external Coulomb field. It will be discussed in detail below.

12.15.3 Anomalous Magnetic Moment

On the right-hand side of the current matrix element (12.401) we replace the γ^μ -term by a combination of vectors $p'^\mu + p^\mu$ and $\sigma^{\mu\nu} q_\nu$, as before in (12.141), and see that the magnetic moment of the free electron acquires a correction factor $1 + G(0)$. Thus the gyromagnetic ratio g in Eq. (12.126) is changes from $g = 2$ to

$$g \equiv 2(1 + a) = 2[1 + G(0) + \dots] \quad (12.416)$$

[recall (12.371)]. The number $G(0)$ yields therefore directly the anomalous magnetic moment:

$$a = G(0). \quad (12.417)$$

In contrast to the charge, this quantity is finite. Its value is [17]

$$a = G(0) = \frac{\alpha}{2\pi} \sim 1\,61\,409\,74292 \times 10^{-12}. \quad (12.418)$$

This result was first calculated by Schwinger [18]. It is about 1.5% larger than the experimental values (12.372) and (12.373). The difference can be explained by higher-order electrodynamic and strong-interaction corrections [19]. By including all diagrams of sixth order in perturbation theory one finds, after a considerable effort (there are 72 Feynman diagrams to sixth order), the expansion

$$a = \frac{\alpha}{2\pi} + c_2 \left(\frac{\alpha}{\pi}\right)^2 + c_3 \left(\frac{\alpha}{\pi}\right)^3 \quad (12.419)$$

with the coefficients [20]

$$c_2 = \frac{197}{144} + \left(\frac{1}{2} - 3 \log 2\right) \zeta(2) + \frac{3}{4} \zeta(4) = -0.328\,478\,965 \dots, r \quad (12.420)$$

$$c_3 = 1.176\,11(42). \quad (12.421)$$

Up to c_2 , the theory is lower than the experimental number by only 1 part in 10^5 . Adding the c_3 -term, the theoretical value becomes

$$a = 1\,159\,652\,140.4(27.1) \times 10^{-12}, \quad (12.422)$$

reducing the discrepancy to 1 part in 10^8 . The error is mainly due to the uncertainty in the fine-structure constant [17].

The above calculation may be used to show that the anomalous magnetic moment of an antiparticle is the same as for a particle. The matrix element of the initial current between positron states is

$$\langle \mathbf{p}', s'_3 | j^\mu(x) | \mathbf{p}, s_3 \rangle = e \langle 0 | b(\mathbf{p}', s'_3) \bar{\psi}(x) \gamma^\mu \psi(x) b^\dagger(\mathbf{p}, s_3) | 0 \rangle = -e \bar{v}(\mathbf{p}', s_3) \gamma^\mu u(\mathbf{p}, s_3) e^{iqx}, \quad (12.423)$$

rather than (12.129). The minus sign is due to the odd number of exchanges of field operators necessary to evaluate the anticommutators. If both momenta are zero, only the zeroth component survives, showing that the charge of the positron is $-e$. For small momentum transfers, we calculate the second spatial component of (12.423) more explicitly as

$$\langle \mathbf{p}', s'_3 | j^2(x) | \mathbf{p}, s_3 \rangle = -e \bar{v}(\mathbf{0}, s_3) \gamma^2 e^{i\zeta^1(i\gamma^0\gamma^1)/2} v(\mathbf{0}, s_3), \quad (12.424)$$

and compare this with (12.134). The linear term in ζ^1 contains the contribution of the charge form factor to the magnetic moment. We see that (12.424) has the opposite overall sign of (12.134) which is compensated by an opposite sign in the exponent of the Lorentz transformation. Thus we obtain the matrix element of j^2 between positrons:

$$-ie\zeta^1 \bar{v}(\mathbf{0}, s_3) S_3 v(\mathbf{0}, s_3) = ie\zeta^1 s_3, \quad (12.425)$$

with an opposite sign in comparison with the electron in (12.135). The sign change at the end is caused by the opposite spin orientation of the two-spinors $\xi(s_3)$ contained in the spinors $v(\mathbf{0}, s_3)$ [recall (4.684), (4.685) and (4.676)].

An opposite sign is also found for the contribution from the second form factor where the matrix element of the electron is

$$e \bar{u}(\mathbf{0}, s_3) \frac{i}{2M} \sigma^{21} q_1 G(0) u(\mathbf{0}, s_3) = -ie \bar{u}(\mathbf{0}, s_3) S_3 \zeta^1 G(0) u(\mathbf{0}, s_3) = -ie \zeta^1 s_3 G(0). \quad (12.426)$$

This produces the correction to the g -factor

$$g = 2[1 + G(0)]. \quad (12.427)$$

For a positron, the matrix element of the current is

$$-e \bar{v}(\mathbf{p}', s'_3) [\gamma^2 F(q^2) + \frac{i}{2M} \sigma^{2\nu} q_\nu G(q^2)] v(\mathbf{p}, s_3), \quad (12.428)$$

and the second term becomes, for $\mathbf{p}' = 0$ and small $\mathbf{p}$ in the x -direction,

$$-e \bar{v}(\mathbf{0}, s_3) \frac{i}{2M} \sigma^{21} q_1 G(0) v(\mathbf{0}, s_3) = ie \bar{v}(\mathbf{0}, s_3) S_3 \zeta^1 G(0) v(\mathbf{0}, s_3) = ie \zeta^1 s_3 G(0), \quad (12.429)$$

which is exactly the opposite of (12.426). Thus a positron has the same correction (12.427) to the g -factor as an electron. Note that the sign change found in (12.425) is present also here, but it is compensated by a minus sign from an extra γ^0 -matrix acting upon $v^\dagger$.

For a muon, the coefficients are [21]

$$\begin{aligned} c_2 &= 0.765\,857\,376(27), & c_3 &= 24.050\,508\,98(44), \\ c_4 &= 24.050\,508\,98(44), & c_5 &= +930(170), \end{aligned} \quad (12.430)$$

leading to

$$a_\mu = 1\,165\,847\,057(29) \times 10^{-12}. \quad (12.431)$$

The strong interactions change this slightly via the composite Feynman diagrams

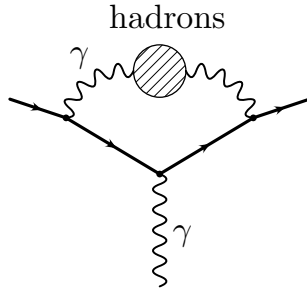


FIGURE 12.24 Leading hadronic vacuum polarization corrections to a_μ .

indicated in Fig. 12.24. Their contribution was estimated in [22] to amount to

$$a_\mu^{\text{str}} = 6\,924(62) \times 10^{-11} \quad \text{to} \quad 6\,988(111) \times 10^{-11}. \quad (12.432)$$

The amplitude is calculated from the formula

$$a_\mu^{\text{str}}(\text{vac. pol.}) = \frac{1}{4\pi^3} \int_{4m_\pi^2}^{\infty} ds K(s) \sigma^0(s)_{e^+e^- \rightarrow \text{hadrons}}, \quad (12.433)$$

where $\sigma^0(s)_{e^+e^- \rightarrow \text{hadrons}}$ is the cross section for the process indicated in the subscript. Some radiative corrections have been taken care of, such as initial state radiation by a subtraction from the measured cross sections. The function $K(s)$ is equal to

$$K(s) = x^2 \left(1 - \frac{x^2}{2}\right) + (1+x)^2 \left(1 + \frac{1}{x^2}\right) \left[\ln(1+x) - x + \frac{x^2}{2} \right] + \frac{1+x}{1-x} x^2 \ln x, \quad (12.434)$$

with

$$x = \frac{1 - \sqrt{1 - 4m_\mu^2/s}}{1 + \sqrt{1 - 4m_\mu^2/s}}. \quad (12.435)$$

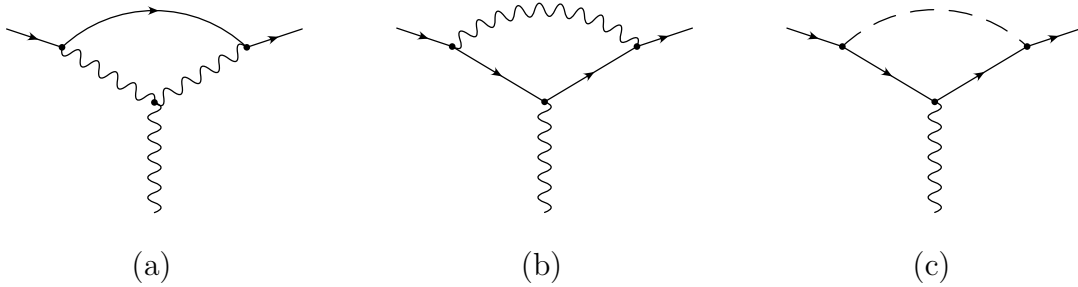
$\sqrt{s}$ (GeV)	$a_\mu^{\text{str}}(\text{vac. pol.}) \times 10^{11}$
$2m_\pi - 1.8$	6343 ± 60
$1.8 - 3.7$	338.7 ± 4.6
$3.7 - 5 + \psi(1S, 2S)$	143.1 ± 5.4
$5 - 9.3$	68.7 ± 1.1
$9.3 - 12$	12.1 ± 0.5
$12 - \infty$	18.0 ± 0.1
Total	6924 ± 62

TABLE 12.1 Different contributions to $a_\mu^{\text{str}}(\text{vac. pol.})$ in the integral 12.433.

It comes from the remaining part of the diagram. The contributions from the different parts of the cross sections to $a_\mu^{\text{str}}(\text{vac. pol.})$ in the integral (12.433) are separately listed in Table 12.15.3. The weak interactions in the standard model add to this [23]

$$a_\mu^{\text{EW}}(1 \text{ loop}) = \frac{5}{3} \frac{G_\mu m_\mu^2}{8\sqrt{2}\pi^2} \left[1 + \frac{1}{5}(1 - 4\sin^2 \theta_W)^2 + \mathcal{O}\left(\frac{m_\mu^2}{M^2}\right) \right] \approx 195 \times 10^{-11}, \quad (12.436)$$

where $G_\mu = 1.16637(1) \times 10^{-5} \text{ GeV}^{-2}$, $\sin^2 \theta_W \equiv 1 - M_W^2/M_Z^2 \simeq 0.223$. and $M = M_W$ or M_{Higgs} . See Fig. 12.25 for the Feynman diagrams.

FIGURE 12.25 One-loop electroweak radiative corrections to a_μ . The wiggly lines are gluons.

Two-loop corrections change this slightly by

$$a_\mu^{\text{weak}}(2 \text{ loop}) = -43(4) \times 10^{-11}, \quad (12.437)$$

if we assume a Higgs particle mass of $m_H \simeq 150 \text{ GeV}$ (with little sensitivity to the exact value). Altogether, we obtain

$$a_\mu^{\text{theory}} = 1\,165\,915\,97(67) \times 10^{-11}, \quad (12.438)$$

in agreement with the experimental numbers [24]

$$a_{\mu}^{\text{exp}} = 11\,659\,204(7) \times 10^{-9}, \quad 11\,659\,202(22) \times 10^{-9}, \quad 11\,659\,204(7) \times 10^{-9}. \quad (12.439)$$

See Fig. 12.26 for a comparison of theory and experiment.

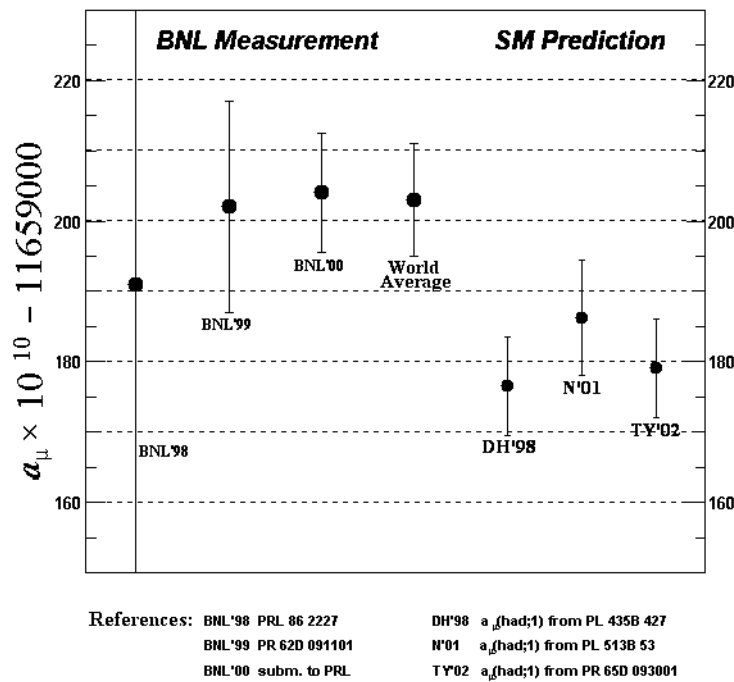


FIGURE 12.26 Measured values of a_{μ} and prediction of the Standard Model (SM). The small error bars of the theoretical value come from the left-hand estimate for the hadron contribution in Eq. (12.432). For sources see Ref. [24].

12.16 Vacuum Polarization

Let us now turn to the vacuum polarization. The lowest-order Feynman diagram is shown in Fig. 12.27.

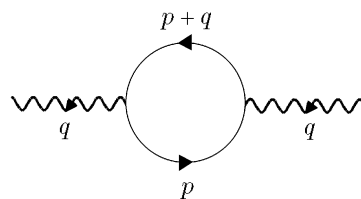


FIGURE 12.27 Lowest-order Feynman diagram for the vacuum polarization.

In general, the propagator of the photon has the form

$$G^{\mu\nu}(q) = i \frac{P^{\mu\nu}(q)}{q^2}, \quad (12.440)$$

where the polarization tensor $P^{\mu\nu}(q)$ depends on the gauge [see (12.111)]. From the lowest-order Feynman diagram in Fig. 12.27, the propagator receives a lowest-order correction

$$G_0^{\mu\nu}(q) [-i\Pi_{\lambda\kappa}(q)] G_0^{\kappa\nu}(q), \quad (12.441)$$

where $-\Pi_{\mu\nu}(k)$ is given by the Feynman integral.

$$-i\Pi_{\mu\nu}(q) = e^2 \int \frac{d^4p}{(2\pi)^4} \frac{\text{tr}[\gamma_\mu(\not{p} + \not{q} + M)\gamma_\nu(\not{p} + M)]}{[(p+q)^2 - M^2](p^2 - M^2)}. \quad (12.442)$$

Using Feynman's formula (11.156)

$$\frac{1}{AB} = \int_0^1 dz \frac{1}{[Az + B(1-z)]^2}, \quad (12.443)$$

we rewrite (12.442) as

$$-i\Pi_{\mu\nu}(q) = e^2 \int_0^1 dz \int \frac{d^4p}{(2\pi)^4} \frac{\text{tr}[\gamma_\mu(\not{p} + \not{q} + M)\gamma_\nu(\not{p} + M)]}{[(p+qz)^2 + q^2(z-z^2) - M^2]^2}. \quad (12.444)$$

This expression is symmetric in μ and ν . A shift in the p -integration by an amount qz brings it to the form

$$-i\Pi_{\mu\nu}(q) = e^2 \int_0^1 dz \int \frac{d^4p}{(2\pi)^4} \frac{\text{tr}\{\gamma_\mu[\not{p} + \not{q}(1-z) + M]\gamma_\nu(\not{p} - \not{q}z + M)\}}{[p^2 + q^2(z-z^2) - M^2]^2}. \quad (12.445)$$

After evaluating the trace, dropping odd terms in p , and using the symmetry in μ and ν , we obtain

$$-i\Pi_{\mu\nu}(q) = 4e^2 \int_0^1 dz \int \frac{d^4p}{(2\pi)^4} \frac{-(-g_{\mu\nu}q^2 + 2q_\nu q_\nu)(z-z^2) - g_{\mu\nu}(p^2 - M^2) + 2p_\mu p_\nu}{[p^2 + q^2(z-z^2) - M^2]^2}. \quad (12.446)$$

Because of the rotational symmetry of the integrand we can use the first replacement rule in Eq. (11.136) to replace $-g_{\mu\nu}(p^2 - M^2) + 2p_\mu p_\nu$ by $-g_{\mu\nu}(p^2/2 - M^2)$.

The momentum integral is quadratically divergent, since there are two more powers of integration variables in the numerator than in the denominator. The situation is improved by imposing the requirement of gauge invariance, $q^\mu \Pi_{\mu\nu}(q) = 0$. This makes the final results independent of the gauge choice in the photon propagator. Thus we postulate, for the moment, the vanishing of the divergent integral

$$-iq^\mu \Pi_{\mu\nu}(q) = e^2 q_\nu 4 \int_0^1 dz \int \frac{d^4p}{(2\pi)^4} \frac{-q^2(z-z^2) - (p^2/2 - M^2)}{[p^2 + q^2(z-z^2) - M^2]^2}. \quad (12.447)$$

We shall verify in the next Subsection that this is guaranteed if we calculate the Feynman diagrams by analytic regularization in D dimensions rather than $D = 4$.

Thus we are left with the logarithmically divergent integral

$$-i\Pi_{\mu\nu}(q) = -(-g_{\mu\nu}q^2 + q_\mu q_\nu) 8e^2 \int_0^1 dz(z - z^2) \int \frac{d^4p}{(2\pi)^4} \frac{1}{[p^2 + q^2(z - z^2) - M^2]^2}. \quad (12.448)$$

Let us define the invariant function that accompanies the tensor $(-g_{\mu\nu}q^2 + q_\mu q_\nu) = q^2 P_{\mu\nu}(q)$ as $-i\Pi(q^2)$, i.e., we write

$$-i\Pi_{\mu\nu}(q) \equiv -iP_{\mu\nu}(q)q^2\Pi(q^2). \quad (12.449)$$

If we expand

$$\Pi(q^2) = \Pi(0) + \Pi'(0)q^2 + \dots, \quad (12.450)$$

we see that only $\Pi(0)$ is logarithmically divergent:

$$-i\Pi(0) = -8e^2 \int_0^1 dz(z - z^2) \int \frac{d^4p}{(2\pi)^4} \frac{1}{(p^2 - M^2)^2}, \quad (12.451)$$

whereas all remaining terms in the expansion (12.450) are finite, for example the first term:

$$-i\Pi'(0) = 16e^2 \int_0^1 dz(z - z^2)^2 \int \frac{d^4p}{(2\pi)^4} \frac{1}{(p^2 - M^2)^3}. \quad (12.452)$$

Since the mass M carries a small negative imaginary part, we now perform a Wick rotation of the integration contour, setting $p^0 = ip^4$ and letting p^4 run from $-\infty$ to ∞ . Thus we substitute $p^2 = -p_E^2$ and $d^4p/(2\pi)^4 = id^4p_E/(2\pi)^4$, and calculate from (12.452):

$$\Pi'(0) = \frac{e^2}{(2\pi)^4} \frac{4}{15} \frac{\pi^2}{M^2} = \frac{\alpha}{6\pi M^2} \frac{1}{5}. \quad (12.453)$$

In the divergent quantity $\Pi(0)$, we perform a Wick rotation so that the integral $d^4p/(2\pi)^4$ turns into an integral over all Euclidean four-momenta $d^4p_E/(2\pi)^4 = S_4 dp_E p_E^3 = dp_E^2 p_E^2/16\pi^2$. If we introduce an ultraviolet momentum cutoff at Λ^2 , we obtain

$$\begin{aligned} \Pi(0) &= 8e^2 \frac{1}{6} \int \frac{d^4p_E}{(2\pi)^4} \frac{1}{(p_E^2 + M^2)^2} = 8e^2 \frac{1}{6} \frac{1}{16\pi^2} \int_0^\infty dp_E^2 \frac{p_E^2}{(p_E^2 + M^2)^2} \\ &= \frac{\alpha}{\pi} \frac{1}{3} \left(\log \frac{\Lambda^2}{M^2} - 1 \right). \end{aligned} \quad (12.454)$$

The complete invariant function of the polarization tensor is therefore

$$\Pi(q^2) = \frac{\alpha}{\pi} \left[\frac{1}{3} \left(\log \frac{\Lambda^2}{M^2} - 1 \right) + \left(\frac{2}{3} + \frac{1}{3 \sin^2 \theta} \right) \left(1 - \frac{\theta}{\tan \theta} \right) - \frac{1}{9} \right]. \quad (12.455)$$

For small q^2 , we expand

$$\Pi(q^2) = \left(\frac{2}{3} + \frac{1}{3 \sin^2 \theta} \right) \left(1 - \frac{\theta}{\tan \theta} \right) = \frac{1}{9} + \frac{4}{15} \theta^2 + \dots, \quad (12.456)$$

and find the bracket to behave like

$$\Pi(0) + \Pi'(0)q^2 + \dots = \frac{\alpha}{\pi} \left[\frac{1}{3} \left(\log \frac{\Lambda^2}{M^2} - 1 \right) + \frac{1}{15} \frac{q^2}{M^2} + \mathcal{O}(q^4) \right]. \quad (12.457)$$

The last term agrees with the result (12.453) of a direct calculation of $\Pi'(0)$. It is gratifying to find out that the condition (12.447) is fulfilled by the dimensional regularization in $d = 4 - \epsilon$ dimensions.

Note that the expression (12.455) is real only for $q^2 < M^2$. When $q^2 > (2M)^2$ the external field can produce electron-positron pairs and $\Pi(q^2)$ acquires an imaginary part. The imaginary part causes a decrease of the probability amplitude for the occurrence of a pure scattering process below the threshold of pair production.

A string of vacuum polarization diagrams produces the geometric series

$$G^{\mu\nu} = G_0^{\mu\nu} + G_0^{\mu\lambda} [-i\Pi_{\lambda\kappa}] G_0^{\kappa\nu} + \dots + G_0^{\mu\lambda} [-i\Pi_{\lambda\kappa}] G_0^{\kappa\sigma} [-i\Pi_{\sigma\tau}] G_0^{\tau\nu} + \dots, \quad (12.458)$$

which can be summed up to

$$G^{\mu\nu}(q) = \{[G_{\mu\nu}^{-1}(q) + i\Pi_{\mu\nu}(q)]^{-1}\}^{-1}. \quad (12.459)$$

Inserting the tensor decomposition (12.449), this can be written as

$$G^{\mu\nu}(q) = i \frac{P^{\mu\nu}(q)}{q^2[1 - \Pi(q^2)]} \approx i \frac{P^{\mu\nu}(q)}{q^2[1 + \Pi(0) + \Pi'(0)q^2 - \dots]} \quad (12.460)$$

For small q^2 , the photon propagator is, therefore,

$$G^{\mu\nu}(q) \approx i \frac{P_{\mu\nu}(q)}{q^2} \left\{ 1 + \Pi(0) + \frac{\alpha}{15\pi M^2} q^2 \right\}^{-1}. \quad (12.461)$$

The divergent number $1 + \Pi(0)$ can be absorbed into the field renormalization factor, after defining

$$A_R^\mu(x) = Z_3^{-1/2} A(x) \quad (12.462)$$

with

$$Z_3 = [1 + \Pi(0)]^{-1} = 1 - \frac{\alpha}{3\pi} \log \frac{\Lambda^2}{m^2} + \dots. \quad (12.463)$$

This corresponds to renormalizing the charge to

$$\alpha_R = Z_3 \alpha. \quad (12.464)$$

The propagator of the renormalized field A_R^μ is then

$$G_R^{\mu\nu}(q) = i \frac{P_{\mu\nu}(q)}{q^2} \left(1 + \frac{\alpha_R}{15\pi} \frac{q^2}{M^2} \right)^{-1}. \quad (12.465)$$

For a given static source of charge Ze at the origin, the Coulomb potential

$$V_C(x) = -\frac{Z\alpha}{r} \quad (12.466)$$

is obtained by applying the free propagator $G_0^{\mu\nu}$ to the current $j^\mu(x) = \delta^\mu_0 Ze\delta^{(3)}(\mathbf{x})$. To lowest order in α , the vacuum polarization changes $G_0^{\mu\nu}(q)$ by a factor

$$\left(1 - \frac{\alpha_R}{15\pi} \frac{q^2}{M^2}\right)$$

which is equivalent to multiplying the potential $V_C(\mathbf{x})$ by a factor

$$\left(1 - \frac{\alpha_R}{15\pi} \frac{\nabla^2}{M^2}\right).$$

The potential is therefore modified to

$$V_C^R(x) = -Z\alpha \left[\frac{1}{r} + \frac{\alpha}{15\pi M^2} 4\pi\delta^{(3)}(\mathbf{x}) \right]. \quad (12.467)$$

A comparison with (12.407)–(12.415) shows that the vacuum polarization decreases the effective radius of the electron (12.411), derived from the vertex correction, by

$$R_e^{2\text{vp}} = -\frac{\alpha}{3\pi M^2} \frac{1}{5}, \quad (12.468)$$

thus giving rise to a total effective radius determined to lowest order in α by:

$$R_e^{2\text{vp}} = -\frac{\alpha}{3\pi M^2} \frac{1}{5} \left(\log \frac{M}{\mu} - \frac{3}{8} - \frac{1}{5} \right). \quad (12.469)$$

Since the finite radius of the electron gives rise to the Lamb shift to be derived below, the vacuum polarization *decreases* the Lamb shift.

12.17 Dimensional Regularization

We still must show that the divergent integral (12.447) is really zero, to ensure the gauge invariance of the self-energy (12.446). In D dimensions, the Dirac matrices have the dimension $2^{D/2}$, and (12.446) reads [26]

$$-i\Pi_{\mu\nu}(q) = 2^{D/2}e^2 \int_0^1 dz \int \frac{d^D p}{(2\pi)^D} \frac{-(-g_{\mu\nu}q^2 + 2q_\nu q_\nu)(z - z^2) - g_{\mu\nu}(p^2 - M^2) + 2p_\mu p_\nu}{[p^2 + q^2(z - z^2) - M^2]^2}. \quad (12.470)$$

Then the previous replacement under the integral $p_\mu p_\nu \rightarrow g_{\mu\nu}/4$ becomes $p_\mu p_\nu \rightarrow g_{\mu\nu}/D$ [recall (11.136)]. The integral $d^D p$ over all four-momenta may now be Wick-rotated to

$$i \int d^D p_E / (2\pi)^D = iS_D / 2(2\pi)^D \int_0^\infty dp_E^2 (p_E^2)^{D/2-1}, \quad (12.471)$$

where S_D is the surface of the unit sphere (11.126). Hence we can rewrite the integral (12.447) in Euclidean spacetime as

$$-iq^\mu \Pi_{\mu\nu}(q) = e^2 q_\nu 2^{D/2} i \int_0^1 dz \int \frac{d^D p_E}{(2\pi)^D} \frac{-q^2(z-z^2) + (1-2/D)p_E^2 + M^2}{[p_E^2 + m^2]^2}, \quad (12.472)$$

where

$$m^2 = m^2(q^2, z) \equiv M^2 - q^2 z(1-z), \quad (12.473)$$

and further as

$$-iq^\mu \Pi_{\mu\nu}(q) = e^2 q_\nu 2^{D/2} i \int_0^1 dz \int \frac{d^D p_E}{(2\pi)^D} \frac{2m^2/D + (1-2/D)(p_E^2 + m^2)}{[p_E^2 + m^2]^2}. \quad (12.474)$$

Now we use Formula (11.130) to replace

$$\int \frac{d^D p_E}{(2\pi)^D} \frac{1}{(p_E^2 + m^2)^\nu} = S_D \frac{\Gamma(D/2)\Gamma(\nu - D/2)}{2} \Gamma(\nu) [m^2]^{D/2-\nu}, \quad (12.475)$$

so that

$$\begin{aligned} -iq^\mu \Pi_{\mu\nu}(q) &= e^2 q_\nu 2^{D/2} i S_D \frac{\Gamma(D/2)}{2} \\ &\times \left[\frac{2}{D} \Gamma(1-D/2) \Gamma(2) + \left(1 - \frac{2}{D}\right) \Gamma(2-D/2) \Gamma(1) \right] \int_0^1 dz [m^2]^{D/2-1} = 0, \end{aligned} \quad (12.476)$$

thus guaranteeing the gauge invariance of the vacuum polarization tensor in any dimension D [10].

12.18 Two-Dimensional QED

If the bare electron mass is zero, an interesting phenomenon arises in two dimensions: The self-energy of the photon makes the photon massive. This happens in spite of gauge invariance of the Lagrangian, as pointed out by Schwinger [6] in 1962. Since this was a surprise, the two-dimensional massless QED is called the *Schwinger model* [27].

Consider the self-energy (12.448) in D spacetime dimensions where the prefactor 4 in Eq. (12.446) is replaced by $2^{D/2}$, so that (12.448) reads

$$-i\Pi_{\mu\nu}(q) = -(-g_{\mu\nu}q^2 + q_\mu q_\nu) 2^{D/2+1} e^2 \int_0^1 dz (z-z^2) \int \frac{d^D p}{(2\pi)^D} \frac{1}{[p^2 + q^2(z-z^2) - M^2]^2}. \quad (12.477)$$

Here the integral over $d^D p$ in momentum spacetime is Wick-rotated, as in (12.471), into the Euclidean momentum integral

$$\frac{S_D}{2(2\pi)^D} i \int_0^\infty dp_E^2 \frac{1}{(p_E^2 + m^2)^2} = \frac{S_D}{2(2\pi)^D} i [m^2]^{D/2-2} \frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)}, \quad (12.478)$$

with m^2 determined by Eq. (12.473). Inserting this into (12.477) yields, for $-i\Pi_{\mu\nu}(q)$ of massless electrons, the tensor

$$-(-g_{\mu\nu}q^2 + q_\mu q_\nu) 2^{D/2+1} e^2 i \int_0^1 dz [z(1-z)]^{D/2-1} (-q^2)^{D/2-2} \frac{S_D}{2(2\pi)^D} \frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)}, \quad (12.479)$$

which is equal to³

$$-(-g_{\mu\nu}q^2 + q_\mu q_\nu) 2^{D/2+1} e^2 i \frac{\Gamma^2(D/2)}{\Gamma(D)} (-q^2)^{D/2-2} \frac{S_D}{2(2\pi)^D} \frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)}, \quad (12.480)$$

so that we obtain, in $D = 2$ dimensions,

$$-i\Pi_{\mu\nu}(q) = -i(-g_{\mu\nu}q^2 + q_\mu q_\nu) \frac{4e^2}{-q^2} \frac{S_2}{2(2\pi)^2} = -i(-g_{\mu\nu}q^2 + q_\mu q_\nu) \frac{e^2}{-\pi q^2} = -iP_{\mu\nu} \frac{e^2}{-\pi q^2}, \quad (12.481)$$

or, recalling (12.449),

$$\Pi(q) = -\frac{e^2}{\pi q^2}. \quad (12.482)$$

Inserting this into (12.460), we obtain the renormalized photon propagator

$$G^{\mu\nu}(q) = i \frac{P^{\mu\nu}(q)}{q^2 + q^2 \Pi(q)} = i \frac{P^{\mu\nu}(q)}{q^2 - e^2/\pi}. \quad (12.483)$$

This shows that the photon has acquired a nonzero mass $m_\gamma^2 = e^2/\pi$. The effective Lagrangian of the photon to this order is

$$\mathcal{L}_{\text{eff}} = -\frac{1}{4} F^{\mu\nu} (1 + m_\gamma^2/\square) F_{\mu\nu}. \quad (12.484)$$

The Schwinger model illustrates the remarkable fact that in spite of the gauge invariance of the theory, a mass term can be generated for the photon by a loop diagram of a massless fermion.

12.19 Self-Energy of Electron

The lowest-order Feynman diagram for the self-energy of the electron is shown in Fig. 12.28. It adds to the electron propagator a term

$$G_0(p)[-i\Sigma(p)]G_0(p), \quad (12.485)$$

where

$$G_0(p) = \frac{i}{\not{p} - M} \quad (12.486)$$

³I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980, Formula 3.191.3.

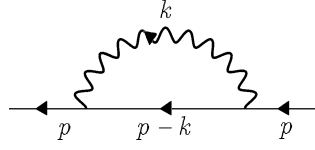


FIGURE 12.28 Lowest-order Feynman diagram for the self-energy of the electron.

is the free Dirac propagator and the self-energy $-i\Sigma(p)$ of the electron is given by the diagram in Fig. 12.28. Explicitly:

$$-i\Sigma(p) = e^2 \int \frac{d^4k}{(2\pi)^4} \gamma^\mu \frac{\not{p} - \not{k} + M}{(p-k)^2 - M^2} \gamma_\mu \frac{1}{k^2}. \quad (12.487)$$

Using the anticommutation rule (12.214), we can simplify, in the numerator,

$$\gamma^\mu (\not{p} - \not{k} + M) \gamma_\mu = -2(\not{p} - \not{k}). \quad (12.488)$$

The integral is logarithmically divergent at large k . It also has an infrared divergence. To enforce convergence, we employ the Pauli-Villars regularization method and modify the photon propagator as follows:

$$\frac{1}{k^2} \rightarrow \frac{1}{k^2 - \mu^2} - \frac{1}{k^2 - \Lambda^2}, \quad (12.489)$$

where Λ is a large cutoff mass and μ is a small photon mass. The self-energy becomes

$$-i\Sigma(p) = e^2 \int \frac{d^4k}{(2\pi)^4} \frac{-2(\not{p} - \not{k}) + 4M}{(p-k)^2 - M^2} \left(\frac{1}{k^2 - \mu^2} - \frac{1}{k^2 - \Lambda^2} \right). \quad (12.490)$$

The mass parameter Λ cuts off the contribution of short-wave photons with $k \gg \Lambda$. At the end we shall take the cutoff to infinity.

By adding the same Feynman diagram repeatedly to an electron line, we obtain the geometric series

$$G_0(p) + G_0(p)[-i\Sigma(p)]G_0(p) + G_0(p)[-i\Sigma(p)]G_0(p)[-i\Sigma(p)]G_0(p) + \dots, \quad (12.491)$$

which can be summed up to

$$G(p) = \frac{i}{\not{p} - M - \Sigma(p)}. \quad (12.492)$$

Using Feynman's formula (12.443), this can be rewritten as

$$\begin{aligned} \Sigma(p) &= -ie^2 \int_0^1 dx \int \frac{d^4k}{(2\pi)^4} \\ &\times \left\{ \frac{-2(\not{p} - \not{k}) + 4M}{[-(k-p)^2 - p^2x(1-x) + M^2x + \Lambda^2(1-x)]^2} - (\Lambda = \mu) \right\}. \end{aligned} \quad (12.493)$$

A simplification occurs by shifting the integration variable from k to $k + px$. Then the terms proportional to k are off in k and can be dropped. After performing a Wick rotation of the integration contour, we obtain

$$\Sigma(p) = \frac{2\pi^2 e^2}{(2\pi)^4} \int_0^1 ds \int_0^1 dk_E k_E^3 \left\{ \frac{-2\not{p}(1-x) + 4M}{[k_E^2 - p^2 x(1-x) + M^2 x + \Lambda^2(1-x)]^2} - (\Lambda=0) \right\}. \quad (12.494)$$

The k_E -integral is easily done, and yields

$$\begin{aligned} \Sigma(p) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx [-2\not{p}(1-x) + 4M] \\ &\times \left\{ \log \left[\frac{-p^2 x(1-x) + M^2 x + \Lambda^2(1-x)}{-p^2 x(1-x) + M^2 x} \right] - (\Lambda = \mu) \right\}. \end{aligned} \quad (12.495)$$

The right-hand side is a 4×4 -matrix in spinor space which may be decomposed into invariant functions

$$\Sigma(p) = (\not{p} - M)A(p^2) + B(p^2), \quad (12.496)$$

where

$$\begin{aligned} A(p^2) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx [-2(1-x)] \left\{ \log f(p^2, x, \Lambda) - (\Lambda = \mu) \right\}, \\ B(p^2) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx 2M(1+x) \left\{ \log f(p^2, x, \Lambda) - (\Lambda = \mu) \right\}, \end{aligned} \quad (12.497)$$

with

$$f(p^2, x, \Lambda) = \frac{-p^2 x(1-x) + M^2 x + \Lambda^2(1-x)}{-p^2 x(1-x) + M^2 x}. \quad (12.498)$$

The invariant functions are logarithmically divergent for large Λ .

We may expand them around the mass shell $p^2 = M^2$ in powers of $p^2 - M^2$. Then only the lowest expansion terms carry the logarithmic divergence:

$$\begin{aligned} A(M^2) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx [-2(1-x)] \log \left[\frac{M^2 x^2 + \Lambda^2(1-x)}{M^2 x^2} \right], \\ B(M^2) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx 2M(1+x) \log \left[\frac{M^2 x^2 + \Lambda^2(1-x)}{M^2 x^2} \right], \\ B'(M^2) &= \frac{\pi^2 e^2}{(2\pi)^4} \int_0^1 dx 2M(1+x)(1-x) \\ &\times \left[\frac{\Lambda^2(1-x)}{M^2 x[M^2 x^2 + \Lambda^2(1-x)]} - \frac{\mu^2(1-x)}{M^2 x[M^2 x^2 + \mu^2(1-x)]} \right]. \end{aligned} \quad (12.499)$$

All higher expansion terms are finite and can be evaluated with an infinite cutoff Λ . We have also dropped all terms that vanish in the limit of zero photon mass μ . Omitting the regular parts of the self-energy, the propagator becomes

$$G(p) = \frac{i}{(\not{p} - M)[1 + A(M^2)] + B(M^2) + B'(M^2)(p^2 - M^2)}$$

$$= \frac{1}{1 + A(M^2) + 2MB'(M^2)} \frac{i}{\not{p} - M - \delta M}, \quad (12.500)$$

where

$$\delta M \equiv -\frac{B(M^2)}{1 + A(M^2) + 2MB'(M^2)}. \quad (12.501)$$

The prefactor in the denominator is commonly denoted by

$$Z_2 \equiv 1 + A(M^2) + 2MB'(M^2). \quad (12.502)$$

It can be removed by renormalizing the field $\psi(x)$ to $\psi_R(x) = Z_2^{1/2}\psi(x)$. The renormalized field has then a propagator with a pole term $i/(\not{p} - M)$. For large Λ^2 , we can simplify the results for Z_2 and δM^2 to order α :

$$\begin{aligned} Z_2 - 1 &= -\frac{\alpha}{2\pi} \int_0^1 dx \left\{ (1-x) \left[\log \frac{\Lambda^2}{M^2} + \log \frac{1-x}{x^2} \right] - 2 \frac{1-x^2}{x} \left[1 - \frac{\mu^2(1-x)}{M^2x^2 + \mu^2(1-x)} \right] \right\}, \\ \delta M^2 &= \frac{\alpha}{2\pi} \int_0^1 dx (1+x) \left[\log \frac{\Lambda^2}{M^2} + \log \frac{1-x}{x^2} \right]. \end{aligned} \quad (12.503)$$

Performing the integrals over x yields

$$\begin{aligned} Z_2 - 1 &= -\frac{\alpha}{2\pi} \left[\log \frac{\Lambda}{M} + \frac{5}{4} + 1 - \log \frac{M^2}{\mu^2} \right], \\ \delta M^2 &= \frac{\alpha}{2\pi} \int_0^1 dx \left[3 \log \frac{\Lambda}{M} + \frac{3}{4} \right]. \end{aligned} \quad (12.504)$$

12.20 Ward-Takahashi Identity

It is important to realize that Z_2 coincides with the renormalization constant $Z_1 = F^{-1}(0)$ defined in Eq. (12.406) by the charge form factor to make the current matrix element finite. This equality is a consequence of the *Ward identity* fulfilled by the vertex correction $\Lambda^\mu(p', p)$ defined in Eq. (12.375):

$$\Lambda^\mu(p, p) = -\frac{\partial}{\partial p_\mu} \Sigma(p). \quad (12.505)$$

For the total Dirac matrix $\Gamma^\mu(p', p) \equiv \gamma^\mu + \Lambda^\mu(p', p)$ in the current (12.375), this implies that

$$\Gamma^\mu(p, p) = \frac{\partial}{\partial p_\mu} [\not{p} - M - \Sigma(p)]. \quad (12.506)$$

This relation holds to all orders in α . For off-diagonal matrix elements of the current, there also exists a more general relation:

$$(p' - p)_\mu \Gamma^\mu(p', p) = [\not{p}' - M - \Sigma(p)] - [\not{p} - M - \Sigma(p)], \quad (12.507)$$

from which (12.506) can be derived in the limit $p' \rightarrow p$. This is the famous *Ward-Takahashi identity*. Its validity for a free theory is obvious. For the interacting theory it will be proved at the end of this section..

A first important consequence of the Ward-Takahashi identity is the equality of the renormalization constants $Z_1 = Z_2$. To derive it, we use (12.506) to rewrite

$$\begin{aligned}\Gamma^\mu(p', p) &= -\frac{\partial}{\partial p_\mu} \Sigma(p) + \Gamma^\mu(p', p) - \Gamma^\mu(p, p) \\ &= -\gamma^\mu + \frac{\partial}{\partial p_\mu} [\not{p} - M - \Sigma(p)] + \Gamma^\mu(p', p) - \Gamma^\mu(p, p).\end{aligned}\quad (12.508)$$

From the renormalization equation of the electron propagator (12.500), we see that

$$\not{p} - M - \Sigma(p) = Z_2^{-1} [\not{p} - M_R - \Sigma_R(p)], \quad (12.509)$$

where $M_R = M + \delta M$. This leads to

$$\Gamma^\mu(p', p) = \gamma^\mu (Z_2^{-1} - 1) - Z_2^{-2} \frac{\partial}{\partial p_\mu} \Sigma_R(p) + \Gamma^\mu(p', p) - \Gamma^\mu(p, p). \quad (12.510)$$

This must be compared with the definition of the renormalized vertex function

$$\Gamma^\mu(p', p) = \gamma^\mu (Z_1^{-1} - 1) + Z_1^{-1} \Gamma_R^\mu(p', p), \quad (12.511)$$

to conclude that

$$\begin{aligned}Z_1 &= Z_2, \\ \Gamma_R^\mu(p', p) &= Z_1 [\Gamma^\mu(p', p) - \Gamma^\mu(p, p)] - \frac{\partial}{\partial p_\mu} \Sigma_R(p).\end{aligned}\quad (12.512)$$

The proof of the Ward-Takahashi identity (12.507) follows from the canonical commutation relations of the current with the fields. These are certainly true in the presence of interactions [28]:

$$\begin{aligned}[j^0(\mathbf{x}, x_0), \psi(\mathbf{x}', x_0)] &= -e\delta^{(3)}(\mathbf{x} - \mathbf{x}')\psi(\mathbf{x}, x_0), \\ [j^0(\mathbf{x}, x_0), \bar{\psi}(\mathbf{x}', x_0)] &= e\delta^{(3)}(\mathbf{x} - \mathbf{x}')\bar{\psi}(\mathbf{x}, x_0).\end{aligned}\quad (12.513)$$

These illustrate Noether's theorem, which makes j^0 the generator of phase transformations [recall Eq. (8.280)]. We now form the derivative of the time-ordered expectation

$$\partial_z^\mu \langle 0 | \hat{T} \psi(x') j_\mu(z) \bar{\psi}(x) | 0 \rangle = e \langle 0 | \hat{T} \psi(x') \bar{\psi}(x) | 0 \rangle [\delta^{(4)}(x' - z) - \delta^{(4)}(z - x)]. \quad (12.514)$$

Expressed in terms of the full propagators, this equation becomes

$$iS(x' - z) \partial_z^\mu \Gamma_\mu(z) iS(z - x) = iS(z - x) - iS(x' - z). \quad (12.515)$$

After a Fourier transformation, it reads

$$S(p')(p' - p)^\mu \Gamma_\mu(p', p) S(p) = S(p) - S(p'), \quad (12.516)$$

or

$$(p' - p)^\mu \Gamma_\mu(p', p) = S^{-1}(p) - S^{-1}(p'), \quad (12.517)$$

which is precisely the Ward-Takahashi identity (12.507).

As a consequence of the equality $Z_1 = Z_2$, we find that the matrix elements of the current between one-loop corrected electron states exhibit a unit charge, rather than the divergent charge that is contained in the charge form factor $F(0) = Z_1^{-1}$. Thus we may conclude the important property of QED that the electric charge remains unrenormalized to all orders in perturbation theory.

12.21 Lamb Shift

One of the most important early confirmations of the correctness of quantum electrodynamics of electrons and photons came from the atomic Lamb shift. According to Dirac's theory, the energy spectrum of an electron in an external Coulomb field is

$$E_{nl} = Mc^2 \left\{ 1 + \frac{\alpha^2 Z^2}{n' + \sqrt{(j + 1/2)^2 - \alpha^2 Z^2}} \right\}^{1/2}, \quad (12.518)$$

where $n' = n - j - 1/2 = 0, 1, 2, \dots$ is the radial quantum number, and $j = 1/2, 3/2, \dots$ the total angular momentum. Up to lowest order in the fine-structure constant $\alpha = e^2/\hbar c$, this is approximately equal to

$$E_{nl} = Mc^2 - \frac{1}{2} \alpha^2 Mc^2 \frac{Z^2}{n^2} \left[1 + \frac{\alpha^2 Z^2}{n} \left(\frac{1}{j + 1/2} - \frac{3}{4n} \right) + \dots \right]. \quad (12.519)$$

These formulas show that the Schrödinger degeneracy, of all levels with the same principal quantum number and different values of the orbital angular l , is modified in Dirac's theory, where levels with the same quantum numbers n and j are degenerate for different l 's. The lowest states, where this degeneracy can be compared with experimental data, are the $n = 2$ - states $2S_{1/2}$ and $2P_{1/2}$. They are found to have slightly different energies, thus contradicting the simple Dirac theory.

The energy difference is explained by quantum electrodynamics, and may be attributed to three physical effects. First, the electron encircling the nucleus is shaken by the vacuum fluctuations of the electromagnetic field over a range of the order of the Compton wavelength. Thus it sees a harmonic average of the Coulomb potential over this length scale. This lifts the level $2S_{1/2}$ against the level $2P_{1/2}$ by roughly 27 MHz. Second, the anomalous magnetic moment of the electron changes slightly the Coulomb attraction. Third, the photon running through the vacuum can excite an electron-positron pair. These three effects together cause an *upwards* shift

of the level $2S_{1/2}$ with respect to the level $2P_{1/2}$ equal to [29] $\Delta E = 1\,010$ MHz, 68 MHz, and -27 MHz, respectively. The sum is roughly $1\,052$ MHz, a number which was confirmed experimentally around 1950 [30]. The calculation of these effects will now be reviewed.

12.21.1 Rough Estimate of the Effect of Vacuum Fluctuations

In order to estimate the first effect, consider a free nonrelativistic electron of mass M in the vacuum. It is shaken by the zero-point oscillation of the electromagnetic field, which causes an acceleration

$$M\dot{\mathbf{x}} = e\mathbf{E}. \quad (12.520)$$

For a given frequency ω , the electron is shaken around its average position by a displacement

$$\Delta\mathbf{x} = -\frac{e}{M}\omega^2\mathbf{E}(\omega). \quad (12.521)$$

Its square-average is

$$\langle(\Delta\mathbf{x})^2\rangle = \frac{e^2}{M^2} \int_0^\infty \frac{d\omega}{\omega^4} \langle\mathbf{E}^2(\omega)\rangle. \quad (12.522)$$

The right-hand side can be estimated from the energy (7.341) of the free electromagnetic field in the vacuum, where it has the value [recall (7.434)]

$$E = \frac{1}{2} \sum_{\mathbf{k}, \lambda} \omega_{\mathbf{k}}. \quad (12.523)$$

The polarization sum runs over the two helicities. Hence, with the usual limiting phase space integral (7.21) for the momentum sum, we have

$$E = \int \frac{d^3k}{(2\pi)^3} \omega_{\mathbf{k}} = \frac{1}{2\pi} \int_0^\infty \frac{d\omega}{\pi} \omega^3. \quad (12.524)$$

Since the vacuum energy is equally distributed between electric and magnetic fields, we find

$$\langle E^2 \rangle = \frac{1}{2\pi} \int_0^\infty \frac{d\omega}{\pi} \omega^3, \quad (12.525)$$

and hence

$$\langle(\Delta\mathbf{x})^2\rangle = \frac{2\alpha}{M^2} \int_0^\infty \frac{d\omega}{\pi} \frac{1}{\omega}. \quad (12.526)$$

The integral is divergent at small and large frequencies ω . A priori, it is unclear which are the relevant frequencies that will contribute in a proper calculation. If we consider only electromagnetic waves with wavelength shorter than the Bohr radius $a_B = 1/\alpha M$, the integral starts at $\omega_{\min} = M\alpha$. Alternatively, we may expect the energy of the atomic electrons to supply the relevant cutoff. Then $\omega_{\min} = M\alpha^2$. On the high-frequency end, we omit wavelengths shorter than the Compton wavelength

of the electron, where classical considerations become invalid. Thus we cut off the integral at $\omega_{\max} = M$. In this way we obtain a mean square somewhere in the range

$$\langle \Delta \mathbf{x} \rangle^2 = \frac{2\alpha}{\pi M} C, \quad (12.527)$$

with a constant C somewhere in the range

$$C \in \left(\log \frac{1}{\omega_{\min}}, 2 \log \frac{1}{\omega_{\min}} \right) \approx 4.92 \times (1, 2). \quad (12.528)$$

The electric interaction energy of an electron shaken over this region is modified as follows. The Hamiltonian at the position $\mathbf{x} + \Delta \mathbf{x}(t)$ is

$$H = e \int d^3x A_0(\mathbf{x} + \Delta \mathbf{x}(t)). \quad (12.529)$$

Averaging over $\Delta \mathbf{x}$ gives

$$\begin{aligned} H &= e \int d^3x \left[A_0(\mathbf{x}) + \frac{1}{2} \langle \Delta x_i \Delta x_j \rangle \partial_i \partial_j A_0(\mathbf{x}) \right] \\ &= e \int d^3x \left[1 + \frac{1}{6} \langle \Delta \mathbf{x} \cdot \Delta \mathbf{x} \rangle \nabla^2 \right] A_0(\mathbf{x}) \\ &= e \int d^3x \left[1 + \frac{1}{3\pi} \frac{\alpha}{M^2} C \nabla^2 \right] A_0(\mathbf{x}). \end{aligned} \quad (12.530)$$

In an atom of nuclear charge Ze with a Coulomb potential (12.413), the Laplace operator yields (12.414), and the potential is changed into an effective one:

$$V_C^{\text{eff}} = -\frac{Z\alpha}{r} + \frac{1}{3\pi} \frac{\alpha}{M^2} C Z \alpha 4\pi \delta^{(3)}(\mathbf{x}). \quad (12.531)$$

For an atomic s -state with wave function ψ_n , we treat the extra potential V_C^{eff} perturbatively. We evaluate its expectation value in a state of principal quantum number n , and find the *positive* energy shift

$$\Delta E_n = \frac{4\alpha}{3M^2} Z \alpha C |\psi_n(\mathbf{0})|^2. \quad (12.532)$$

Thus, the present rough estimate of the effect of vacuum fluctuations produces the same term as before in (12.415), except for a different logarithmic factor (12.411).

For a hydrogen atom we insert

$$\psi_n(\mathbf{0}) = \frac{1}{\sqrt{n^3\pi}} \left(\frac{1}{a_B} \right)^{3/2}, \quad (12.533)$$

where $a_B = 1/M\alpha$ is the Bohr radius. If the nuclear charge is Z , then a_B is diminished by this factor. Thus, we obtain the energy shift

$$\Delta E_n = \frac{4\alpha^2 Z}{3M^2} (MZ\alpha)^3 \frac{1}{n^3\pi} C. \quad (12.534)$$

For a hydrogen atom with $n = 2$, this becomes

$$\Delta E_2 = \frac{\alpha^3}{6\pi} \alpha^2 M C. \quad (12.535)$$

The quantity $M\alpha^2$ is the unit energy of atomic physics determining the hydrogen spectrum to be $E_n = -M\alpha^2/2n^2$. Thus

$$M\alpha^2 = 4.36 \times 10^{-11} \text{erg} = 27.21 \text{eV} = 2 \text{ Ry} = 2 \cdot 3.288 \times 10^{15} \text{Hz}. \quad (12.536)$$

Inserting this, together with $\alpha \approx 1/137.036$, into (12.542) yields⁴

$$\Delta E_2 \approx 135.6 \text{MHz} \times C, \quad (12.537)$$

which amounts to the theoretical estimate

$$667.15 \text{ MHz} < \Delta E_2 < 1334.3 \text{ MHz}. \quad (12.538)$$

The experimental Lamb shift⁵

$$\Delta E_{\text{Lamb shift}} \approx 1057 \text{ MHz}, \quad (12.539)$$

is indeed contained in this range.

12.21.2 Relativistic Estimate

The above simple estimate of the effect of vacuum fluctuations produces the same type of correction to the Coulomb potential as the vertex correction in Eq. (12.415), and the vacuum polarization in (12.467). Those two corrections yield an energy shift in an s -state $\psi_n(\mathbf{x})$ of principal quantum number n :

$$\Delta E_n = \frac{4\alpha}{3M^2} Z\alpha |\psi_n(\mathbf{0})|^2 C_{\text{rel}} = \frac{4\alpha^3 Z^4}{3\pi n^3} \alpha^2 M C_{\text{rel}}, \quad (12.540)$$

with the constant C_{rel} :

$$C_{\text{rel}} \equiv \log \frac{M}{\mu} - \frac{3}{8} - \frac{1}{5}. \quad (12.541)$$

For a hydrogen atom in an s -state of principal quantum number $n = 2$ with $n = 2$, this implies

$$\Delta E_2 = \frac{\alpha^3}{6\pi} M \alpha^2 C_{\text{rel}} \approx 135.641 \text{ MHz} \times C_{\text{rel}}. \quad (12.542)$$

The result is not completely determined since it contains an infrared cutoff μ in the constant C_{rel} of Eq. (12.541). In a first approximation, we may imagine the atomic energy $M\alpha^2$ to provide the infrared cutoff for the photon energies. This leads to an estimate for the energy shift of the $2S_{1/2}$ levels with respect to the $2P_{1/2}$ levels of

⁴The precise value of the *Lamb constant* $\alpha^4 M/6\pi$ is $135.641 \pm 0.004 \text{ MHz}$.

⁵See Notes and References.

the hydrogen atom that is about 6% smaller than the larger of the nonrelativistic estimates (12.538):

$$\Delta E_2 \approx (1\,334.3 - 51 - 27.3) \text{ MHz.} \approx 1\,256 \text{ MHz.} \quad (12.543)$$

The intermediate expression exhibits the contribution of the terms $-3/8$ and $-1/5$ in (12.541) (thus showing that vacuum polarization gives a negative shift -27.31 MHz). This shift was first calculated by Uehling [31], who initially thought that vacuum polarization was the main cause of the Lamb shift. He was disappointed to see it contributing only with about 3%. In muonic atoms, however, vacuum polarization does produce the dominant contribution to the Lamb shift for a simple reason: While the above-calculated energy shifts contain a factor $1/M^2$ in formulas such as (12.593), where M is the mass of the muon, the leading vacuum polarization graph still involves an electron loop containing the electron mass, thus being enhanced by a factor $(M_\mu/M_e)^2 \approx 210^2$.

12.21.3 Effect of Wave Functions

In the above calculations the finite size of the electron was derived from a one-loop Feynman-diagram in which the electron lines describe free particles. In an atom, however, the electrons move in a Coulomb potential. The electron is bound to the nucleus. A more accurate calculation should take into account the atomic wave functions of the electron. This is most simply done in an approximation which treats the electrons as nonrelativistic particles. Such an approximation carries an intrinsic error caused by the fact that if a nonrelativistic electron emits a photon with energy of the order Mc^2 and larger, the recoil will necessarily make the electron relativistic. Such an error can, however, be avoided by separating the relativistic from the nonrelativistic contributions. In the first contribution, the effect of the atomic binding of the electrons is negligible, so that the electrons can be treated as free relativistic particles. In the second contribution, the electrons remain approximately nonrelativistic. There exists a natural energy scale $K = M\alpha$ which is much larger than the atomic energy $M\alpha^2$, but much smaller than the rest energy of the electron M . The energy scale K serves to make the separation quantitative. For photons in the upper energy regime, to be referred to as the *hard-photon regime*, we may equip the photon with a mass $\alpha^2 M \gg \mu \ll \alpha M$, and deduce the Lamb shift from Eq. (12.540) to be

$$\Delta E_n = \frac{4\alpha}{3M^2} Z\alpha |\psi_n(\mathbf{0})|^2 C_{\text{hard}} = \frac{4\alpha^3 Z^4}{3\pi n^3} \alpha^2 M C_{\text{hard}}, \quad (12.544)$$

with the constant

$$C_{\text{hard}} \equiv \log \frac{M}{\mu} - \frac{3}{8} - \frac{1}{5}. \quad (12.545)$$

The renormalization procedure has removed the ultraviolet divergences occurring in the calculation of vertex corrections and vacuum polarizations. In the *soft-photon regime*, this leaves us with the task of calculating the contribution from the photons of low energy where the electrons stay nonrelativistic. In the transverse gauge with

$\nabla \mathbf{A}(x) = 0$, the Hamiltonian has the form (12.160), with the Coulomb Hamiltonian (12.161). The radiation field (12.162) contains, in the soft-photon regime under consideration, only photon energies within the limited interval $\omega \in (0, K)$ where K satisfies $M\alpha^2 \ll K \ll M$. The radiation field is expanded in terms of photon creation and annihilation operators as in Eq. (7.350):

$$\hat{A}^\mu(x) = \sum_{\mathbf{k}, \lambda} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[e^{-ikx} \epsilon^\mu(\mathbf{k}, \lambda) \hat{a}_{\mathbf{k}, \lambda} + \text{h.c.} \right]. \quad (12.546)$$

The hats above the field operators are displayed, for clarity. To estimate the expected effects we consider first the influence of the radiation field upon a free electron.

Effect of Vacuum Oscillations upon Free Electron

Let us first calculate the size of the energy shift for a free electron. This is the quantum-mechanical version of the calculation in Subsection 9.10.1.

The Hamilton operator of a free electron of momentum $\mathbf{p}$ is $\hat{H}_0 = \hat{\mathbf{p}}^2/2M$, and the wave functions is a plane wave

$$\langle \mathbf{x} | \mathbf{p} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{p}\mathbf{x}} \quad (12.547)$$

of energy $E_{\mathbf{p}} = \mathbf{p}^2/2M$. If the electromagnetic field is quantized, there is a ground state for the fluctuating vector potential, which is the vacuum state $|0\rangle$ of the photon field. The combined state will be denoted by $|\mathbf{p}; 0\rangle$. The calculation is done perturbatively. Thus we expand the energy shift in powers of the coupling constant:

$$\Delta E_{\mathbf{p}} = \Delta E_{\mathbf{p}}^{(1)} + \Delta E_{\mathbf{p}}^{(2)} + \dots, \quad (12.548)$$

assuming the charge e to be sufficiently small. The first-order shift $\Delta E_{\mathbf{p}}^{(1)}$ is simply the expectation value of the interaction operator

$$\hat{H}^{\text{int}} = -\frac{e}{Mc} \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}(\mathbf{x}) + \frac{e^2}{M^2 c^2} \hat{\mathbf{A}}^2(\mathbf{x}). \quad (12.549)$$

Since this is odd in the field $\mathbf{A}(\mathbf{x})$ which has no expectation value, the first-order energy shift vanishes. Thus we turn to the second-order shift $\Delta E_{\mathbf{p}}^{(2)}$, in which we may ignore the second term in the interaction (called the *seagull term*) that contributes equally to all atomic levels. Then we have

$$\Delta E_{\mathbf{p}} = \frac{e^2}{(Mc)^2} \langle \mathbf{p}; 0 | \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}(\mathbf{x}) \frac{1}{E_{\mathbf{p}} - \hat{H}_0} \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}(\mathbf{x}) | \mathbf{p}; 0 \rangle. \quad (12.550)$$

Inserting a complete set of intermediate electron-plus-single photon states $|\mathbf{p}; k\rangle$, we find, in natural units with $c = 1, \hbar = 1$,

$$\Delta E_{\mathbf{p}} = \frac{e^2}{M^2} \int d^3x \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \lambda, \lambda' = 1, 2}} \frac{1}{\sqrt{2V|\mathbf{k}|}} \frac{1}{\sqrt{2V|\mathbf{k}'|}} \frac{[\mathbf{p} \cdot \boldsymbol{\epsilon}(\mathbf{k}, \lambda) e^{i\mathbf{k}\mathbf{x}}] [\mathbf{p} \cdot \boldsymbol{\epsilon}^*(\mathbf{k}', \lambda') e^{-i\mathbf{k}'\mathbf{x}}]}{\frac{\mathbf{p}^2}{2M} - \frac{1}{2M}(\mathbf{p} - \mathbf{k}')^2 - |\mathbf{k}'|}$$

$$= \frac{e^2}{M^2} \sum_{\mathbf{k}, \lambda=1,2} \frac{1}{2V|\mathbf{k}|} \frac{|\mathbf{p} \cdot \boldsymbol{\epsilon}(k, \lambda)|^2}{\frac{\mathbf{p} \cdot \mathbf{k}}{M} - \frac{\mathbf{k}^2}{2M} - |\mathbf{k}|}. \quad (12.551)$$

Performing the polarization sum

$$\sum_{\lambda=1,2} |\mathbf{p} \cdot \boldsymbol{\epsilon}(k, \lambda)|^2 = \mathbf{p}^2 - \frac{(\mathbf{p} \cdot \mathbf{k})^2}{\mathbf{k}^2}, \quad (12.552)$$

and replacing the sum over momenta by a phase space integral, $V \int d^3k/(2\pi)^3$, we obtain

$$\Delta E_{\mathbf{p}} = \frac{\mathbf{p}^2}{2M} J_M(p^2) \quad (12.553)$$

with

$$J_M(p^2) = \frac{e^2}{M} \int \frac{d^3k}{(2\pi)^3} \frac{1}{|\mathbf{k}|} \left[1 - \frac{(\mathbf{p} \cdot \mathbf{k})^2}{\mathbf{p}^2 \mathbf{k}^2} \right] \frac{1}{\frac{\mathbf{p} \cdot \mathbf{k}}{M} - \frac{\mathbf{k}^2}{2M} - |\mathbf{k}|}. \quad (12.554)$$

Writing the last factor as

$$-\frac{1}{k} + \frac{1}{k} \frac{\frac{k^2}{2M} - \frac{\mathbf{p} \cdot \mathbf{k}}{M}}{\frac{k^2}{2M} - \frac{\mathbf{p} \cdot \mathbf{k}}{M} + k}, \quad (12.555)$$

we obtain

$$J_M(p^2) = J_M(0) + J'_M(p^2) \quad (12.556)$$

with

$$J_M(0) = -\frac{e^2}{M} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} \left[1 - \frac{(\mathbf{p} \cdot \mathbf{k})^2}{p^2 k^2} \right] \frac{1}{k} \quad (12.557)$$

and

$$J'_M(p^2) = \frac{e^2}{M} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} \left[1 - \frac{(\mathbf{p} \cdot \mathbf{k})^2}{p^2 k^2} \right] \frac{\frac{k^2}{2M} - \frac{\mathbf{p} \cdot \mathbf{k}}{M}}{\frac{k^2}{2M} - \frac{\mathbf{p} \cdot \mathbf{k}}{M} + k}. \quad (12.558)$$

The first term can easily be calculated:

$$\begin{aligned} J_M(0) &= -\frac{e^2}{4\pi^2 M} \int_0^\infty dk \int_0^\infty d\cos\theta (1 - \cos^2\theta) \\ &= -\frac{4\alpha}{3\pi M} \int_0^\infty dk. \end{aligned} \quad (12.559)$$

Being in the soft-photon regime, a quadratic divergence at large k is avoided. The integral is cut off at $k = K \ll M$. With the resulting finite $J_M(0)$, the kinetic energy of the electron is changed from $E(\mathbf{p}) = \mathbf{p}^2/2M$ to the renormalized energy

$$E_R(\mathbf{p}) = \frac{\mathbf{p}^2}{2M} [1 + J_M(0)]. \quad (12.560)$$

Such a factor may be absorbed in the mass of the electron, by defining a renormalized mass

$$M_R = \frac{M}{1 + J_M(0)} \sim M - MJ_M(0). \quad (12.561)$$

In terms of this and the subtracted function $J'_M(p^2)$ of Eq. (12.558), we find the full momentum dependence of the energy to order α :

$$E_R(\mathbf{p}) = \frac{\mathbf{p}^2}{2M_R} [1 + J'_{M_R}(p^2)]. \quad (12.562)$$

Effect of Vacuum Oscillations upon Bound Electron

We now perform the same calculation once more in the presence of the Coulomb potential $V_C(\mathbf{x})$, and study an electron in an orbit of principal quantum number n with a wave function $\psi_n(\mathbf{x})$, moving through a photon vacuum $|0\rangle$. Then Eq. (30B.18) becomes

$$\Delta E_n = \frac{e^2}{M^2} \langle n; 0 | \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}(\mathbf{x}) \frac{1}{E_n - \hat{H}_C} \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}(\mathbf{x}) | n; 0 \rangle. \quad (12.563)$$

Inserting a complete set of states $|n'; 0\rangle$ between the operators in Eq. (12.563) leads to

$$\Delta E_n = \frac{e^2}{M^2} \sum_n \sum_{\lambda, \lambda'} \int \frac{d^3k}{(2\pi)^3} \frac{1}{2V|\mathbf{k}|} \frac{(\hat{\mathbf{p}}e^{i\mathbf{k}\mathbf{x}})_{nn'} \boldsymbol{\epsilon}(\mathbf{k}, \lambda) (\hat{\mathbf{p}}e^{-i\mathbf{k}\mathbf{x}})_{n'n} \boldsymbol{\epsilon}^*(\mathbf{k}, \lambda)}{E_n - E_{n'} - k} \quad (12.564)$$

where $(\hat{\mathbf{p}}e^{i\mathbf{k}\mathbf{x}})_{nn'}$ denotes the matrix elements

$$(\hat{\mathbf{p}}e^{i\mathbf{k}\mathbf{x}})_{nn'} \equiv \int d^3x \psi_n(\mathbf{x}) (\hat{\mathbf{p}}e^{i\mathbf{k}\mathbf{x}})_{nn'} \psi_{n'}(\mathbf{x}). \quad (12.565)$$

A Schrödinger wave function corresponds graphically to an infinite set of static photon exchanges. The energy shift to be calculated from Eq. (12.563) has therefore the following graphical representation: The additional photon provides a radiative

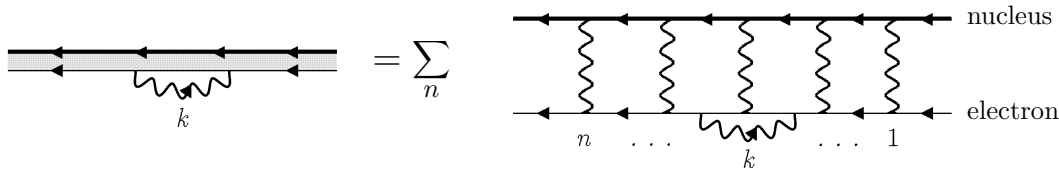


FIGURE 12.29 Diagrammatic content in the calculation of the energy shift with the help of Schrödinger wave functions. A hydrogen atom is represented by the fat line on the left which results from an infinite sum of photon exchanges.

correction to the static photons which creates the bound state. The sum over n' must, of course, include also an integral over the continuous wave functions. By rewriting, as in (12.555),

$$\frac{1}{E_n - E_{n'} - k} = -\frac{1}{k} + \frac{E_{n'} - E_n}{k(E_{n'} - E_n + k)}, \quad (12.566)$$

we obtain

$$\begin{aligned} \Delta E_n &= \frac{e^2}{M^2} \sum_{n'} (\hat{p}_i e^{i\mathbf{k}\mathbf{x}})_{nn'} (\hat{p}_j e^{-i\mathbf{k}\mathbf{x}})_{n'n} \\ &\times \int \frac{d^3k}{(2\pi)^3} \frac{1}{2k^2} \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \left[-1 + \frac{E_{n'} - E_n}{E_{n'} - E_n + k} \right]. \end{aligned} \quad (12.567)$$

The $|\mathbf{k}|$ -integration is again restricted to the soft-photon regime $|\mathbf{k}| < K \ll M$. In the integral involving only the first term in the brackets of (12.567), the energies $E_{n'}$ are absent and we can replace the sum over all wave functions $|n'\rangle$ by an integral over plane waves. Then we obtain the expectation value of the energy calculated for a free electron in Eq. (12.560):

$$-\frac{1}{2M} \langle n | \mathbf{p}^2 | n \rangle J_M(0). \quad (12.568)$$

This produces the same mass renormalization as before. Subtracting this from ΔE_n , we are left with

$$\begin{aligned} \Delta E'_n &= \frac{e^2}{2M^2} \sum_{n'} (\hat{p}_i e^{i\mathbf{k}\mathbf{x}})_{nn'} (\hat{p}_j e^{-i\mathbf{k}\mathbf{x}})_{n'n} \\ &\times \int \frac{d^3k}{(2\pi)^3} \frac{1}{k^2} \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \frac{E_{n'} - E_n}{E_{n'} - E_n + k}. \end{aligned} \quad (12.569)$$

In order to understand the behavior of the integral, it is useful to further split the k -integral in the soft-photon regime. Thus we introduce the energies $M\alpha^2 \ll K' \ll K = M\alpha$, and distinguish an upper regime with wave number $K' < k < K$ and a lower regime with $M\alpha^2 \ll k < K'$. The corresponding energy shifts are denoted by $\Delta_{\text{low}} E'_n$ and $\Delta_{\text{up}} E'_n$, respectively. In the upper regime we may approximate (12.569) by

$$\begin{aligned} \Delta_{\text{up}} E'_n &= \frac{e^2}{4M^2} \left[\sum_{n'} (\hat{p}_i e^{i\mathbf{k}\mathbf{x}})_{nn'} (\hat{p}_j e^{-i\mathbf{k}\mathbf{x}})_{n'n} (E_{n'} - E_n) + (i \leftrightarrow j) \right] \\ &\times \int \frac{d^3k}{(2\pi)^3} \frac{1}{k^2} \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right). \end{aligned} \quad (12.570)$$

The sum over n' can now be expressed with the help of the Hamilton operator $\hat{H}_C$ of the Coulomb system as

$$\sum_{n'} (\hat{p}_i e^{i\mathbf{k}\mathbf{x}})_{nn'} (\hat{p}_j e^{-i\mathbf{k}\mathbf{x}})_{n'n} (E_{n'} - E_n) + (i \leftrightarrow j) = \langle n | [\hat{p}_i e^{i\mathbf{k}\mathbf{x}} [\hat{H}_C, \hat{p}_j e^{-i\mathbf{k}\mathbf{x}}]] | n \rangle. \quad (12.571)$$

Working out the commutators, this reduces to

$$[\hat{p}_i e^{i\mathbf{k}\mathbf{x}}, [\hat{H}_C, \hat{p}_j e^{-i\mathbf{k}\mathbf{x}}]] = \partial_i \partial_j V_C(\mathbf{x}) + \dots, \quad (12.572)$$

where the omitted terms contain a factor k_i , k_j , or both. Due to their longitudinal nature, they do not contribute to (12.571), where they are contracted with the transverse projection tensor $\delta_{ij} - k_i k_j / k^2$. Thus we find

$$\Delta_{\text{up}} E'_n = \frac{e^2}{4M^2} \langle n | \partial_i \partial_j V_C(\mathbf{x}) | n \rangle \int_{K > |\mathbf{k}| > K'} \frac{d^3 k}{(2\pi)^3} \frac{1}{k^3} \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right). \quad (12.573)$$

Doing the integral over all $\mathbf{k}$ -directions yields

$$\Delta_{\text{up}} E'_n = \frac{e^2}{4M^2} \langle n | \nabla^2 V_C(\mathbf{x}) | n \rangle \frac{1}{3\pi^2} \int_{K'}^K \frac{dk}{k}. \quad (12.574)$$

Inserting

$$\nabla^2 V_C(x) = 4\pi Z\alpha \delta^{(3)}(\mathbf{x}), \quad (12.575)$$

this can be rewritten as

$$\Delta_{\text{up}} E'_n = \frac{4\alpha Z}{3\pi M^2} |\psi_n(\mathbf{0})|^2 \log \frac{K}{K'}. \quad (12.576)$$

Note that this expression matches smoothly with the energy shift (12.544) caused by hard photons. By adding the two results, the intermediate energy scale K cancels, producing an energy shift depending only on the separation parameter K' :

$$(\Delta_{\text{hard}} + \Delta_{\text{up}}) E'_n = \frac{4\alpha}{3\pi M^2} |\psi_n(\mathbf{0})|^2 \left(\log \frac{M}{K'} - \frac{3}{8} - \frac{1}{5} \right). \quad (12.577)$$

Consider now the lower soft-photon part of the integral (12.569). Here we take advantage of the fact that, due to the presence of the atomic probability distribution $|\psi_n(\mathbf{x})|^2$, the integration over $\mathbf{x}$ is limited to a range $|\mathbf{x}| \lesssim a_B = 1/\alpha M$. Since $|\mathbf{k}| < K' \ll \alpha M$ we see that

$$|\mathbf{k}\mathbf{x}| \ll 1, \quad (12.578)$$

so that we can neglect the exponential $e^{i\mathbf{k}\mathbf{x}}$ in the matrix elements $(\hat{\mathbf{p}} e^{i\mathbf{k}\mathbf{x}})_{nn'}$. Thus we may evaluate the simpler expression

$$\Delta_{\text{low}} E'_n \approx \frac{e^2}{2M^2} \sum_{n'} (p_i)_{nn'} (p_j)_{n'n} \int_0^K \frac{d^3 k}{(2\pi)^3} \frac{1}{k^2} \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \frac{E_{n'} - E_n}{E_{n'} - E_n + k}. \quad (12.579)$$

This approximation amounts to neglecting the recoil of the atom. Performing the integral over all $\mathbf{k}$ -directions yields

$$\Delta_{\text{low}} E'_n \approx \sum_{n'} \frac{|\mathbf{p}_{nn'}|^2}{2M} J_M(n, n') \quad (12.580)$$

with

$$J_M(n, n') = \frac{2\alpha}{\pi M} \frac{2}{3} \int_0^{K'} dk \frac{E_{n'} - E_n}{E_{n'} - E_n + k}. \quad (12.581)$$

After doing the k -integral, this becomes

$$J_M(n, n') \approx \frac{4\alpha}{3\pi M} (E_{n'} - E_n) \left[\log \frac{K'}{|E_{n'} - E_n|} + i\pi\Theta(E_n - E_{n'}) \right]. \quad (12.582)$$

The imaginary part contributes to the decay rate of an atom from the state n into a lower state n' . It can be dropped in the final formula for the energy shift.

Let us decompose

$$\log \frac{K'}{E_{n'} - E_n} = \log \frac{K'}{2E_{1S}} - \log \frac{E_{n'} - E_n}{2E_{1S}}, \quad (12.583)$$

thus separating (12.580) into two sums $\Delta_{\text{low}}^{(1)} E_n$ and $\Delta_{\text{low}} E_n$. The first of these sums can be treated the same way as in (12.571) and yields a contribution

$$\Delta_{\text{low}}^{(1)} E_n' = \frac{4\alpha Z}{3\pi M^2} |\psi_n(\mathbf{0})|^2 \log \frac{K'}{2E_{1S}}. \quad (12.584)$$

Together with the energy shift (12.577), this becomes

$$(\Delta_{\text{hard}} + \Delta_{\text{up}} + \Delta_{\text{low}}^{(1)}) E_n' = \frac{4\alpha Z}{3\pi M^2} |\psi_n(\mathbf{0})|^2 \bar{C} = \frac{4\alpha^3 Z^4}{3\pi n^3} \alpha^2 M \bar{C} \quad (12.585)$$

with the constant

$$\bar{C} = \log \frac{M}{2E_{1S}} - \frac{3}{8} - \frac{1}{5} = \log \frac{1}{\alpha^2} - \frac{3}{8} - \frac{1}{5} \approx 9.265. \quad (12.586)$$

The separation parameter K' has disappeared, and the result is unambiguous.

For the $n = 2$ -state of the hydrogen atom, the numerical value is

$$\begin{aligned} (\Delta_{\text{hard}} + \Delta_{\text{up}} + \Delta_{\text{low}}^{(1)}) E_n' &\approx 135.6 \text{ MHz} \times \bar{C} \\ &\approx (1334 - 51) \text{ MHz} \approx 1283 \text{ MHz}. \end{aligned} \quad (12.587)$$

This is still larger than the experimental value 1057 MHz. The relativistic treatment of the hard regime together with the upper soft-photon regime have produced a number which lies about 4% below the upper rough estimate (12.538).

It remains to calculate the second sum $\Delta_{\text{low}} E_n'$ in the lower soft-photon regime which contains the effect of the wave functions in an essential way. This sum is slightly more involved and requires evaluating a detailed spectral sum. We shall write it as

$$\Delta_{\text{low}} E_n' = -\frac{2\alpha}{3\pi} M^2 S_n \quad (12.588)$$

where S_n denotes the sum

$$S_n = \sum_{n'} |\mathbf{p}_{nn'}|^2 (E_{n'} - E_n) \log \frac{|E_{n'} - E_n|}{2E_{1S}}. \quad (12.589)$$

It is convenient to define an average energy E^{av} by the relation

$$S_n = \left[\sum_{n'} |\mathbf{p}_{nn'}|^2 (E_{n'} - E_n) \right] \log \frac{E^{\text{av}}}{2E_{1S}}. \quad (12.590)$$

The bracket is, by virtue of (12.571), equal to

$$\begin{aligned} \sum_{n'} |\mathbf{p}_{nn'}|^2 (E_{n'} - E_n) &= \frac{1}{2} \langle n | [\hat{\mathbf{p}} e^{i\mathbf{k}\mathbf{x}} [\hat{H}_C, \hat{\mathbf{p}} e^{-i\mathbf{k}\mathbf{x}}]] | n \rangle = \frac{1}{2} \langle n | \nabla^2 V_C | n \rangle \\ &= \frac{1}{2} 4\pi Z\alpha |\psi_n(\mathbf{0})|^2 = \frac{2Z^4\alpha}{n^3}. \end{aligned} \quad (12.591)$$

This provides a useful check for the convergence of the calculation. An explicit evaluation of the sum gives, for the $2S$ level [32]:

$$E^{\text{av}} = 8.320 \alpha^2 M. \quad (12.592)$$

By writing S_n in the form (12.590), the effect of the correction is to subtract a term $\log(2E_{1S}/E^{\text{av}})$ from $\bar{C}$ in (12.585), thus producing the result

$$\Delta E_n = \frac{4\alpha}{3\pi M^2} |\psi_n(\mathbf{0})|^2 C_2 = \frac{4\alpha^3 Z^4}{3\pi n^3} \alpha^2 M C_2, \quad (12.593)$$

with

$$C_{2S^{1/2}}^{\text{tot}} = \bar{C} - \log \frac{2E_{1S}}{E^{\text{av}}} = \log \frac{1}{\alpha^2} - \frac{3}{8} - \frac{1}{5} - \log \frac{2E_{1S}}{E^{\text{av}}} \approx 7.146. \quad (12.594)$$

In combining the hard-photon with the two soft-photon results we have been a bit careless since the first result (12.544) was derived with a finite photon mass $\alpha^2 M \gg \mu \ll \alpha M$ as an infrared cutoff parameter. The calculation of the finite correction (12.595) should be done in the same way, i.e., we should integrate

$$\begin{aligned} \Delta_{\text{low}} E'_n &\approx \frac{e^2}{2M^2} \sum_{n'} (p_i)_{nn'} (p_j)_{n'n} \\ &\times \int_0^K \frac{d^3 k}{(2\pi)^3} \frac{1}{k^2 + \mu^2} \left(\delta_{ij} - \frac{k_i k_j}{k^2 + \mu^2} \right) \frac{E_{n'} - E_n}{E_{n'} - E_n + \sqrt{k^2 + \mu^2}}. \end{aligned} \quad (12.595)$$

The photon mass changes (12.581) into

$$J'_M(n, n') = \frac{2\alpha}{\pi M} \int_0^{K'} dk \left(1 - \frac{1}{3} \frac{k^2}{k^2 + \mu^2} \right) \frac{E_{n'} - E_n}{E_{n'} - E_n + \sqrt{k^2 + \mu^2}}. \quad (12.596)$$

The difference between the two integrals is

$$J'_M(n, n') - J_M(n, n') = \frac{4\alpha}{3\pi M} (E_{n'} - E_n) \left[\log \frac{\mu}{2|E_{n'} - E_n|} + \frac{5}{6} + i\pi \Theta(E_n - E_{n'}) \right]. \quad (12.597)$$

A comparison with (12.582) shows that the constant $C_{2S^{1/2}}^{\text{tot}}$ in (12.594) receives an additional correction of $5/6 - \log 2 \approx 0.140$, bringing it up to

$$C_{2S^{1/2}}^{\text{tot}} = \log \frac{M}{2E_{1S}} - \frac{3}{8} - \frac{1}{5} - \log \frac{2E_{1S}}{E_{\text{av}}} + \frac{5}{6} - \log 2 \approx 7.286, \quad (12.598)$$

corresponding to an energy shift

$$\Delta E_{2S^{1/2}} \approx (1\,334.3 - 51 - 27.3 - 287 + 20) \text{ MHz} \approx 989 \text{ MHz}, \quad (12.599)$$

which is smaller than the experimental value 1 057 MHz.

An important correction is missing in this calculation: the one caused by the anomalous magnetic moment of the electron. This produces an energy shift of about 68.5 MHz, which brings the Lamb shift from the value (12.599) up to 1 057.5 MHz, in excellent agreement with the experimental number 1 057 MHz.

This contribution will be calculated in the next subsection. Before we come to that, however, we want to observe that, while the relativistic Lamb shift was applied only to s -waves, the effect of the wave functions changes also the energy of states with orbital angular momenta $l \geq 0$. For such wave functions, we may define an average energy analog to (12.590) as

$$S_n = \left[\sum_{n'} |\mathbf{p}_{nn'}|^2 (E_{n'} - E_n) \right]_{l=0} \log \frac{E_{\text{av}}}{2E_{1S}}. \quad (12.600)$$

The bracket must be taken for $l = 0$ since it vanishes for $l > 0$ by virtue of the same commutator calculation as in (12.591), to be evaluated between $l \neq 0$ -states. By doing the spectral sum one finds the average energy [33]

$$E_{2P}^{\text{av}} = 0.9704 \alpha^2 M. \quad (12.601)$$

This raises the p -wave slightly by

$$\Delta^{\text{av}} E_{2P} = \frac{\alpha^3}{6\pi} \alpha^2 M C_{2P}^{\text{av}}, \quad (12.602)$$

with

$$C_{2P}^{\text{av}} = \log \frac{2E_{1S}}{2E_{2P}^{\text{av}}} \approx 0.03, \quad (12.603)$$

i.e., by

$$\Delta^{\text{av}} E_{2P} \approx 135.6 \text{ MHz} \times C_{2P}^{\text{av}} \approx 4 \text{ MHz}. \quad (12.604)$$

12.21.4 Effect of the Anomalous Magnetic Moment

The relativistic current of the electron was found in Eq. (12.401) to have the form

$$\langle \mathbf{p}' | j^\mu | \mathbf{p} \rangle = e \bar{u}(\mathbf{p}') \left[\gamma^\mu F(q^2) + \frac{i}{2M} \sigma^{\mu\nu} q_\nu G(q^2) \right] u(\mathbf{p}), \quad (12.605)$$

with the form factors $F(q^2)$ and $G(q^2)$ given by Eqs. (12.403) and (12.391). For small momentum transfers, these can be approximated by [recall (12.407) and (12.418)]

$$\begin{aligned} F(q^2) &\approx 1 + q^2 R_e^{\text{vc}2}, & R_e^{\text{vc}2} &= \frac{\alpha}{3\pi M^2} \left(\log \frac{M}{\mu} - \frac{3}{8} \right), \\ G(q^2) &\approx \frac{\alpha}{2\pi}. \end{aligned} \quad (12.606)$$

In configuration space, this amounts to an effective extra electromagnetic interaction of the Dirac field of the electron which can be written as a Lagrangian density

$$\mathcal{L}_{\text{eff}} = -e\bar{\psi}(x) \left\{ \gamma^\mu \left[1 - R_e^{\text{vc}2} \square \right] A_\mu(x) + \frac{i}{2M} \sigma^{\mu\nu} i \frac{\alpha}{2\pi} \partial_\nu A_\mu(x) \right\} \psi(x). \quad (12.607)$$

In a static electric field, the radiative corrections provide a solution of the Dirac equation $\psi_{njm}(\mathbf{x})$ with an additional energy

$$\Delta E = e\bar{\psi}(\mathbf{x}) \left[\gamma^0 R_e^{\text{vc}2} \nabla^2 A_0(\mathbf{x}) + \frac{i\alpha}{4\pi M} \boldsymbol{\gamma} \cdot \mathbf{E}(\mathbf{x}) \right] \psi(\mathbf{x}). \quad (12.608)$$

To lowest order in α , we approximate the solutions to the Dirac equation by combinations of the nonrelativistic Schrödinger wave functions ψ_{nlm} with rest spinors $u(\mathbf{0}, s_3)$, combining them to state of total angular momentum j with the help of Clebsch-Gordan coefficients, as shown in Eq. (6.184). The first term in (12.608) leads precisely to the relativistic energy shift $\Delta_{\text{hard}} E$ calculated in (12.544). However, that calculation lacked the energy shift due to the second term, which arises from the anomalous magnetic moment:

$$\Delta E^{\text{a}} = i \frac{e\alpha}{4\pi M} \int d^3x \bar{\psi}(\mathbf{x}) \boldsymbol{\gamma} \psi(\mathbf{x}) \mathbf{E}(\mathbf{x}). \quad (12.609)$$

In order to calculate this we have to approximate the solutions of the Dirac equations a little better than so far. We go to the Dirac representation of the gamma matrices and decompose the bispinor into two simple spinors, as in Eq. (6.184),

$$\psi(\mathbf{x}) = \begin{pmatrix} \xi(x) \\ \eta(x) \end{pmatrix}. \quad (12.610)$$

These satisfy the Dirac equation (4.500). We observed in (4.580) that the lower, small components are related to the upper large ones by [see also (6.113)]

$$\eta(\mathbf{x}) = -i \frac{\nabla \cdot \boldsymbol{\sigma}}{M} \xi(\mathbf{x}) + \mathcal{O}(\alpha). \quad (12.611)$$

Neglecting the corrections of the order of α and inserting (12.611) into (12.610) and (12.609), thereby using the explicit form of the electric field

$$\mathbf{E}(\mathbf{x}) = -Z\alpha \frac{\mathbf{x}}{|\mathbf{x}|^3}, \quad (12.612)$$

the integrand is found to contain an expression

$$\begin{aligned}\bar{\psi}(\mathbf{x})\boldsymbol{\gamma} \cdot \frac{\mathbf{x}}{|\mathbf{x}|^3}\psi(\mathbf{x}) &= \xi^\dagger(\mathbf{x})\frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{|\mathbf{x}|^3}\eta(\mathbf{x}) - \eta^\dagger(\mathbf{x})\boldsymbol{\gamma}\frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{|\mathbf{x}|^3}\xi(\mathbf{x}) \\ &\approx \frac{1}{2Mi} \left[\xi^\dagger(\mathbf{x})\frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{|\mathbf{x}|^3}\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}\xi(\mathbf{x}) + \text{h.c.} \right].\end{aligned}\quad (12.613)$$

After an integration by parts this leads to

$$\int d^3x \bar{\psi}(\mathbf{x})\boldsymbol{\gamma} \cdot \frac{\mathbf{x}}{|\mathbf{x}|^3}\psi(\mathbf{x}) \approx \xi^\dagger(\mathbf{x}) \left[\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}, \frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{|\mathbf{x}|^3} \right] \xi(\mathbf{x}). \quad (12.614)$$

We now observe that

$$\boldsymbol{\nabla} \cdot \frac{\mathbf{x}}{|\mathbf{x}|^3} = -\boldsymbol{\nabla}^2 \frac{1}{|\mathbf{x}|} = 4\pi\delta^{(3)}(\mathbf{x}), \quad (12.615)$$

which allows us to calculate the commutator, using the chain rule, as being

$$\left[\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}, \frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{|\mathbf{x}|^3} \right] = -\boldsymbol{\nabla}^2 \frac{1}{|\mathbf{x}|} - 2i\boldsymbol{\sigma} \cdot (\mathbf{x} \times \boldsymbol{\nabla}) \frac{1}{|\mathbf{x}|^3} = 4\pi\delta^{(3)}(\mathbf{x}) + 4\frac{1}{|\mathbf{x}|^3}\mathbf{L} \cdot \mathbf{S}. \quad (12.616)$$

The first term gives rise to another energy shift for s -waves, which may be written in the same general form as the previous ones:

$$\Delta E_n = \frac{4\alpha}{3M^2} Z\alpha |\psi_n(\mathbf{0})|^2 C^a, \quad (12.617)$$

with the constant being now

$$C^a \equiv \frac{3}{8}. \quad (12.618)$$

The second term depends on the angular momentum of the Dirac wave function. Writing $2\mathbf{L} \cdot \mathbf{S} = \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2$, the eigenvalues of $\mathbf{L} \cdot \mathbf{S}$ are $j(j+1) - l(l+1) - 3/4$. The expectation value of $1/|\mathbf{x}|^3$ in $l \neq 0$ -states is

$$\langle nlm | \frac{1}{|\mathbf{x}|^3} | nlm \rangle = \frac{2}{l(l+1)(2l+1)n^3} (Z\alpha M)^3. \quad (12.619)$$

Thus we obtain an energy shift for $l \neq 0$ -states:

$$\Delta E_n = \frac{4\alpha}{3M^2} Z\alpha |\psi_n(\mathbf{0})|^2 C_{j,l}^a = \frac{4\alpha^3 Z^4}{3\pi n^3} \alpha^2 M C_{j,l}^a \quad (12.620)$$

with

$$C_{j,l}^a \equiv \frac{3}{8} \frac{1}{2l+1} \begin{cases} \frac{1}{l+1} & \text{for } j = l + \frac{1}{2}, \\ -\frac{1}{l} & j = l - \frac{1}{2}; \quad (l \geq 1). \end{cases} \quad (12.621)$$

This leads for a level shift of the s -wave

$$\Delta^a E_{2S^{1/2}} = \frac{\alpha^3}{6\pi} \alpha^2 M C_{1/2,0}^a, \quad (12.622)$$

with

$$C_{1/2,0}^a = \frac{3}{8}. \quad (12.623)$$

Remarkably, the anomalous magnetic moment causes a small energy shift also in states of higher angular momenta. The $2P^{1/2}$ -state of the relativistic hydrogen atom is shifted opposite to the $2S^{1/2}$ -state by

$$\Delta^a E_{2P^{1/2}} = \frac{\alpha^3}{6\pi} \alpha^2 M C_{1/2,1}^a, \quad (12.624)$$

with

$$C_{1/2,1}^a \equiv -\frac{1}{8}. \quad (12.625)$$

Together with the s -wave splitting (12.623) this leads to the total *Lamb shift*:

$$\Delta^a E = \frac{\alpha^3}{6\pi} \alpha^2 M (C_{1/2,0}^a - C_{1/2,1}^a) = \frac{\alpha^3}{6\pi} \alpha^2 M C_{\text{Lamb}}^a, \quad (12.626)$$

with

$$C_{\text{Lamb}}^a = \frac{3}{8} + \frac{1}{8} = \frac{1}{2}, \quad (12.627)$$

i.e., by

$$\Delta^a E \approx 135.6 \text{ MHz} \times C_{\text{Lamb}}^a \approx 68.9 \text{ MHz}. \quad (12.628)$$

Recently, Lamb shifts have been measured also in heavy atoms where the atomic levels are accessible to X-ray spectroscopy. There the theoretical analysis is much more difficult due to the narrowness of the atomic wave functions and the large size of the nucleus [35].

Appendix 12A Calculation of the Dirac Trace in the Klein-Nishina Formula

The trace (12.289) can be expanded as

$$F = \frac{1}{M^2} \left[\frac{t_1^8 + M^2 t_1^6}{(2pk)^2} + \frac{t_2^8 + M^2 t_2^6}{(2pk)(2p'k')} + \frac{t_3^8 + M^2 t_3^6}{(2pk)(2pk')} + \frac{t_4^8 + M^2 t_4^6}{(2pk')^2} \right], \quad (12A.1)$$

where t_j^i denotes the following Dirac traces involving i gamma matrices:

$$\begin{aligned} t_1^8 &= \frac{1}{4} \text{tr}(\not{\epsilon}' \not{k} \not{\epsilon} \not{p} \not{\epsilon} \not{k} \not{\epsilon}' \not{p}'), & t_2^8 &= \frac{1}{4} \text{tr}(\not{\epsilon}' \not{k} \not{\epsilon} \not{p} \not{\epsilon}' \not{k}' \not{\epsilon} \not{p}'), \\ t_3^8 &= \frac{1}{4} \text{tr}(\not{\epsilon} \not{k}' \not{\epsilon}' \not{p} \not{\epsilon} \not{k} \not{\epsilon}' \not{p}'), & t_4^8 &= \frac{1}{4} \text{tr}(\not{\epsilon} \not{k}' \not{\epsilon}' \not{p} \not{\epsilon}' \not{k}' \not{\epsilon} \not{p}'), \\ t_1^6 &= \frac{1}{4} \text{tr}(\not{\epsilon}' \not{k} \not{\epsilon} \not{\epsilon} \not{k} \not{\epsilon}'), & t_2^6 &= \frac{1}{4} \text{tr}(\not{\epsilon}' \not{k} \not{\epsilon} \not{\epsilon}' \not{k}' \not{\epsilon}'), \\ t_3^6 &= \frac{1}{4} \text{tr}(\not{\epsilon} \not{k}' \not{\epsilon}' \not{\epsilon} \not{k} \not{\epsilon}'), & t_4^6 &= \frac{1}{4} \text{tr}(\not{\epsilon} \not{k}' \not{\epsilon}' \not{\epsilon}' \not{k}' \not{\epsilon}'). \end{aligned} \quad (12A.2)$$

For brevity, we have omitted the symbols of complex conjugation on the outgoing polarization vectors, which may be taken to be real and purely spatial, corresponding to linear polarizations.

Traces involving an odd number of gamma matrices have been omitted, since they vanish. We now use the crossing symmetry (12.286) to rewrite F as

$$F = \frac{1}{M^2} \left[\frac{t_1^8 + M^2 t_1^6}{(2pk)^2} + \frac{t_2^8 + M^2 t_2^6}{(2pk)(2p'k')} + (\epsilon \leftrightarrow \epsilon', k \leftrightarrow -k') \right]. \quad (12A.3)$$

The traces are evaluated using the Wick expansion (12.253), together with the properties

$$p^2 = p'^2 = M^2, \quad k^2 = k'^2 = 0, \quad \epsilon^2 = \epsilon'^2 = -1. \quad (12A.4)$$

Using further the properties in the laboratory frame with $p = (M, 0, 0, 0)$:

$$\begin{aligned} \epsilon p &= \epsilon' p = 0, \\ \epsilon' p' &= \epsilon'(p + k - k') = \epsilon' k, \end{aligned}$$

we calculate t_1^8 as follows: First we use $\epsilon^2 = -1$, and the Dirac relation (12.249) to reduce

$$\not{\epsilon} \not{p} \not{\epsilon} = -\not{p} \not{\epsilon} \not{\epsilon} = \not{p}. \quad (12A.5)$$

Similarly, $k^2 = 0$ allows us to rewrite

$$\not{k} \not{p} \not{k} = -\not{k} \not{k} \not{p} + 2(kp)\not{k} = 2(kp)\not{k}. \quad (12A.6)$$

Then t_1^8 becomes

$$t_1^8 = 2(pk) \frac{1}{4} \text{tr}(\not{\epsilon}' \not{k} \not{\epsilon}' \not{p}'). \quad (12A.7)$$

Now there are only three Wick contractions in the expansion à la (12.253):

$$t_1^8 = 2(pk) [(\epsilon' k)(\epsilon' p') - (\epsilon' \epsilon')(kp') + (\epsilon' p')(k\epsilon')], \quad (12A.8)$$

which yield

$$t_1^8 = 2(pk) [2(\epsilon' k)(\epsilon' p') + (kp')]. \quad (12A.9)$$

With the help of the substitution

$$kp' = -\frac{1}{2}[(p' - k)^2 - M^2] = -\frac{1}{2}[(p - k')^2 - M^2] = pk', \quad (12A.10)$$

this becomes

$$t_1^8 = 4(pk)(\epsilon' k)^2 + 2(pk')(pk). \quad (12A.11)$$

Note that the similar relation

$$kp = \frac{1}{2}[(p + k)^2 - M^2] = \frac{1}{2}[(p' + k')^2 - M^2] = p'k', \quad (12A.12)$$

leads to

$$t_4^8 = -4(pk')(\epsilon k')^2 + 2(pk')(pk) \quad (12A.13)$$

arising from t_1^8 via the crossing operation (12.286). The other traces are

$$t_1^6 = t_4^6 = 0, \quad (12A.14)$$

since they contain, in the middle, the products $\not{k} \not{\epsilon} \not{\epsilon} \not{k} = -\not{k} \not{k} = -k^2 = 0$ and $\not{k}' \not{\epsilon}' \not{\epsilon}' \not{k}' = -\not{k}' \not{k}' = -k'^2 = 0$. We further find

$$t_2^6 = t_3^6 = \frac{1}{4} \text{tr}(\not{\epsilon}' \not{\epsilon} \not{\epsilon}' \not{k} \not{k}') = M^2 [2(kk')(\epsilon \epsilon')^2 - 2(\epsilon \epsilon')(k\epsilon')(k'\epsilon) - (kk')], \quad (12A.15)$$

and finally,

$$\begin{aligned} t_2^8 = t_3^8 = & -4(\epsilon \epsilon')^2 (kp)(k'p) + 2(\epsilon \epsilon')^2 (kk')M^2 - 2(\epsilon \epsilon')(\epsilon k')(k'\epsilon)M^2 - 2(\epsilon k')^2 (kp) \\ & + 2(\epsilon k)^2 (k'p) - (kk')M^2 + 2(kp)(k'p). \end{aligned} \quad (12A.16)$$

Hence

$$\begin{aligned} \frac{1}{2M^2} \left[\frac{t_1^8 + M^2 t_1^6}{(2pk)^2} + \frac{t_2^8 + M^2 t_2^6}{(2pk)(2p'k')} \right] (\epsilon \leftrightarrow \epsilon', k \leftrightarrow k') = \frac{1}{2M^2} \left\{ 2(\epsilon\epsilon')^2 \right. \\ \left. + \left[\frac{1}{2(pk)(pk')} ((\epsilon k')^2(kp) + (\epsilon' k)^2(k'p) - (kk')(k'p)) + (\epsilon \leftrightarrow \epsilon', k \leftrightarrow k') \right] \right\}. \end{aligned}$$

The bracket is, explicitly,

$$\frac{1}{2(pk)(pk')} \{ (kk')[(kp) - (k'p)] \}, \quad (12A.17)$$

which can be simplified to

$$\frac{1}{2(pk)(pk')} (kk')^2, \quad (12A.18)$$

using the equation

$$kk' = k(p + k - p') = kp - kp' = kp - k'p. \quad (12A.19)$$

Thus we obtain [34]

$$F = \frac{1}{2M^2} \left[\frac{(k'k)^2}{(pk)(pk')} + 4(\epsilon'\epsilon)^2 \right]. \quad (12A.20)$$

In the laboratory frame where

$$pk' = M\omega', \quad pk = M\omega, \quad (12A.21)$$

and Compton's relation ensures that (12.264),

$$k'k = \omega'\omega(1 - \cos\theta) = M\omega'\omega \left(\frac{1}{\omega'} - \frac{1}{\omega} \right) = M(\omega - \omega'),$$

$$pk' = M\omega', \quad pk = M\omega, \quad (12A.22)$$

and expression (12A.20) reduces to (12.254).

In the electron-positron annihilation process, the trace in Eq. (12.289) becomes

$$F = \frac{1}{M^2} \left[\frac{t_1^8 - M^2 t_1^6}{(2pk)^2} + \frac{t_2^8 - M^2 t_2^6}{(2pk)(2p'k')} + (\epsilon \leftrightarrow \epsilon', k \leftrightarrow k') \right], \quad (12A.23)$$

and we find, after the replacement $p' = k + k' - p$,

$$F = \frac{1}{2M^2} \left\{ \frac{(k'k)[(kp) + (k'p)]}{(kp)(k'p)} - 4(\epsilon'\epsilon)^2 \right\}. \quad (12A.24)$$

Inserting (12.305) and using $kp = \omega M$ and $k'p = \omega' M$, this becomes

$$F = \frac{1}{2M^2} \left[\frac{(k'k)^2}{4(kp)(k'p)} - 4(\epsilon'\epsilon)^2 \right], \quad (12A.25)$$

instead of (12A.20), thus yielding Eq. (12.290) which we wanted to derive.

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*If you lose the path
you get to know it better.*
TANZANIAN PROVERB

13

Formal Properties of Perturbation Theory

In Chapter 10 we have observed simple composition rules which help to construct all Feynman diagrams of a field theory from connected diagrams which, in turn, can be decomposed in a simple way into one-particle irreducible ones. These composition rules can be derived by applying simple functional operations upon certain generating functionals [1, 2].

13.1 Connectedness Structure of Feynman Diagrams

In view of the applications to come, we write the action in a rather general form

$$\mathcal{A}[\varphi] = \mathcal{A}^0[\varphi] + \mathcal{A}^{\text{int}}[\varphi], \quad (13.1)$$

with a free action

$$\mathcal{A}^0[\varphi] = \frac{1}{2} \int d^D x' d^D x \varphi(x) iG_0^{-1}(x', x) \varphi(x) \quad (13.2)$$

and an interaction

$$\begin{aligned} \mathcal{A}^{\text{int}}[\varphi] = & -\frac{1}{3!} \int d^D x_1 d^D x_2 d^D x_3 V_3(x_1, x_2, x_3) \varphi(x_1) \varphi(x_2) \varphi(x_3) \\ & -\frac{1}{4!} \int d^D x_1 d^D x_2 d^D x_3 d^D x_4 V_4(x_1, x_2, x_3, x_4) \varphi(x_1) \varphi(x_2) \varphi(x_3) \varphi(x_4). \end{aligned} \quad (13.3)$$

In the relativistic scalar theory discussed in the previous chapter, the operator iG_0^{-1} between the φ -fields had the specific form

$$iG_0^{-1}(x, x') = \delta^{(D)}(x - x')(-\partial^2 - m^2). \quad (13.4)$$

We shall find it convenient to introduce a short notation and write (13.2) as

$$\mathcal{A}^0[\varphi] = \frac{1}{2} \varphi iG_0^{-1} \varphi. \quad (13.5)$$

Here the fields are considered as vectors with continuous indices x , whereas $G_0^{-1}(x, x')$ is a corresponding matrix. Such objects will be referred to as functional

vectors and matrices, respectively. This notation will permit an immediate adaptation of all formulas to many different field theories. With x being considered as a functional index, $V_3(x_1, x_2, x_3)$ and $V_4(x_1, x_2, x_3, x_4)$ may be viewed as functional tensors which are symmetric in all indices. We can save many integral symbols by rewriting (13.3) by analogy with (13.5) in the short form

$$\mathcal{A}^{\text{int}}[\varphi] = -\frac{1}{3!}V_3\varphi^3 - \frac{1}{4!}V_4\varphi^4, \quad (13.6)$$

where the successive contraction of the functional indices x_1, x_2, x_3, x_4 is tacitly implied.

For the above general action and in this notation, the Heisenberg field operator φ satisfies an equation of motion

$$iG_0^{-1}\varphi + \frac{\delta\mathcal{A}^{\text{int}}[\varphi]}{\delta\varphi} = 0, \quad (13.7)$$

or explicitly

$$iG_0^{-1}\varphi(x) - \frac{V_3}{2!}\varphi^2 - \frac{V_4}{3!}\varphi^3 = 0. \quad (13.8)$$

13.2 Functional Differential Equations

The operator equation (13.8) can be used to derive a differential equation for the generating functional $Z[j]$ of the theory defined in Eq. (7.840). In the functional vector notation introduced above, we shall write the generating functional as

$$Z[j] = \langle Te^{ij\varphi} \rangle. \quad (13.9)$$

In order to apply (13.8), we form the derivative

$$\frac{\delta}{i\delta j}Z[j] = \langle T\varphi e^{ij\varphi} \rangle \quad (13.10)$$

and multiply this by the functional matrix iG_0^{-1} . When passing iG_0^{-1} to the right-hand side of the time-ordering operator, we generate the φ^2 - and φ^3 -terms of (13.8). These can also be obtained from higher derivatives $(\delta/\delta j)^2$ and $(\delta/\delta j)^3$ applied to $Z[j]$. The passage through the time-ordering operator produces some additional terms in the same way as in the derivation of the equations (7.43)–(7.45) for the Green functions. Its calculation requires the use of canonical equal-time commutation rules. Since these are the same for interacting and free fields, we can evaluate them for the free fields and consider taking iG_0^{-1} to the right of the time-ordering operator in the free-field expression

$$iG_0^{-1} \frac{\delta}{i\delta j} Z_0[j]. \quad (13.11)$$

The free partition function was calculated in Section 7.18. In Eqs. (7.843) and (7.844) we found

$$Z^0[j] = e^{-\frac{1}{2}j G_0 j}, \quad (13.12)$$

satisfying the functional differential equation

$$iG_0^{-1} \frac{\delta}{i\delta j(x)} Z^0[j] + j(x) Z^0[j] = 0. \quad (13.13)$$

The generalization to the interacting case follows directly by adding the interaction terms of (13.8) expressed in terms of derivatives with respect to the current:

$$\left[iG_0^{-1} \frac{\delta}{i\delta j} - \frac{V_3}{2!} \left(\frac{\delta}{i\delta j} \right)^2 - \frac{V_4}{3!} \left(\frac{\delta}{i\delta j} \right)^3 + j \right] Z[j] = 0. \quad (13.14)$$

For the subsequent development it is useful to introduce the short-hand notation

$$\frac{\delta}{i\delta j} \frac{\delta}{i\delta j} \cdots \frac{\delta}{i\delta j} Z[j] = Z_{jj\dots j}[j], \quad (13.15)$$

with the arguments $x_1, \dots, x_n$ of the currents suppressed. Then we may write (13.14) as

$$iG_0^{-1} \frac{1}{i} Z_j - \frac{V_3}{2!} \frac{1}{i^2} Z_{jj} - \frac{V_4}{3!} \frac{1}{i^3} Z_{jjj} + jZ = 0. \quad (13.16)$$

This equation can be used to calculate $Z[j]$ recursively. However, we have seen in the previously discussed example of the φ^4 -theory, that $Z[j]$ is not a very economic quantity to deal with. Its expansion coefficients, the n -point Green functions, contain many disconnected pieces. A substantial simplification arises by going over to the functional $iW[j]$ defined by

$$iW[j] = \log Z[j]. \quad (13.17)$$

It serves as a generating functional for the connected part of the Green functions which are obtained from

$$G_c^{(n)}(x_1, \dots, x_n) = \frac{\delta}{i\delta j(x_1)} \cdots \frac{\delta}{i\delta j(x_n)} iW[j]. \quad (13.18)$$

Using the differential equation (13.16) we are able to prove quite generally that these Green functions do deserve their name since their graphical representation consists only of connected diagrams. The connected Green functions collect precisely all the connected diagrams in $G^{(n)}(x_1, \dots, x_n)$.

Conversely, given all connected Green functions $G_c^{(n)}(x_1, \dots, x_n)$, the full Green functions $G^{(n)}(x_1, \dots, x_n)$ can be recovered in a simple way. We prove this by deriving the general relationship between the two types of Green functions. This relationship serves to transform the functional differential equation (13.16) for $Z[j]$ into a more useful equation for $W[j]$, and showing that its functional derivatives render precisely all connected Green functions $G_c^{(n)}(x_1, \dots, x_n)$.

13.3 Decomposition of Green Functions into Connected Green Functions

Using the exponential relation (13.17) between iW and Z we can now derive general relations between the n -point functions and the connected ones. For the one-point function we find

$$G^{(1)}(x) = Z^{-1}[j] \frac{\delta}{i\delta j(x)} Z[j] = \frac{\delta}{\delta j} W[j] = G_c^{(1)}(x). \quad (13.19)$$

Thus the one-point function, which represents the ground state expectation value of the field, is always connected:

$$\langle \varphi(x) \rangle \equiv G^{(1)}(x) = G_c^{(1)}(x). \quad (13.20)$$

We may convince ourselves that this is indeed true by drawing the Feynman diagrams corresponding to the formula

$$G^{(1)}(x) = \frac{\langle 0 | T \varphi(x) e^{i\mathcal{A}_{\text{int}}^{[\varphi]} + j\varphi} | 0 \rangle}{\langle 0 | T e^{i\mathcal{A}_{\text{int}}^{[\varphi]}} | 0 \rangle}. \quad (13.21)$$

All disconnected pieces cancel when forming the quotient.

Consider now the two-point function where

$$\begin{aligned} G^{(2)}(x_1, x_2) &= Z^{-1}[j] \frac{\delta}{i\delta j(x_1)} \frac{\delta}{i\delta j(x_2)} Z[j] \\ &= Z^{-1}[j] \frac{\delta}{i\delta j(x_1)} \left\{ \left(\frac{\delta}{i\delta j(x_2)} iW[j] \right) Z[j] \right\} \\ &= Z^{-1}[j] \left\{ \frac{1}{i} W_{j(x_1)j(x_2)} + W_{j(x_1)} W_{j(x_2)} \right\} Z[j] \\ &= G_c^{(2)}(x_1, x_2) + G_c^{(1)}(x_1) G_c^{(1)}(x_2). \end{aligned} \quad (13.22)$$

In addition to the connected diagrams with two ends there are two connected diagrams ending in a single line. These are absent in a pure φ^4 -theory at $j = 0$ if the ground state of the system is normal, a specification which we are going to understand only later when discussing phase transitions.

For the three-point function we find

$$\begin{aligned} G^{(3)}(x_1, x_2, x_3) &= Z^{-1}[j] \frac{\delta}{i\delta j(x_1)} \frac{\delta}{i\delta j(x_2)} \frac{\delta}{i\delta j(x_3)} Z[j] \\ &= Z^{-1}[j] \frac{\delta}{i\delta j(x_1)} \frac{\delta}{i\delta j(x_2)} \left\{ \left[\frac{\delta}{i\delta j(x_3)} iW[j] \right] Z[j] \right\} \\ &= Z^{-1}[j] \frac{\delta}{i\delta j(x_1)} \left\{ \left[\frac{1}{i} W_{j(x_2)j(x_3)} + W_{j(x_2)} W_{j(x_3)} \right] Z[j] \right\} \\ &= Z^{-1}[j] \left\{ \frac{1}{i^2} W_{j(x_1)j(x_2)j(x_3)} + i \left(W_{j(x_1)} W_{j(x_2)j(x_3)} + W_{j(x_2)} W_{j(x_1)j(x_3)} \right. \right. \\ &\quad \left. \left. + W_{j(x_3)} W_{j(x_1)j(x_2)} \right) + W_{j(x_1)} W_{j(x_2)} W_{j(x_3)} \right\} Z[j] \\ &= G_c^{(3)}(x_1, x_2, x_3) + \left[G_c^{(1)}(x_1) G_c^{(2)}(x_2, x_3) + 2 \text{ perm} \right] + G_c^{(1)}(x_1) G_c^{(1)}(x_2) G_c^{(1)}(x_3), \end{aligned} \quad (13.23)$$

and for the four-point function

$$\begin{aligned}
G^{(4)}(x_1, \dots, x_4) &= G_c^{(4)}(x_1, \dots, x_4) + [G_c^{(3)}(x_1, x_2, x_3) G_c^{(1)}(x_4) + 3 \text{ perm}] \\
&+ [G_c^{(2)}(x_1, x_2) G_c^{(2)}(x_3, x_4) + 2 \text{ perm}] \\
&+ [G_c^{(2)}(x_1, x_2) G_c^{(1)}(x_3) G_c^{(1)}(x_4) + 4 \text{ perm}] \\
&+ G_c^{(1)}(x_1) \cdots G_c^{(1)}(x_4).
\end{aligned} \tag{13.24}$$

In the pure φ^4 -theory (and in normal systems) there are no odd Green functions and we remain with (10.73), which was observed there diagrammatically up to second order in the perturbation expansion.

For the general Green function $G^{(n)}$, the total number of terms is most easily retrieved by dropping all indices and factors i and differentiating with respect to j (the prime stands for $\delta/\delta j$)

$$\begin{aligned}
G^{(1)} &= e^{-W} (e^W)_j = W_j = G_c^{(1)} \\
G^{(2)} &= e^{-W} (e^W)_{jj} = W_{jj} + W_j^2 = G_c^{(2)} + G_c^{(1)2} \\
G^{(3)} &= e^{-W} (e^W)_{jjj} = W_{jjj} + 3W_{jj}W_j + W_j^3 = G_c^{(3)} + 3G_c^{(2)}G_c^{(1)} + G_c^{(1)3} \\
G^{(4)} &= e^{-W} (e^W)_{jjjj} = W_{jjjj} + 4W_{jjj}W_j + 3W_{jj}^2 + 6W_{jj}W_j^2 + W_j^4 \\
&= G_c^{(4)} + 4G_c^{(3)}G_c^{(1)} + 3G_c^{(2)2} + 6G_c^{(2)}G_c^{(1)2} + G_c^{(1)4}.
\end{aligned} \tag{13.25}$$

All relations follow from the recursion relation

$$G^{(n)} = G_j^{(n-1)} + G^{(n-1)}G_c^{(1)}, \quad n > 2, \tag{13.26}$$

after setting $G_{cj}^{(n-1)} = G_c^{(n)}$ and using the initial relation $G^{(1)} = G_c^{(1)}$.

If we compare the first four relations with the explicit equations (13.22)–(13.24), we see that the numerical factors on the right-hand side of (13.25) refer to the permutations of the arguments $x_1, x_2, x_3, \dots$ of otherwise equal expressions. Since there is no problem in reconstructing the explicit permutations, we shall write from now on all composition laws in the short-hand notation (13.25).

The formula (13.25) and its generalization is often referred to as *cluster decomposition* or also as the *cumulant expansion* of the Green functions.

Let us now prove the statement that the connected Green functions collect precisely all connected diagrams contained in the n -point functions. For this we observe that the decomposition rules can be inverted by simply writing $iW[j] = \log Z[j]$ and by functionally differentiating this equation repeatedly with respect to j . This leads to the sequence of equations:

$$\begin{aligned}
G_c^{(1)} &= G^{(1)} \\
G_c^{(2)} &= G^{(2)} - G^{(1)}G^{(1)} \\
G_c^{(3)} &= G^{(3)} - 3G^{(2)}G^{(1)} + 2G^{(1)3} \\
G_c^{(4)} &= G^{(4)} - 4G^{(3)}G^{(1)} + 12G^{(2)}G^{(1)2} - 3G^{(2)2} - 6G^{(1)4}.
\end{aligned} \tag{13.27}$$

Each equation follows from the previous one by differentiation with respect to j , and replacing the derivatives on the right-hand side according to the rule

$$G_j^{(n)} = G^{(n+1)} - G^{(n)}G^{(1)}. \quad (13.28)$$

As before, the numerical factors imply different permutations of the arguments, and the primes denote functional differentiations with respect to j .

Now it is obvious that any connected diagram contained in $G^{(n)}$ must also be contained in $G_c^{(n)}$, since all added or subtracted terms in (13.27) are products of $G^{(n)}$'s and thus necessarily disconnected.

The proof that $G_c^{(n)}$ collects *only* connected diagrams, is somewhat more involved and requires the use of the equations of motion (13.8). Since the information on G_c is contained most directly in $W[j]$, we shall first translate the equations of motion into a functional differential equation for $W[j]$.

13.4 Functional Differential Equation for $W[j]$

Since we already know the consequences of the equation of motion for $Z[j]$ we may simply insert (13.17) into (13.16) and find directly the following differential equation for $W[j]$:

$$iG_0^{-1}W_j - \frac{1}{2!}V_3\frac{1}{i^2}\left(iW_{jj} - W_j^2\right) - \frac{1}{3!}V_4\frac{1}{i^3}\left(iW_{jjj} - 3W_{jj}W_j - iW_j^3\right) + j = 0. \quad (13.29)$$

Multiplying this by $-iG_0$ gives

$$W_j = -iG_0\frac{1}{2!}V_3\frac{1}{i^2}\left(iW_{jj} - W_j^2\right) - iG_0\frac{1}{3!}V_4\frac{1}{i^3}\left(iW_{jjj} - 3W_{jj}W_j - iW_j^3\right) + iG_0j. \quad (13.30)$$

This may be expressed in terms of the connected Green function

$$G_c^{(1)} = W_j(x) \quad (13.31)$$

and its functional derivatives with respect to j as

$$\begin{aligned} G_c^{(1)} &= -G_0\frac{V_3}{2!}\left(G_{cj}^{(1)} + iG_c^{(1)}G_c^{(1)}\right) \\ &\quad + G_0\frac{V_4}{3!}\left(iG_{cjj}^{(1)} - 3G_{cj}^{(1)}G_c^{(1)} - iG_c^{(1)3}\right) + iG_0j. \end{aligned} \quad (13.32)$$

13.5 Iterative Solution

Equation (13.30) can best be solved graphically as shown in Fig. 13.1. To lowest,

$$\begin{aligned}
\text{---}\bigcirc &= -\frac{1}{2!} \left(\text{---}\bigcirc\bigcirc + i \text{---}\bigcirc\bigcirc \right) \\
&+ \frac{1}{3!} \left(\text{---}\bigcirc\bigcirc - 3 \text{---}\bigcirc\bigcirc - i \text{---}\bigcirc\bigcirc \right) + i \text{---}\bigotimes \\
\\
\curvearrowright \text{---}\bigcirc &= i \text{---}\bigotimes - \frac{1}{2!} \left(i \text{---}\bigcirc - i \text{---}\bigcirc\bigcirc \right) + \frac{1}{3!} \left(3 \text{---}\bigcirc\bigcirc - i \text{---}\bigcirc\bigcirc \right) + \dots \\
\curvearrowright W[j] &= \frac{i}{2} \bigotimes\bigotimes - \frac{i}{2!} \bigotimes\bigcirc + \frac{i}{3!} \bigotimes\bigcirc\bigcirc + \frac{1}{4} \bigotimes\bigcirc\bigcirc - \frac{1}{24} \bigotimes\bigotimes\bigotimes + \dots \\
\\
\text{---}\bigcirc &= G_c^{(1)} = W[j] \\
\\
\begin{array}{c} n \\ \diagup \quad \diagdown \\ \diagdown \quad \diagup \\ 1 \quad 2 \quad 3 \end{array} &= G_c^{(1)} j \dots j = i^{n-1} G_c^{(n)} \\
\\
\text{---} &= G_0 \quad \bigtimes = V_4 \\
\text{---} &= V_3 \quad \text{---}\bigotimes = i
\end{aligned}$$

FIGURE 13.1 Graphical solution of the recursion relation (13.30) for the generating functional $W[j]$ of all connected Green functions.

i.e., zeroth order in V_3 and V_4 , we have¹

$$G_c^{(1)} = iG_0 j. \quad (13.33)$$

From this we find the zeroth order generating functional $W[j]$ by functional integration

$$W^0[j] = \int \mathcal{D}j W_j^{(0)}[j] = \int \mathcal{D}j G_c^{(1)} = \frac{i}{2} j G_0 j, \quad (13.34)$$

a result already known from previous discussions.

Reinserting (13.34) on the right-hand side of (13.32) we find the first-order equation

$$G_c^{(1)} = -G_0 \frac{V_3}{2!} (iG_0 - iG_0 j G_0 j) + G_0 \frac{V_4}{3!} [3G_0 G_0 j - (G_0 j)^3] + iG_0 j. \quad (13.35)$$

This can be integrated functionally to obtain $W[j]$ up to first order in the potentials. Graphically, this process amounts to multiplying the open line in each diagram by a current j and dividing the resulting powers j^n by n . Thus we have (see Fig. 13.1)

$$W^0[j] + W^1[j] = \frac{i}{2} j G_0 j - \frac{i}{2!} j G_0 V_3 G_0 + \frac{i}{3!} V_3 (G_0 j)^3$$

¹The superscripts (1), (2), ... of Green functions $G_c^{(1)}$, $G_c^{(2)}$, ... refer to the number of points in the connected Green function. This is in contrast to the superscripts 1, 2, ... of W^1 , W^2 , ... which record the order in the interactions $V_{3,4}$ of the perturbative expressions for $W[j]$.

$$+ \frac{1}{4} V_4 G_0 (G_0 j)^2 - \frac{1}{24} V_4 (G_0 j)^4. \quad (13.36)$$

This procedure can be continued to any order in V_3 and V_4 .

We are now in a position to confirm the statement made above that the generating functional $W[j]$ collects *only* connected diagrams in its Taylor coefficients $\delta^n W / \delta j(x_1) \dots \delta j(x_n)$. Recall that we convinced ourselves by the argument after Eq. (13.28) that these were *all* connected diagrams contained in $G^{(n)}(x_1, \dots, x_n)$. For the lowest two orders we can verify the connectedness directly by inspecting the third line in Fig. 13.1. After this, the diagrammatic form of the recursion relation shows that this topological property remains true to all orders in $V_{3,4}$, by induction. Indeed, if it was true for some n , then all $G_c^{(1)}$ to be inserted on the right-hand side are connected, and so are the diagrams constructed from these giving $G_c^{(1)}$ to $(n+1)$ st order. Note that this calculation is unable to recover the value of $W[j]$ at $j=0$ since this is an unknown integration constant of the functional differential equation. For the purpose of generating Green functions, this constant is irrelevant. We have seen in Eq. (10.81) that $Z[0]$ consists of the sum of all connected vacuum diagrams contained in $W[0]$.

13.6 Vertex Functions

Having understood the connectedness structure of Feynman diagrams, we now turn to the second important property, the significance of one-particle irreducible graphs. We remind the reader of the crucial role in the perturbation expansions of Chapter 10 played by the vertex functions, which are the one-particle irreducible amputated Green functions introduced in Subsection 10.6.1. Here we shall describe their properties by functional differential equations. In particular, we shall present a simple algorithm yielding the composition rules of connected diagrams into one-particle irreducible ones.

13.7 The Generating Functional for Vertex Functions

First we introduce a new generating functional $\Gamma[\Phi]$ which is defined as the Legendre transform of $W[j]$:

$$\Gamma[\Phi] \equiv W[j] - W_j j, \quad (13.37)$$

where $W_j j$ is a short-hand notation for

$$W_j j = \int d^D x W_j(x) j(x), \quad (13.38)$$

and the new variable Φ is the functional derivative of $W[j]$:

$$\Phi(x) \equiv \frac{\delta W[j]}{\delta j(x)} \equiv W_j = \langle \varphi \rangle_j. \quad (13.39)$$

It gives the ground state expectation of the interacting field operator in the presence of the current j . The physical situation corresponds to $j = 0$ and we shall denote the associated field expectation by

$$\Phi_0 = \langle \varphi \rangle|_{j=0}, \quad (13.40)$$

which may be zero or non-zero and space-time dependent. The most common situation found in quantum field theoretic systems is $\Phi_0 = 0$. In many interesting physical applications to many-body systems, however, the state Φ_0 at $j = 0$ is non-zero and in fact, not even isotropic, but it carries interesting structures: It may be perforated by vortices, as in superconductors, exhibit a plane wave-like modulation, as in magnetic superconductors and pion condensates, or occur in a lattice-like modulation, as in the blue phase of cholesteric liquid crystals. At present we shall allow any such possibility.

In this section we want to demonstrate an important property of the functional derivatives of $\Gamma[\Phi]$, to be denoted by

$$\Gamma_{\Phi \dots \Phi}^{(n)}(x_1, \dots, x_n) \equiv \frac{\delta}{\delta \Phi(x_1)} \dots \frac{\delta}{\delta \Phi(x_n)} \Gamma[\Phi]. \quad (13.41)$$

They collect precisely all OPI vertex diagrams formed with vertices $V_3 + V_4\Phi$ and V_4 , connected by propagators $G_c^{(2)} \equiv \mathcal{A}_{\Phi\Phi}^{-1}$. The expression $V_4\Phi$ is the short notation for $\int d^D x V_4(x_1, x_2, x_3, x_4)\Phi(x_4)$. In the previously discussed special case of a φ^4 -theory with $\Phi_0 = \langle \varphi \rangle = 0$, the vertex functions (13.41) for $\Phi = 0$ coincide with those defined graphically in Eq. (10.6.1), for example.

In order to prove this, we employ a functional differential equation for $\Gamma[\Phi]$. This can be derived quite simply from that for $W[j]$. First we observe that $G_c^{(1)}$ is simply the field expectation Φ . Second we see that

$$iG_c^{(2)} = G_j^{(1)} = W_{jj} = \frac{\delta \Phi}{\delta j} = \left(\frac{\delta j}{\delta \Phi} \right)^{-1} = -\Gamma_{\Phi\Phi}^{-1}. \quad (13.42)$$

Here the inverse is to be understood in the functional sense, i.e.,

$$\Gamma_{\Phi\Phi}^{-1}(x, y) \equiv \left[\frac{\delta^2 \Gamma}{\delta \Phi(x) \delta \Phi(y)} \right]^{-1} \quad (13.43)$$

is the functional matrix that satisfies

$$\int dy \Gamma_{\Phi\Phi}^{-1}(x, y) \Gamma_{\Phi\Phi}(y, z) = \delta(x - z). \quad (13.44)$$

Equation (13.42) says that the second derivative of the generating functional $\Gamma[\Phi]$ determines directly the propagator of the interacting theory in the presence of the external source j . Since j is an auxiliary quantity which eventually has to be turned off such that Φ becomes Φ_0 , the actual physical propagator is given by

$$G = G_c^{(2)} = i\Gamma_{\Phi\Phi}^{-1}, \quad (13.45)$$

evaluated at $\Phi = \Phi_0$. The third relation to be used follows from (13.42) by deriving W_{jj} once more functionally with respect to j and applying the chain rule to find

$$W_{jjj} = \Gamma_{\Phi\Phi}^{-2} \Gamma_{\Phi\Phi\Phi} \frac{\delta\Phi}{\delta j} = -\Gamma_{\Phi\Phi}^{-3} \Gamma_{\Phi\Phi\Phi} = -iG^3 \Gamma_{\Phi\Phi\Phi}. \quad (13.46)$$

This equation has a simple physical meaning. The third derivative of $W[j]$ on the left-hand side is the full three-point function (up to the sign), so that

$$G^{(3)} = -W_{jjj} = iG^3 \Gamma_{\Phi\Phi\Phi}. \quad (13.47)$$

This equation states that the full three-point function arises from a third derivative of $\Gamma[\Phi]$ by attaching to each derivation a full propagator. This is exactly the structure observed before in (10.86) for the four-point function.

We shall express Eq. (13.52) graphically as follows:

$$\text{Diagram: a circle with three external lines} = i \text{ Diagram: a shaded circle with three external lines}$$

where

$$\text{Diagram: a circle with } n \text{ external lines labeled } 1, 2, \dots, n \equiv G_c^{(n)}$$

denotes the connected n -point function and

$$\text{Diagram: a shaded circle with } n \text{ external lines labeled } 1, 2, \dots, n \equiv \Gamma_{\Phi_1 \dots \Phi_n}$$

the n -point vertex function.

Thus $\Gamma_{\Phi\Phi\Phi}$ seems to be a three-point vertex function in the same sense as defined graphically in Subsection 10.6.1. For this it has to contain all OPI diagrams. This will emerge from the discussion to follow.

To go on to higher orders, we observe that (13.46) states that the functional derivative of the full propagator G with respect to the current j is

$$\frac{1}{i} G_j = -W_{jjj} = G^{(3)} = iG^3 \Gamma_{\Phi\Phi\Phi}. \quad (13.48)$$

This is pictured graphically as follows:

$$\frac{d}{i dj} \text{Diagram: a circle with one external line} = i \text{ Diagram: a shaded circle with three external lines}.$$

This equation may be differentiated further with respect to the current j by graphical methods. From the definition (13.18) we deduce the trivial recursion relation

$$G_c^{(n)}(x_1, \dots, x_n) = \frac{\delta}{i\delta j(x_1)} G_c^{(n-1)}(x_2, \dots, x_n), \quad (13.49)$$

which is represented graphically as

$$\frac{d}{i\delta j} \begin{array}{c} n \quad n-1 \\ \diagup \quad \diagdown \\ \circ \\ \diagdown \quad \diagup \\ 1 \quad 2 \end{array} \vdots = \begin{array}{c} n+1 \quad n \quad n-1 \\ \diagup \quad \diagdown \quad \diagup \\ \circ \\ \diagdown \quad \diagup \quad \diagdown \\ 1 \quad 2 \end{array} \vdots \quad n > 2.$$

Thus, by applying $\delta/i\delta j$ repeatedly to Eq. (13.48), we generate all higher connected Green functions. On the right-hand side of (13.48), the differentiation of each line is done using once more (13.48), which changes a line into a three-point function. It remains to find the derivative of the vertex function. This is calculated via the chain rule as

$$\Gamma_{\Phi \dots \Phi j} = \Gamma_{\Phi \dots \Phi \Phi} \frac{\delta \Phi}{\delta j} = \Gamma_{\Phi \dots \Phi \Phi} iG, \quad (13.50)$$

which is represented graphically as

$$\frac{d}{i\delta j} \begin{array}{c} n \quad n-1 \\ \diagup \quad \diagdown \\ \text{\textcircled{X}} \\ \diagdown \quad \diagup \\ 1 \quad 2 \end{array} \vdots = \begin{array}{c} n+1 \quad n \quad n-1 \\ \diagup \quad \diagdown \quad \diagup \\ \text{\textcircled{X}} \\ \diagdown \quad \diagup \quad \diagdown \\ 1 \quad 2 \end{array} \vdots.$$

With these graphical rules, we can differentiate (13.46) any number of times, and derive the graphical structure of the connected Green functions with an arbitrary number of external legs. The result up to $n = 5$ is shown in Fig. 13.2.

The diagrams generated in this way have a tree-like structure which is why they are called *tree diagrams*. The tree decomposition reduces all diagrams to their one-particle irreducible contents.

The one-particle reducible structure of all graphs can be illustrated in another way. Let us separate the effective action into a free and a nontrivial part

$$\begin{aligned} \Gamma[\Phi] &\equiv \Gamma^0[\Phi] + \Gamma^{\text{int}}[\Phi] = \frac{1}{2}(\partial\Phi)^2 - \frac{m^2}{2}\Phi^2 + \Gamma^{\text{int}}[\Phi] \\ &= \frac{1}{2}\Phi iG_0^{-1}\Phi + \Gamma^{\text{int}}[\Phi]. \end{aligned} \quad (13.51)$$

The free part coincides with the free action $\mathcal{A}^0[\Phi]$ in Eq. (13.2), except that the fluctuating field φ is replaced by its expectation value Φ . The same decomposition is done with the generating functional $W[j]$ [recall (13.34)]:

$$W[j] = W^0[j] + W^{\text{int}}[j] = \frac{i}{2}j G_0 j + W^{\text{int}}[j]. \quad (13.52)$$

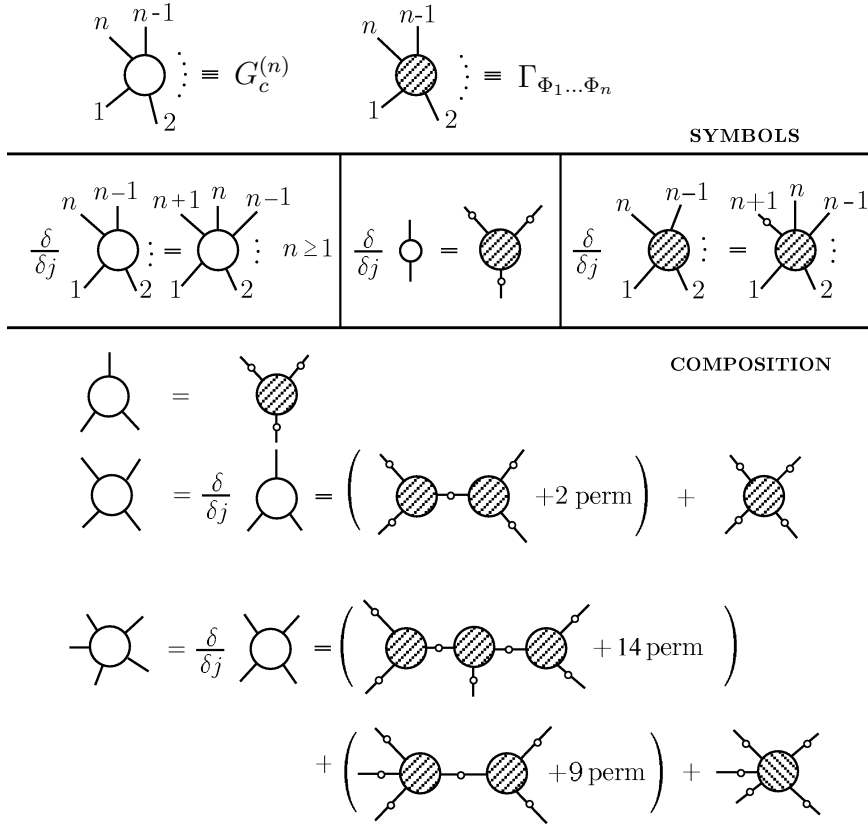


FIGURE 13.2 Tree decomposition of connected Green functions into one-particle irreducible parts.

Then we see that

$$\begin{aligned} \Gamma^{\text{int}}[\Phi] &= W^{\text{int}}[j] - \frac{i}{2} \Phi G_0^{-1} \Phi \\ &\quad + \frac{i}{2} j G_0 j - j \Phi. \end{aligned} \quad (13.53)$$

But using the equation for the current

$$j = -\Gamma_{\Phi} = -\Gamma_{\Phi}^{\text{int}} - i G_0^{-1} \Phi \quad (13.54)$$

we find

$$\frac{i}{2} \Gamma_{\Phi}^{\text{int}} G_0 \Gamma_{\Phi}^{\text{int}} = \frac{i}{2} j G_0 j - \frac{i}{2} \Phi G_0^{-1} \Phi - j \Phi, \quad (13.55)$$

which is obviously a one-particle reducible contribution. Inserting this into (13.53), we may write

$$W^{\text{int}}[j] = \Gamma^{\text{int}}[\Phi] - \frac{i}{2} \Gamma_{\Phi}^{\text{int}} G_0 \Gamma_{\Phi}^{\text{int}}. \quad (13.56)$$

This equation shows explicitly how the sum of all connected diagrams in $W^{\text{int}}[j]$ is composed of all one-particle *irreducible* connected diagrams in $\Gamma^{\text{int}}[\Phi]$ plus all one-particle *reducible* diagrams.

The effective action $\Gamma[\Phi]$ can also be used to prove the fact that the full propagator can be expressed as a geometric series (10.85) of repetitions of the self-energy, a fact that was observed graphically to low orders in Subsection 10.6.1. We take once more the decomposition (13.51):

$$\Gamma[\Phi] = \Gamma^0[\Phi] + \Gamma^{\text{int}}[\Phi]. \quad (13.57)$$

Differentiating this twice with respect to Φ , we obtain

$$\begin{aligned} \Gamma_{\Phi\Phi} &= iG_0^{-1} + \Gamma_{\Phi\Phi}^{\text{int}}, \\ \Gamma_{\Phi\Phi\Phi} &= \Gamma_{\Phi\Phi\Phi}^{\text{int}}, \end{aligned} \quad (13.58)$$

and (13.45) can be rewritten as

$$G = G_0 \left(1 - iG_0 \Gamma_{\Phi\Phi}^{\text{int}} \right)^{-1}. \quad (13.59)$$

Expanding the denominator and recollecting terms, this can also be written as an integral equation

$$G = G_0 + iG_0 \Gamma_{\Phi\Phi}^{\text{int}} G. \quad (13.60)$$

In this equation we recognize the self-energy

$$\Sigma = -\Gamma_{\Phi\Phi}^{\text{int}}. \quad (13.61)$$

This was introduced graphically in Eq. (10.85), where it was *defined* by the relation

$$G \equiv i[G_0^{-1} - \Sigma]^{-1}, \quad \Sigma \equiv iG_0^{-1} - iG^{-1}. \quad (13.62)$$

Comparison with (13.59) shows that (13.61) is the correct identification.

Thus the self-energy is given by the interacting part of the second derivative of the effective action. This proves the statement that, in general, all Feynman diagrams in the propagator can be obtained by a geometric series type of repetition of self-energy diagrams. What we do not know as yet, but what will become clear immediately in the next section, is the fact that the self-energy collects precisely all one-particle irreducible amputated two-point functions.

13.8 Functional Differential Equation for $\Gamma[\Phi]$

We shall now prove the fact that $\Gamma[\Phi]$ contains only one-particle irreducible diagrams by means of a functional differential equation for $\Gamma[\Phi]$. For a cubic and quartic interaction, this is immediately obtained from the differential equation (13.29) for $W[j]$. We simply substitute

$$W_j \rightarrow \Phi, \quad j \rightarrow \Gamma_\Phi, \quad W_{jj} \rightarrow iG, \quad W_{jjj} \rightarrow -G^{(3)} = -iG^3 \Gamma_{\Phi\Phi\Phi}, \quad (13.63)$$

make use of the separation (13.57), and find for the interacting part the functional differential equation

$$\Phi \Gamma_{\Phi}^{\text{int}} = -\frac{1}{2!} V_3 \Phi^3 - \frac{1}{3!} V_4 \Phi^4 - \frac{1}{2!} \Phi (V_3 + V_4 \Phi) G - \frac{1}{3!} \Phi V_4 i G^3 \Gamma_{\Phi\Phi\Phi}^{\text{int}}. \quad (13.64)$$

This equation can be solved iteratively together with (13.59). Before starting, it is useful to observe that there exists a trivial relation between $\Gamma[\Phi]$ and $\Phi \Gamma_{\Phi}^{\text{int}}$ which merely consists in a factor $1/n$ in front of every power Φ^n . Thus the diagrams in $\Gamma[\Phi]$ differ from those in $\Phi \Gamma[\Phi]$ only by numerical prefactors. The resulting equations are displayed graphically in Fig. 13.3. First we neglect Γ^{int} on the right-hand side of the equation and find the first-order correction $\Gamma^1[\Phi]$ to the interacting part $\Gamma^{\text{int}}[\Phi]$:

$$\Gamma^1[\Phi] = -\frac{1}{3!} V_3 \Phi^3 - \frac{1}{4!} V_4 \Phi^4 - \frac{1}{2} V_3 G_0 \Phi - \frac{1}{4} V_4 G_0 \Phi^2. \quad (13.65)$$

The first two terms are simply the interacting parts of the original action $\mathcal{A}^{\text{int}}[\Phi]$ (13.3), with φ replaced by Φ . The remaining two terms are new. They may be obtained by partial contractions in the interacting part of the original interaction (13.3), and by setting $\varphi = \Phi$ in the remaining uncontracted fields:

$$\begin{aligned} -\frac{1}{3!} V_3 \varphi^3 &\rightarrow -\frac{1}{3!} V_3 3 \varphi \overline{\varphi} \varphi \Phi, \\ -\frac{1}{4!} V_4 \varphi^4 &\rightarrow -\frac{1}{4!} V_4 \frac{4 \cdot 3}{2!} \varphi \overline{\varphi} \varphi \Phi. \end{aligned} \quad (13.66)$$

The iteration has been continued graphically up to the second order in the interactions in Fig. 13.3.

The lowest term $\Gamma^1[\Phi]$ obviously contains only OPI diagrams. The graphical iteration shows that this property persists to all orders. If all diagrams of n th order are OPI, those composed to next order on the right-hand side of Eq. (13.64) always contain at least two more lines and thus do not decompose by cutting a single line. They therefore are OPI (in normal field theories in which the expectation Φ_0 vanishes at zero external source j). This proves the statement made on that behalf in the beginning. It is thereby confirmed that the self-energy collects only one-particle irreducible vertex diagrams. Thus the full propagator is indeed obtained from the geometric iteration of such diagrams implied by (13.59):

$$G = G_0 + G_0(-i\Sigma)G_0 + G_0(-i\Sigma)G_0(-i\Sigma)G_0 + \dots \quad (13.67)$$

As argued before, all OPI two-point vertex diagrams must be contained in $\Sigma = -i\Gamma_{\Phi\Phi}^{\text{int}}$. If it occurs in G it must also occur in Σ .

We have also proved another important statement observed graphically in the low-order diagrams of Chapter 10. All n -point functions can be obtained by composing all OPI vertex diagrams and all full Green functions from tree diagrams. The composition rules were derived above.

$$\begin{aligned}
\Sigma &= -\Gamma_{\Phi\Phi}^{\text{int}} \\
\Phi\Gamma_{\Phi}^{\text{int}} &= -\frac{1}{2!} \text{ (3-vertex) } - \frac{1}{3!} \text{ (4-vertex) } \\
&\quad - \frac{1}{2!} \text{ (loop with 3-vertex) } - \frac{1}{2!} \text{ (loop with 4-vertex) } - \frac{1}{3!} \text{ (triangle loop) } \\
\text{---}\bigcirc\text{---} &= \text{---} - i \text{---}\bigcirc\text{---} \\
\text{---} &= G_0 \quad \text{---}\bigcirc\text{---} = G \\
\text{Y} &= V_3 \quad \text{---}\bigcirc\text{---} = \Gamma_{\Phi\Phi}^{\text{int}} \equiv -\Sigma \\
\text{X} &= V_4 \quad \text{---}\bigcirc\text{---} = \Gamma_{\Phi\Phi\Phi}^{\text{int}} \\
\text{---} &= \Phi
\end{aligned}$$

$$\begin{aligned}
\Gamma^1 &= -\frac{1}{3!} \text{ (3-vertex) } - \frac{1}{4!} \text{ (4-vertex) } - \frac{1}{2} \text{ (loop) } - \frac{1}{4} \text{ (triangle loop) } \\
\text{---}\bigcirc\text{---} &= \text{---} - i \left(\text{---}\bigcirc\text{---} + \frac{1}{2} \text{ (3-vertex) } + \frac{1}{2} \text{ (loop) } \right) \\
\text{---}\bigcirc\text{---} &= -\text{Y} - \text{X} \\
\Gamma^2 &= \frac{1}{4} \text{ (loop with 3-vertex) } + \frac{i}{4} \text{ (loop with 4-vertex) } + \frac{i}{4} \text{ (triangle loop) } \\
&\quad + \frac{i}{16} \text{ (triangle loop with 3-vertex) } + \frac{i}{8} \text{ (triangle loop with 4-vertex) } + \frac{i}{3!} \left(\text{---}\bigcirc\text{---} + \frac{1}{2} \text{ (loop) } \right)
\end{aligned}$$

FIGURE 13.3 Graphical solution of the functional differential equation (13.64) for the interacting part $\Gamma^{\text{int}}[\Phi]$ of effective action.

For completeness, let us treat the functional differential equation for $\Gamma[\Phi]$ once more in a different way in a non-normal system (corresponding to a magnetized phase in solid-state physics) with a nonvanishing field expectation $\Phi_0 = \langle \varphi \rangle \neq 0$ for $j = 0$, keeping explicit reference to Φ_0 . Setting

$$\Phi = \Phi_0 + \Phi' \quad (13.68)$$

we define

$$\Gamma'[\Phi'] \equiv \Gamma[\Phi_0 + \Phi'] \quad (13.69)$$

which then satisfies the equation

$$\begin{aligned} iG_0^{-1}\Phi_0 - \frac{1}{2!}V_3(\Phi'_0 + 2\Phi_0\Phi') - \frac{1}{3!}V_4(\Phi_0^3 + 3\Phi_0^2\Phi' + 3\Phi_0\Phi'^2) \\ - \frac{1}{2}V_4i\Gamma'_{\Phi\Phi'}\Phi_0 - \frac{1}{2!}V_3(i\Gamma'_{\Phi\Phi'}\Phi_0 + \Phi'^2) \\ - \frac{1}{4!}V_4(\Gamma'_{\Phi\Phi'}{}^3\Gamma_{\Phi'\Phi'\Phi'} + 3i\Gamma_{\Phi\Phi'}\Gamma'_{\Phi'\Phi'} + \Phi'^3 + 2\Phi_0^2\Phi'^2) - \Gamma'_{\Phi'} = 0. \end{aligned} \quad (13.70)$$

Let us now split

$$\Gamma'[\Phi'] = \Gamma'^0[\Phi'] + \Gamma'^{\text{int}}[\Phi'], \quad (13.71)$$

with

$$\Gamma^0[\Phi'] = \mathcal{A}[\Phi_0] + \mathcal{A}_\Phi[\Phi_0]\Phi' + \frac{1}{2}\mathcal{A}_{\Phi\Phi}[\Phi_0]\Phi'\Phi'. \quad (13.72)$$

Inserting this into (13.70), we find for Γ' the functional differential equation

$$\begin{aligned} \Phi'\Gamma'_{\Phi'} = -\frac{1}{2!}\Phi'(V_3 + V_4\Phi_0)(i\Gamma'_{\Phi'\Phi'} + \Phi'^2) \\ - \frac{1}{3!}\Phi'V_4(\Gamma'_{\Phi'\Phi'}{}^3\Gamma_{\Phi'\Phi'\Phi'} + 3i\Gamma_{\Phi\Phi'}\Gamma'_{\Phi'\Phi'} + \Phi'^3). \end{aligned} \quad (13.73)$$

Here we insert

$$\Gamma'_{\Phi\Phi'} = \mathcal{A}_{\Phi\Phi}[\Phi_0] + \Gamma'^{\text{int}}_{\Phi'\Phi'}, \quad (13.74)$$

and

$$\Gamma'_{\Phi'\Phi'\Phi'} = \Gamma'^{\text{int}}_{\Phi'\Phi'\Phi'}. \quad (13.75)$$

Then Eq. (13.73) becomes structurally identical with (13.64), only that V_3, V_4 are replaced by $(V_3 + V_4\Phi_0)$ and V_4 , respectively, and the free Green function G_0 by

$$G_0^{\Phi_0} = i \left[iG_0^{-1} - V_3\Phi_0 - \frac{V_4}{2}\Phi_0^2 \right]. \quad (13.76)$$

Thus $\Gamma^{\text{int}}[\Phi]$, when expanded in powers of Φ' , does indeed collect only one-particle irreducible diagrams. This is what we wanted to prove in the general case $\Phi_0 \neq 0$ [see (13.41)]:

$$\Gamma_{\Phi' \dots \Phi'}^{(n)} = \frac{\delta^n \Gamma}{\delta \Phi(x) \dots \delta \Phi(x_n)} \Big|_{\Phi=\Phi_0}. \quad (13.77)$$

13.9 Effective Action as Basis for Variational Calculation

In the last section we have seen that the effective action contains all information necessary to construct all n -point functions. Moreover, its calculation requires only a certain restricted class of Feynman diagrams, namely those which are OPI. There is, however, another important feature which makes the effective action a powerful tool in the study of physical properties of a system and which, finally, justifies its name: A physical configuration of the field expectation $\Phi = \langle \varphi \rangle|_j$ that extremizes $\Gamma[\Phi]$ at $j = 0$. This is a direct consequence of the definition (13.37). If we write $\Gamma[\Phi]$ in the form

$$\Gamma[\Phi] = W[j] - \int d^D x \Phi(x) j(x), \quad (13.78)$$

we find

$$\frac{\delta \Gamma}{\delta \Phi} = \int d^D x \left(\frac{\delta W}{\delta j} - \Phi \right) \frac{\delta j}{\delta \Phi} - j(x) = -j(x), \quad (13.79)$$

implying that, in the absence of the auxiliary external source j , $\Gamma[\Phi]$ is indeed extremal. The functional $\Gamma[\Phi]$ has thus exactly the same property in quantum theory as the usual action $\mathcal{A}[\Phi]$ in classical theory.

13.10 Effective Potential

A special role in the extraction of observational consequences from a theory is played by the effective potential. Remember that in classical mechanics, the potential is defined by the action evaluated for a time-independent orbit $q(t)$ as

$$\mathcal{A} = \int_{t_a}^{t_b} dt \mathcal{L}(q, \dot{q}) \Big|_{q=\text{const}} = -TV(q), \quad T \equiv t_b - t_a. \quad (13.80)$$

By analogy, we define the effective potential of a field theory, if it has the special property $\Phi_0 = \text{const}$, by

$$\Gamma[\Phi] \Big|_{\Phi=\text{const}} = -TL^3V(\Phi), \quad L^3 = \text{spatial volume}. \quad (13.81)$$

Comparing this with (13.41) we see that the effective potential has the expansion

$$TL^3V(\Phi) = - \sum \frac{1}{n!} \int d^D x_1 \cdots d^D x_n \Gamma^{(n)}(x_1, \dots, x_n) (\Phi - \Phi_0) \cdots (\Phi - \Phi_0). \quad (13.82)$$

Introducing the Fourier transforms

$$\Gamma^{(n)}(q_1, \dots, q_n) \equiv \int d^D x_1 \cdots d^D x_n e^{i(q_1 x_1 + \dots + q_n x_n)} \Gamma^{(n)}(x_1, \dots, x_n), \quad (13.83)$$

and removing the overall δ -function of energy-momentum conservation contained in $\Gamma^{(n)}(q_1, \dots, q_n)$ due to the translational invariance of $\Gamma^{(n)}(x_1, \dots, x_n)$,

$$\Gamma^{(n)}(q_1, \dots, q_n) \equiv (2\pi)^D \delta^{(D)}(q_1 + \dots + q_n) \bar{\Gamma}^{(n)}(q_1, \dots, q_n), \quad (13.84)$$

we can write (13.86) as

$$V(\Phi) = - \sum \frac{1}{n!} \bar{\Gamma}^{(n)}(q_1, \dots, q_n) \Big|_{q_i=0} (\Phi - \Phi_0) \dots (\Phi - \Phi_0). \quad (13.85)$$

The discussion has been given for a single Bose field. For a set of Bose fields φ_a , the index a may be imagined as being included in the spacetime index x . Thus Eq. (13.86) reads more explicitly:

$$V(\Phi_a) = - \sum \frac{1}{n!} \bar{\Gamma}^{(n)}(q_1, \dots, q_n) \Big|_{q_i=0} (\Phi - \Phi_0)_{a_1} \dots (\Phi - \Phi_0)_{a_n}. \quad (13.86)$$

13.11 Higher Effective Actions

Effective actions are an important theoretical tool to find extremal principles in quantum field theory and statistical mechanics [20]. Their history goes back to the extremal principles of Lee and Yang [21]. C. de Dominicis, P.C. Martin, and others [3]. The functional $\Gamma[G]$ is specified in terms of a graphical expansion according to the number of fermion loops. We shall sketch this formalism in real time, where the lowest contributions lead directly to the famous time-dependent Hartree-Fock-Bogoliubov equations. Higher corrections are found from a graphical iteration procedure. Let us briefly recall that procedure for a fermion system. We shall derive an effective action functional $\Gamma[G]$, whose extrema yield the bilocal density matrix G of the interacting Fermi liquid.

Starting point is an action of the form (13.1) with an arbitrary two-body force. It will be expressed in terms of the quasi-real doubled field

$$\varphi = \begin{pmatrix} \psi \\ \psi^* \end{pmatrix}, \quad \text{with} \quad \bar{\varphi} \equiv c\varphi^\dagger = \varphi, \quad c = \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (13.87)$$

as

$$\mathcal{A}[\varphi] = \frac{1}{2} \varphi G_0^{-1} \varphi - \frac{1}{4!} v \varphi \varphi \varphi \varphi, \quad (13.88)$$

with G_0^{-1} being now

$$G_0^{-1} = c \begin{pmatrix} \partial_\tau + \hat{\mathbf{p}}^2/2 + V_1(\mathbf{x}) - \mu^T & 0 \\ 0 & -\partial_\tau - \hat{\mathbf{p}}^2/2 - V_1(\mathbf{x}) + \mu \end{pmatrix}. \quad (13.89)$$

More explicitly, the matrix elements of G_0 contain the free correlation functions

$$G(\mathbf{x}, t; \mathbf{x}', t') \equiv \begin{pmatrix} \langle T_t \psi_\alpha(\mathbf{x}, t) \psi_\beta(\mathbf{x}', t') \rangle_0 & \langle T_t \psi_\alpha(\mathbf{x}, t) \psi_\beta^\dagger(\mathbf{x}', t') \rangle_0 \\ \langle T_t \psi_\alpha^\dagger(\mathbf{x}, t) \psi_\beta(\mathbf{x}', t') \rangle_0 & \langle T_t \psi_\alpha^\dagger(\mathbf{x}, t) \psi_\beta^\dagger(\mathbf{x}', t') \rangle_0 \end{pmatrix}. \quad (13.90)$$

where α, β are spin indices, all being suppressed in (13.88) and the subsequent formulas.

To the action (13.88) we add a bilocal source term and form the generating functional

$$Z[K] \equiv \int \mathcal{D}\varphi \exp \left\{ i \left[\mathcal{A}[\varphi] + \frac{1}{2} \varphi K \varphi \right] \right\}, \quad (13.91)$$

where

$$K \equiv c \begin{pmatrix} \kappa & \lambda \\ \lambda^\dagger & -\kappa^T \end{pmatrix},$$

and $\varphi K \varphi$ stands short for $\int dt dt' \varphi_a(t) K_{ab}(t, t') \varphi_b(t')$. The superscript T denotes functional transposition, i.e., if spin indices are displayed: $K_{ab}^T(t, t') \equiv K_{ba}(t', t)$, $\mu_{\alpha\beta}^T(t, t) \equiv \mu_{\beta\alpha}(t', t)$. Note that the potential v with four doubled indices is antisymmetric.

Formally, $Z[K]$ can be calculated by removing the interacting part from the integral via functional derivatives, writing

$$Z[K] = \exp \left(-\frac{i}{6} v \frac{\delta}{i\delta K} \frac{\delta}{i\delta K} \right) Z_0[K], \quad (13.92)$$

where $Z_0[K]$ is given by a Gaussian functional integral, which can be performed to give

$$Z_0[K] = \int \mathcal{D}\varphi \exp \left[\frac{i}{2} \varphi i G_K^{-1} \varphi \right] = \exp \left[\frac{1}{2} \text{Tr} \log i G_K^{-1} \right], \quad (13.93)$$

with $G_K^{-1} = G_0^{-1} + K$. Obviously, G_K is the Green function of the fermions in the presence of an external field K . Expanding Z in powers of v results in the standard diagrammatic rules of perturbation theory. If we form the logarithm generating functional

$$iW[K] = \log Z[K], \quad (13.94)$$

this contains all connected vacuum graphs formed with four-vertices and propagators G_K . Because of the fermion nature of φ these are one-particle irreducible graphs which look as follows (we drop all diagrams with three-vertices):

$$\begin{aligned} W[K] = & \frac{1}{8} \text{diagram}_1 - \frac{1}{2!} \left[\frac{1}{8} \text{diagram}_2 + \frac{1}{24} \text{diagram}_3 + \frac{1}{6} \text{diagram}_4 \right] \\ & + \frac{1}{3!} \left[\frac{3}{16} \text{diagram}_5 + \frac{1}{8} \text{diagram}_6 + \frac{1}{4} \text{diagram}_7 + \frac{1}{8} \text{diagram}_8 + \frac{3}{4} \text{diagram}_9 + \frac{3}{4} \text{diagram}_{10} \right]. \end{aligned} \quad (13.95)$$

Given $W[K]$, it is easy to find the exact density matrix of the system

$$\frac{1}{2} G = \frac{\delta W[K]}{\delta K} = -\frac{\delta}{\delta K} W[K]. \quad (13.96)$$

An effective action $\Gamma[G]$ of the system is now introduced as the Legendre transform

$$\Gamma[G] \equiv W[K] - \frac{1}{2} \text{Tr}(KG) \Big|_{K=K[G]} \quad (13.97)$$

such that (13.96) amounts to

$$\frac{\delta \Gamma[G]}{\delta G} = -\frac{1}{2} K. \quad (13.98)$$

At the end, the auxiliary source K is set equal to 0. Equation (13.98) implies that the physical density matrix extremizes $\Gamma[G]$, thus providing us with an extremal principle.

Let us evaluate the lowest contributions explicitly: At the one-loop level we have

$$W^{(1)}[K] = -\frac{i}{2} \text{Tr} \log iG_K^{-1} \quad (13.99)$$

and (13.96) yields $G = G_K$. Reinserting this into (13.97), we obtain

$$\Gamma[G] \equiv \Gamma^{(0)}[G] + \Gamma^{(1)}[G] = \frac{i}{2} \text{Tr}(G_0^{-1}G) - \frac{i}{2} \text{Tr} \log iG^{-1}. \quad (13.100)$$

The extremum of this functional provides us with the density matrix of the free fermion system $G = G_0$.

We now add to $W[K]$ the lowest two-loop correction in (13.96):

$$W^{(2)}[K] = -\frac{1}{8}v G_K G_K. \quad (13.101)$$

Exhibiting upper and lower spin components, as well as other particle indices, this contains again Hartree, Fock, and Bogoliubov contributions, whose explicit spin-up and spin-down configurations are

$$-\frac{1}{24}g_{\alpha\beta\gamma\delta}[(G_K)_{\alpha\downarrow\beta\uparrow}(G_K)_{\gamma\downarrow\delta\uparrow} - (G_K)_{\alpha\downarrow\delta\uparrow}(G_K)_{\gamma\downarrow\beta\uparrow} - (G_K)_{\alpha\downarrow\gamma\downarrow}(G_K)_{\beta\uparrow\delta\uparrow}]. \quad (13.102)$$

By differentiating $W_2[K] = W^{(0)}[K] + W^{(1)}[K] + W^{(2)}[K]$ with respect to K according to (13.96), we obtain

$$G = G_K - \frac{i}{2}G_K(vG_K)G_K, \quad (13.103)$$

which is solved for

$$K = iG^{-1} - iG_0^{-1} + \frac{1}{2}vG, \quad (13.104)$$

to be reinserted into $W_2[K]$, yielding via (13.97):

$$\Gamma^{(2)}[G] = -\frac{1}{8}gGG. \quad (13.105)$$

Extremizing $\Gamma_2[K] = \Gamma^{(0)}[K] + \Gamma^{(1)}[K] + \Gamma^{(2)}[K]$, we find:

$$G = i \left[iG_0^{-1} - \frac{1}{2}vG \right]^{-1}. \quad (13.106)$$

This is precisely the well-known time-dependent Hartree-Fock-Bogoliubov equation.

Let us indicate how to proceed in this fashion to higher-loop corrections. Most efficiently we may use the obvious functional identity

$$\int D\varphi \frac{\delta}{\delta\varphi} \varphi \exp \left[i\mathcal{A}[\varphi] + \frac{i}{2} \varphi K \varphi \right] = 0, \quad (13.107)$$

and work out the differentiations and derive the functional differential equation

$$(iG_0^{-1} + K)W_{,K} + \frac{i}{3}v(W_{,KK} + iW_{,K}^2) - \frac{i}{2} = 0. \quad (13.108)$$

A subscript separated by a comma indicates functional differentiation with respect to that variable. Using the relation (13.96) and the equation obtained from the second derivative of $W[K]$:

$$-iW_{,KK} = G_{,K}/2 = K_{,G}^{-1}/2 = -\Gamma_{,GG}^{-1}/4, \quad (13.109)$$

we find

$$(iG_0^{-1} - 2\Gamma_{,G})G - \frac{1}{3!}v(i\Gamma_{,GG}^{-1}) - i = 0. \quad (13.110)$$

By separating out the trivial parts the interacting part satisfies the coupled equations

$$\Gamma_{,G}^{\text{int}}[G]G = -\frac{1}{4}vGG + \frac{i}{12}vG^4\alpha, \quad (13.111)$$

$$\alpha = -4\Gamma_{,GG}^{\text{int}}(1 - 2iGG\Gamma_{,GG}^{\text{int}})^{-1} = -4\Gamma_{,GG}^{\text{int}} + 2i\Gamma_{,GG}^{\text{int}}GG\alpha. \quad (13.112)$$

The quantity α represents the exact four-particle vertex function of the theory. The equations are pictured in Fig. 13.4. They generate precisely those vacuum graphs

$$\begin{aligned} \Gamma_G^{\text{int}} G &= -\frac{1}{4} \text{---}\bigcirc\bigcirc\text{---} + \frac{i}{12} \text{---}\bigcirc\bigcirc\bigcirc\bigcirc\text{---} \\ \text{---}\bigcirc\bigcirc\text{---} &= -4 \text{---}\boxed{\Gamma_{GG}^{\text{int}}}\text{---} + 2i \text{---}\boxed{\Gamma_{GG}^{\text{int}}}\text{---}\bigcirc\bigcirc\text{---} \bigg|_{\text{symm}} \end{aligned}$$

FIGURE 13.4 Recursion relation for two-particle-irreducible graphs in the effective action $\Gamma^{\text{int}}[G]$.

which do not fall into disjoint pieces when cutting two lines, i.e., they consist of all two-particle irreducible diagrams. Up to two loops, we have

$$\Gamma[G] \equiv \Gamma^{(0)}[G] + \Gamma^{(1)}[G] + \Gamma^{\text{int}}[G], \quad (13.113)$$

with

$$\Gamma^{\text{int}}[G] = \frac{1}{8} \text{---}\bigcirc\bigcirc\text{---} - \frac{1}{24} \text{---}\bigcirc\bigcirc\bigcirc\bigcirc\text{---} + \frac{1}{48} \text{---}\bigcirc\bigcirc\bigcirc\bigcirc\text{---} + \dots \quad (13.114)$$

In general, effective action has the expansion

$$\Gamma[\Sigma, G] = -\frac{i}{2}\text{Tr} \log(iG_0^{-1} - \Sigma) - \frac{1}{2}\text{Tr}(G\Sigma) - \frac{1}{8}vGG + \sum_{n \geq 3}^{\infty} \Gamma^{(n)}[G], \quad (13.115)$$

with $\Gamma^{(n)}$ collecting all two-particle-irreducible graphs with n loops. The extremality condition $\Gamma_G[G] = 0$ produces a Green function

$$G = i\{G_0^{-1} - \Sigma[G]\}^{-1}, \quad (13.116)$$

with a self-energy

$$\frac{1}{2}\Sigma[G] = -\Gamma_G^{\text{int}}[G] = \frac{1}{4}vG - \frac{i}{12}vG^3\alpha = \frac{1}{4}vG - \sum_{n \geq 3}^{\infty} \Gamma_{,G}^{(n)}[G]. \quad (13.117)$$

Equation (13.116) was first used by Dyson [20] with the prescription that $\Sigma[G]$ contains all those self-energy graphs which are one-particle irreducible, i.e., which do not fall apart when cutting one line. Obviously, this agrees precisely with the present procedure, since removing one line from all two-particle irreducible diagrams produces all one-particle irreducible diagrams of the self-energy.

We remark that large amplitude collective excitations are studied by solving the above equations semiclassically. For any periodic state one chooses some initial self-energy Σ , and solves the eigenvalue equation

$$\{iG_0^{-1} - \Sigma\}\chi_k(t) = \lambda_k\chi_k(t), \quad (13.118)$$

where $\chi_k(t)$ are antiperiodic wave functions and ν_k the corresponding Bloch-Floquet indices. Then one determines

$$\begin{aligned} G(t, t') &= \sum_k \sum_n \frac{i}{\omega_n - \nu_k} \exp[-i\omega_n(t - t')] \chi_k(t) \chi_k(t') \\ &= \sum_k \frac{1}{\exp(i\lambda_k T) + 1} \exp[-i\nu_k(t - t')] \chi_k(t) \chi_k(t'), \end{aligned} \quad (13.119)$$

where the Fermi distribution contains the period of the oscillations T like an imaginary temperature, as a result of the sum over the frequencies $\omega_n = 2\pi(n + 1/2)/T$. This Green function (13.119) is inserted into (13.118) for a next iteration. The static case follows by taking the limit $T \rightarrow \infty$, in which the sum reduces to the states below the Fermi surface, and $\chi_k(t)$ become time-independent wave functions.

The resulting G can be inserted into the effective action $\Gamma[G]$ for a quantization of the large-amplitude oscillating orbits (or for a determination of the energy in the case of static G configurations, $E = -\Gamma[G]/T$). For this purpose one only has to form the semiclassical quantum propagator as the Fourier transform [4]

$$\int \frac{dT}{2\pi} \exp(i\Gamma[G] + ET) \equiv \frac{\partial W(E)}{\partial E} \exp[iW(E)], \quad (13.120)$$

where T is the period of the orbit. Running through the same orbit many times and inserting a phase -1 for each turning point gives a Green function

$$\partial W/\partial E \sum_{n=1}^{\infty} \exp[inW(E)] = \partial W/\partial E \exp[iW(E)] \frac{1}{1 + \exp[iW(E)]}, \quad (13.121)$$

which has poles at $W(E_n) = 2\pi(n + 1/2)$ [4].

If an imaginary-time solution passes through a potential barrier, then the Boltzmann factor $\exp(-TE) = \exp\{i\Gamma[G]\}$ gives the amplitude of barrier penetration [5].

13.12 High Orders in a Simple Model

It is instructive to apply the treatment to an exactly solvable model where one can calculate the higher effective action to arbitrary order. Consider the classical partition function of the anharmonic oscillator in zero dimensions, where it is given by the simple integral

$$Z = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi/\beta\omega^2}} e^{-\beta(\omega^2 x^2/2 + gx^4/4!)}. \quad (13.122)$$

It is easy to expand this in powers of g as $Z = \sum_{k=0}^{\infty} z^{(k)} g'^k$ where $g' \equiv g/\beta\omega^4$. The coefficients are

$$z^{(k)} = \frac{(-1)^k}{6^k k!} \frac{\Gamma(2k + 1/2)}{\Gamma(1/2)} \quad (13.123)$$

starting out like $\frac{1}{8}, \frac{35}{384}, \frac{385}{3072}, \frac{25025}{98304}, \frac{1616615}{2359296}, \frac{260275015}{113246208}, \frac{929553625}{100663296}, \frac{835668708875}{19327352832}, \dots$. For large k , they grow like $(-1)^k (2/3)^k k! / k\pi\sqrt{2}$. The series is divergent, but Borel-summable. It possesses an absolutely convergent strong-coupling expansion in powers of $1/\sqrt{g'}$. This is found by rewriting (13.122) as

$$Z = g'^{-1/4} \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{dy}{\sqrt{y}} e^{-y/\sqrt{g'}} e^{-y^2} \quad (13.124)$$

and expanding the first exponential. The result is the absolutely convergent strong-coupling series:

$$Z = (g')^{-1/4} \sum_{k=0}^{\infty} \xi_k \left(\frac{1}{\sqrt{g'}} \right)^k \quad (13.125)$$

with coefficients

$$\xi_k = \frac{1}{2\sqrt{\pi}} (-1)^k \frac{\Gamma(k/2 + 1/4)}{k!}. \quad (13.126)$$

The series may be expressed in terms of well-known mathematical functions as

$$Z = e^{1/8g'} W_{0,-1/4}(1/4g') = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2g'} \right)^{1/2} e^{1/8g'} K_{1/4}(1/8g'), \quad (13.127)$$

where $W_{0,-1/4}(z)$ is Whittaker's function and $K_{1/4}(z)$ the modified Bessel function. For $g \rightarrow \infty$ the function approaches the limit

$$Z \xrightarrow{g \rightarrow \infty} \lambda_0 (g'/6)^{-1/4} \quad (13.128)$$

with

$$\lambda_0 = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{dy}{\sqrt{y}} e^{-y^2} = \frac{\Gamma(1/4)}{2\sqrt{\pi}} \approx 1.0228 \quad (13.129)$$

The free energy of the model is defined by $Z \equiv e^{-\beta F}$. It has the power series expansion

$$\beta F = \sum_{n=1}^{\infty} f_n \cdot \left(\frac{g}{\beta \omega^4} \right)^n, \quad (13.130)$$

with the expansion coefficients f_n being equal to

$$f_n = \left(\frac{1}{8}, -\frac{1}{12}, \frac{11}{96}, -\frac{17}{72}, \frac{619}{960}, -\frac{709}{324}, \frac{858437}{96768}, -\frac{54193}{1296}, \frac{18639247}{82944}, \dots \right). \quad (13.131)$$

The function Z is plotted in Fig. 13.5.

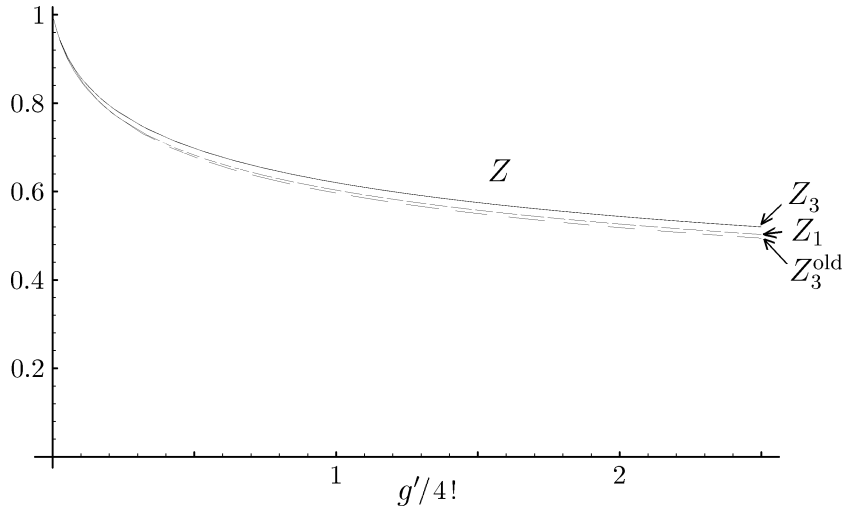


FIGURE 13.5 The anharmonic model integral Z as a function of $g' = g/\omega^4$ in comparison with three variational approximations: Z_1 (long-dashed) coming from the Hartree-Fock-Bogoliubov approximation to the energy, Z_3 from the new extended approximation, and Z_3^{old} from the much worse old extension derived from the higher effective action. The new extension Z_3 is not distinguishable from Z on this plot, lying less than 0.1% below Z at $g'/4! = 2.5$. Observe that the old extension Z_3^{old} is worse than Z_1 .

How well is this classical partition function reproduced by the Hartree-Fock approximation and its successive improvements?

The function $\Gamma[G, \Sigma[G]]$ of Eq. (13.115) becomes, for $\beta = 1$:

$$\Gamma[G, \Sigma[G]] = \frac{1}{2} \log \frac{\Omega^2}{\omega^2} + \frac{\omega^2 - \Omega^2}{2} a^2 + 3ga^4 - \frac{1}{48} g^2 a^8 + \frac{1}{48} g^3 a^{12} - \frac{5}{128} g^4 a^{16} + \frac{101}{960} g^5 a^{20} - \dots \quad (13.132)$$

with $a^2 = 1/\Omega$, where the higher terms can be calculated to all orders. They have the form $(-1)^{n-1}c_n g^n a^{4n}$ with c_n satisfying the recursion relation

$$c_n = \frac{1}{2n} \left[-\frac{1}{6}c_{n-1}(2n-2)(2n-3) + 8 \sum_{m=1}^{n-1} (n-m)m(2m-1)c_m c_{n-m} \right], \quad (13.133)$$

starting out with $c_1 = 1/8$, $c_2 = 1/48$, and continuing with $\frac{5}{128}$, $\frac{101}{960}$, $\frac{93}{256}$, $\frac{8143}{5376}$, $\frac{271217}{36864}$, ...

The Hartree-Fock-Bogoliubov approximation $\Gamma_1(a) \equiv \Gamma_1[G, \Sigma[G]]$ is obtained by truncating the expansion after $c_1 = 1/8$ and setting all c_i with $i > 1$ equal to zero. An important feature this approximation is that it explains quite well the strong-coupling behavior $g \rightarrow \infty$ of the system. In this limit, we see from the first-order terms in (13.132) that the extremal Ω^2 diverges for large g like $d(g/6)^{1/2}$, and that $Z_1 \rightarrow e^{1/4}/\sqrt{d}(g/6)^{1/4}$. Indeed, the associated approximation for Z at $g = 6$ is $e^{1/4}/\sqrt{d} \approx 0.9756$. This compares reasonably with the correct value λ_0 in (13.129).

The curve denoted by Z_3 in Fig. 13.5 comes from the extended approximation obtained by setting the c_i 's equal to zero for $i > 3$. The curve Z_3^{old} is obtained by minimization of the effective action of the same order. In the figure, the curve looks acceptable. However, when trying to calculate the behavior in the presence of higher-order correction terms, we find a severe weakness of the associated correction scheme: The extremality equation to be solved for d becomes, if we include higher-order corrections to the Hartree-Fock-Bogoliubov approximation:

$$-d + \frac{3}{d} - \left(\frac{6}{d^3} + \frac{810}{d^7} + \frac{16362}{d^9} \dots \right) = 0. \quad (13.134)$$

The factorial growth of the coefficients makes it impossible to extract a solution without resummation procedures. This is seen in Fig. (13.6), where the third-order approximation is worse than the first-order one.

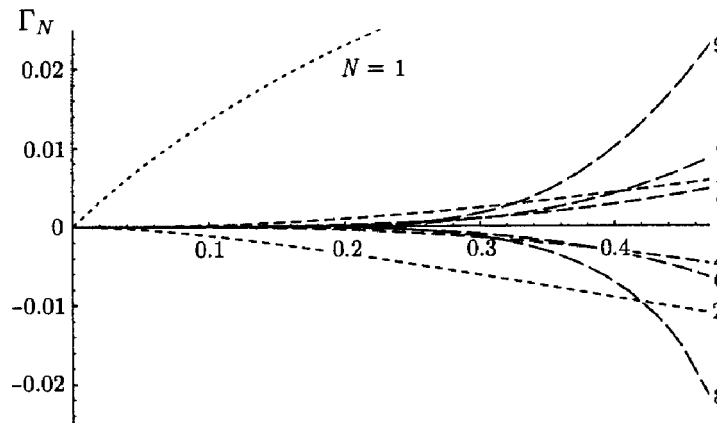


FIGURE 13.6 Approximations to βF obtained from the extrema of the higher effective action $\Gamma[G, \Sigma[G]]$ in Eq. (13.132) up to order g^N , denoted by Γ_N . The errors increase rapidly with increasing g and there is no uniform convergence.

The only scheme to converge at higher order is the one based on variational perturbation theory (VPT). It was developed in Refs. [6, 7] and applied in Chapter 3 (for the history see the first citation there) and Section 22.5.

Notes and References

In this chapter we follow mainly the review paper [1].

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*Perfection is achieved, not when there is nothing more to add,
but when there is nothing left to take away.*
ANTOINE DE SAINT-EXUPÈRY (1900–1944)

14

Functional-Integral Representation of Quantum Field Theory

In Chapter 7 we have quantized various fields with the help of canonical commutation rules between field variables and their canonical conjugate field momenta. From these and the temporal behavior of the fields determined by the field equations of motion we have derived the Green functions of the theory. These contain all experimentally measurable informations on the quantum field theory. They can all be derived from functional derivatives of certain generating functionals. For a real scalar field this was typically an expectation value

$$Z[j] \equiv \langle 0|T[j]|0\rangle \quad (14.1)$$

where $T[j]$ was the time-ordered product in (7.827)

$$T[j] \equiv \hat{T} e^{i \int d^4x j(x)\phi(x)}. \quad (14.2)$$

Here the Green functions can all be obtained from functional derivatives of $Z[j]$ of the type (7.841).

For complex scalar fields, the corresponding generating functional is given by the expectation value (7.849). Now the Green functions can all be obtained from functional derivatives of the type (7.850).

In theoretical physics, Fourier transformations have always played an important role in yielding complementary insights into mathematical structures. Due to the conjugate appearance of fields $\phi(x)$ and sources $j(x)$ in expressions like (14.2), this is also true for generating functionals and constitutes a basis for the functional-integral formalism of quantum field theory.

14.1 Functional Fourier Transformations

An important observation is now that instead of calculating these generating functionals as done in Chapter 7 from a formalism of field theory, in which $\phi(x)$ is a field

operator, they can also be derived from a functional Fourier transform of another functional $\tilde{Z}[\phi]$ that depends on a *classical* field $\phi(x)$:

$$Z[j] \equiv \int \mathcal{D}\phi \tilde{Z}[\phi] e^{i \int d^D x j(x)\phi(x)}. \quad (14.3)$$

The symbol $\int \mathcal{D}\phi(x)$ in this expression is called a *functional integral*.

The mathematics of functional integration is an own discipline that is presented in many textbooks [1, 2]. Functional integrals were first introduced in ordinary quantum mechanics by R.P. Feynman [3], who used them to express physical amplitudes without employing operators. The uncertainty relation that can be expressed by an equal-time commutation relation $[x(t), p(t)] = i\hbar$ between $x(t)$ and the conjugate variable $p(t)$ of quantum mechanics is the consequence of quantum fluctuations of the classical variables $x(t)$ and $p(t)$. In quantum mechanics, the functional integral is merely a *path integral* of a fluctuation variable $x(t)$. In field theory, there is a fluctuating path for each space point $\mathbf{x}$. Instead of a time-dependent variable $x(t)$ one deals with more general dynamical variables $\phi_{\mathbf{x}}(t) = \phi(\mathbf{x}, t) = \phi(x)$, one for each spacepoint $\mathbf{x}$. The path integrals over all $x(t)$ go over into functional integrals over all fluctuating fields $\phi(x)$.

Functional integrals may be defined most simply in a discretized approximation. Spacetime is grated into a fine spacetime lattice. For every spacetime coordinate x^μ we introduce a discrete lattice point close to it

$$x^\mu \rightarrow x_n^\mu \equiv n\epsilon, \quad n = 0, \pm 1, \pm 2, \pm 3, \quad (14.4)$$

where ϵ is a very small lattice spacing. Then we may approximate integrals by sums:

$$\int d^D x j(x)\phi(x) \approx \epsilon^D \sum_{\mathbf{n}} j(x_{\mathbf{n}})\phi(x_{\mathbf{n}}) \equiv \epsilon^D \sum_{\mathbf{n}} j_{\mathbf{n}}\phi_{\mathbf{n}} \quad (14.5)$$

where $\mathbf{n}$ is to be read as a D -dimensional index $(n_0, n_1, \dots, n_D)$, one for each component of the spacetime vector x^μ . Now we define $\int \mathcal{D}\phi(x)$ as the infinite product of integrals over $\phi_{\mathbf{n}}$ at each point $x_{\mathbf{n}}$:

$$\int \mathcal{D}\phi(x) = \prod_{\mathbf{n}} \int \frac{d\phi_{\mathbf{n}}}{\sqrt{2\pi i/\epsilon^D}}. \quad (14.6)$$

Operations with functional integrals are very similar to those with ordinary integrals. For example, the Fourier transform of (14.3) can be inverted, by analogy with ordinary integrals, to obtain:

$$\tilde{Z}[\phi] \equiv \int \mathcal{D}j(x) Z[j] e^{-i \int d^D x j(x)\phi(x)}. \quad (14.7)$$

There are functional analogs of the Dirac δ -function:

$$\int \mathcal{D}j(x) e^{-i \int d^D x j(x)\phi(x)} = \delta[\phi], \quad (14.8)$$

$$\int \mathcal{D}\phi(x) e^{i \int d^D x j(x)\phi(x)} = \delta[j], \quad (14.9)$$

called δ -functionals. In the lattice approximation corresponding to (14.6), they are defined as infinite products of ordinary δ -functions

$$\delta[\phi] = \prod_{\mathbf{n}} \sqrt{2\pi i/\epsilon^D} \delta(\phi_{\mathbf{n}}), \quad \delta[j] = \prod_{\mathbf{n}} \sqrt{2\pi i/\epsilon^D} \delta(j_{\mathbf{n}}). \quad (14.10)$$

They have the obvious property

$$\int \mathcal{D}\phi \delta[\phi] = 1, \quad \int \mathcal{D}j \delta[j] = 1. \quad (14.11)$$

A commonly used notation for the measure (14.6) of functional integrals employs continuously infinite product of integrals which must be imagined as the continuum limit of the lattice product (14.6). In this notation one writes

$$\int \mathcal{D}\phi(x) = \prod_x \int \frac{d\phi(x)}{\sqrt{2\pi i}}, \quad \int \mathcal{D}j(x) = \prod_x \int \frac{dj(x)}{\sqrt{2\pi i}}, \quad (14.12)$$

and the associated δ -functionals as

$$\delta[\phi] = \prod_x \sqrt{2\pi i} \delta(\phi(x)), \quad \delta[j] = \prod_x \sqrt{2\pi i} \delta(j(x)). \quad (14.13)$$

14.2 Gaussian Functional Integral

Only very few functional integrals can be solved explicitly. The simplest nontrivial example is the Gaussian integral¹

$$\int \mathcal{D}j(x) e^{-\frac{i}{2} \int d^D x d^D x' j(x) M(x, x') j(x')}. \quad (14.14)$$

In the discretized form, this can be written as

$$\left[\prod_{\mathbf{n}} \int \frac{dj_{\mathbf{n}}}{\sqrt{2\pi i/\epsilon^D}} \right] e^{-\frac{i}{2} \epsilon^{2D} \sum_{\mathbf{n}, \mathbf{m}} j_{\mathbf{n}} M_{\mathbf{n}\mathbf{m}} j_{\mathbf{m}}}. \quad (14.15)$$

We may assume M to be a real symmetric functional matrix, since its antisymmetric part would not contribute to (14.14). Such a matrix may be diagonalized by a rotation

$$j_{\mathbf{n}} \rightarrow j'_{\mathbf{n}} = R_{\mathbf{n}\mathbf{m}} j_{\mathbf{m}}, \quad (14.16)$$

which leaves the measure of integration invariant

$$\frac{\partial(j_1, \dots, j_{\mathbf{n}})}{\partial(j'_1, \dots, j'_{\mathbf{n}})} = \det R^{-1} = 1. \quad (14.17)$$

¹Mathematically speaking, integrals with an imaginary quadratic exponent are more accurately called *Fresnel integrals*, but field theorists do not make this distinction.

In the diagonal form, the multiple integral (14.15) factorizes into a product of Gaussian integrals, which are easily calculated:

$$\prod_{\mathbf{n}} \int \frac{dj'_{\mathbf{n}}}{\sqrt{2\pi i/\epsilon^D}} e^{-\frac{i}{2}\epsilon^{2D} \sum_{\mathbf{n}} j'_{\mathbf{n}} M_{\mathbf{n}} j'_{\mathbf{n}}} = \prod_{\mathbf{n}} \frac{1}{\sqrt{-\epsilon^D M_{\mathbf{n}}}} = \det^{-1/2}(-\epsilon^D M). \quad (14.18)$$

On the right-hand side we have used the fact that the product of diagonal values $M_{\mathbf{n}}$ is equal to the determinant of M . The final result

$$\left[\prod_{\mathbf{n}} \int \frac{dj_{\mathbf{n}}}{\sqrt{2\pi i/\epsilon^D}} \right] e^{-\frac{i}{2}\epsilon^{2D} \sum_{\mathbf{n}, \mathbf{m}} j_{\mathbf{n}} M_{\mathbf{nm}} j_{\mathbf{m}}} = \det^{-1/2}(-\epsilon^D M) \quad (14.19)$$

is invariant under rotations, so that it holds also without diagonalizing the matrix.

This formula can be taken to the continuum limit of infinitely fine gratings $\epsilon \rightarrow 0$. Recall the well-known matrix formula

$$\det A = e^{\log \det A} = e^{\text{tr} \log A}, \quad (14.20)$$

and expand $\text{tr} \log A$ into power series as follows

$$\text{tr} \log A = \text{tr} \log [1 + (A - 1)] = -\text{tr} \sum_{k=1}^{\infty} \frac{(-)^k}{k} (A - 1)^k. \quad (14.21)$$

The advantage of this expansion is that when approximating the functional matrix A by the discrete matrix $\epsilon^D M$, the traces of powers of $\epsilon^D M$ remain well-defined objects in the continuum limit $\epsilon \rightarrow 0$:

$$\begin{aligned} \text{tr}(\epsilon^D M) &= \epsilon^D \sum_{\mathbf{n}} M_{\mathbf{nn}} \rightarrow \int d^D x M(x, x) \equiv \text{Tr} M, \\ \text{tr}(\epsilon^D M)^2 &= \epsilon^{2D} \sum_{\mathbf{n}, \mathbf{m}} M_{\mathbf{nm}} M_{\mathbf{mm}} \rightarrow \int d^D x d^D x' M(x, x') M(x', x) \equiv \text{Tr} M^2, \\ &\vdots \end{aligned} \quad (14.22)$$

We therefore rewrite the right-hand side of (14.19) as $\exp[-(1/2)\text{tr} \log(-\epsilon^D M)]$, and expand

$$\begin{aligned} \text{tr} \log(-\epsilon^D M) &= \text{tr} \log [1 + (-\epsilon^D M - 1)] \\ &\xrightarrow{\epsilon \rightarrow 0} - \sum_{k=1}^{\infty} \frac{(-)^k}{k} \int d^D x_1 \cdots d^D x_k \left[-M(x_1, x_2) - \delta^{(D)}(x_1 - x_2) \right] \times \cdots \\ &\quad \times \left[-M(x_2, x_3) - \delta^{(D)}(x_2 - x_3) \right] \left[-M(x_k, x_1) - \delta^{(D)}(x_k - x_1) \right]. \end{aligned} \quad (14.23)$$

The expansion on the right-hand side defines the trace of the logarithm of the functional matrix $-M(x, x')$, and will be denoted by $\text{Tr} \log(-M)$. This, in turn,

serves to define the *functional determinant* of $-M(x, x')$ by generalizing formula (14.20) to functional matrices:

$$\text{Det}(-M) = e^{\log \det(-M)} = e^{\text{Tr} \log(-M)}. \quad (14.24)$$

Thus we obtain for the functional integral (14.14) the result:

$$\int \mathcal{D}j(x) e^{-\frac{i}{2} \int d^D x d^D x' j(x) M(x, x') j(x')} = \text{Det}^{-1/2}(-M) = e^{-\frac{1}{2} \text{Tr} \log(-M)}. \quad (14.25)$$

This formula can be generalized to complex integration variables by separating the currents into real and imaginary parts, $j(x) = [j_1(x) + i j_2(x)]/\sqrt{2}$. Each integral gives the same functional determinant so that

$$\int \mathcal{D}j^*(x) \mathcal{D}j(x) e^{-i \int d^D x d^D x' j^*(x) M(x, x') j(x')} = e^{-\text{Tr} \log M}. \quad (14.26)$$

Here $M(x, x')$ is an arbitrary *Hermitian* matrix, and the measure of integration for complex variables $j(x)$ is defined as the product of the measures for real and imaginary parts: $\mathcal{D}j^*(x) \mathcal{D}j(x) \equiv \mathcal{D}j_1(x) \mathcal{D}j_2(x)$.

14.3 Functional Formulation for Free Quantum Fields

Having calculated the Gaussian functional integrals (14.25) and (14.26) we are able to perform the functional integrations over the generating functional (14.3) to derive its Fourier transform $\tilde{Z}[\phi]$. First we shall do so only for the free-field generating functional (7.843), which we shall equip with a subscript 0 to emphasize the free situation:

$$Z_0[j] = e^{-\frac{1}{2} \int d^4 y_1 d^4 y_2 j(y_1) G_0(y_1, y_2) j(y_2)}. \quad (14.27)$$

By writing $M(x, x')$ as

$$M(x, x') = -i G_0(x, x'), \quad (14.28)$$

the Gaussian functional integral (14.14) becomes

$$\int \mathcal{D}j(x) e^{-\frac{1}{2} \int d^D x d^D x' j(x) G_0(x, x') j(x')} = \text{Det}^{-1/2}(-i G_0). \quad (14.29)$$

This result can immediately be extended to calculate the functional Fourier transform of the generating functional $Z_0[j]$ defined in (14.3). Thus we want to form

$$\tilde{Z}_0[\phi] = \int \mathcal{D}j(x) e^{-\frac{1}{2} \int d^D x d^D x' j(x) G_0(x, x') j(x') + i \int j(x) \phi(x)}. \quad (14.30)$$

The extra term linear in $j(x)$ does not change the harmonic nature of the exponent. The integral can be reduced to the Gaussian form (14.29) by a simple quadratic completion process. For this manipulation it is useful to omit the spacetime indices, and use an obvious functional vector notation to rewrite (14.30) as

$$\tilde{Z}_0[\phi] = \int \mathcal{D}j e^{-\frac{i}{2} j^T \frac{1}{i} G_0 j + i j^T \phi}. \quad (14.31)$$

The exponent may be completed quadratically as

$$-\frac{i}{2} \left(j^T + iG_0^{-1} \phi \right)^T \frac{1}{i} G_0 \left(j + iG_0^{-1} \phi \right) + \frac{i}{2} \phi^T iG_0^{-1} \phi. \quad (14.32)$$

We now replace the variable $j + iG_0^{-1} \phi$ by j' which, in each of the infinite integrals, amounts only to a trivial shift of the center of integration. Thus

$$\tilde{Z}_0[\phi] = \left(\int \mathcal{D}j' e^{-\frac{i}{2} j'^T \frac{1}{i} G_0 j'} \right) e^{\frac{i}{2} \phi^T iG_0^{-1} \phi}. \quad (14.33)$$

We can now apply formula (14.26) and find

$$\tilde{Z}_0[\phi] = \text{Det}(M)^{1/2} e^{\frac{i}{2} \int d^D x d^D x' \phi(x) M^{-1}(x, x') \phi(x')}, \quad (14.34)$$

Inserting for $M(x, x')$ the functional matrix (14.28) we see that the exponent contains the free-particle Green function:

$$M^{-1}(x, x') = -iG_0(x, x') = (-\partial^2 - m^2) \delta^{(D)}(x - x'). \quad (14.35)$$

The determinant is a constant prefactor which does not depend on the field ϕ . We shall abbreviate it as a normalization factor

$$\mathcal{N} = \text{Det}^{-1/2}(-iG_0) = \text{Det}^{-1/2}(-\partial^2 - m^2). \quad (14.36)$$

With the help of Eq. (14.20), this can be rewritten as

$$\mathcal{N} = \exp \left\{ -\frac{1}{2} \text{Tr} \log(-\partial^2 - m^2) \right\}. \quad (14.37)$$

Inserting into (14.34) the differential operator (14.35), and performing a partial integration in spacetime, we can rewrite it as

$$\tilde{Z}_0[\phi] = \mathcal{N} e^{i \int d^D x \left[\frac{1}{2} (\partial \phi)^2 - \frac{m^2}{2} \phi^2 \right]} = \mathcal{N} e^{i \int d^D x \mathcal{L}_0(\phi, \partial \phi)}. \quad (14.38)$$

Thus the Fourier-transformed generating functional is, up to the normalization factor $\mathcal{N}$, just the exponential of the classical free-field action under consideration.

By Fourier-transforming $\tilde{Z}[\phi]$ according to formula (14.3), we recover the initial generating functional $Z_0[j]$. This procedure yields the famous functional integral representation for the free-particle generating functional

$$Z_0[j] = \mathcal{N} \int \mathcal{D}\phi(x) e^{i \int d^D x [\mathcal{L}_0(\phi, \partial \phi) + j(x) \phi(x)]}. \quad (14.39)$$

In this representation, the field is no longer an operator but a real variable that contains all quantum information via its field fluctuations. The functional integral over the ϕ -field is defined in (14.6). By analogy with (14.25), we have for the real field fluctuations the Gaussian formula

$$\int \mathcal{D}\phi(x) e^{\frac{i}{2} \int d^D x d^D x' \phi(x) M^{-1}(x, x') \phi(x')} = (\text{Det } M)^{\frac{1}{2}}, \quad (14.40)$$

valid for real symmetric functional matrices $M(x, x')$.

For complex fields $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$, there is a similar functional integral formula

$$\int \mathcal{D}\phi^*(x) \mathcal{D}\phi(x) e^{i \int d^D x d^D x' \phi^*(x) M^{-1}(x, x') \phi(x')} = \text{Det } M, \quad (14.41)$$

in which $M(x, x')$ is a Hermitian functional matrix. This follows directly from (14.26).

Let us use the formula (14.40) to cross-check the proper normalization of (14.39). At zero source, $Z_0[j]$ has to be equal to unity [compare (14.27)]. This is ensured if

$$\mathcal{N}^{-1} = \text{Det}^{1/2}(-iG_0) = \int \mathcal{D}\phi(x) e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)}. \quad (14.42)$$

Indeed, after a spacetime integration by parts, the right-hand side may be written as

$$\int \mathcal{D}\phi e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)} = \int \mathcal{D}\phi e^{i \int d^D x \frac{1}{2}[(\partial\phi)^2 - m^2\phi^2]} = \int \mathcal{D}\phi e^{i \int d^D x \phi(x) M^{-1}(x, x') \phi(x')}. \quad (14.43)$$

Applying now formula (14.39), and using (14.36), we verify that $Z_0[0] = 1$.

Using the expression (14.42) for the normalization factor, we can rewrite Eq. (14.38) for the Fourier transform $\tilde{Z}_0[\phi]$ as

$$\tilde{Z}_0[\phi] = \frac{e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)}}{\int \mathcal{D}\phi(x) e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)}}. \quad (14.44)$$

This ratio is obviously normalized:

$$\int \mathcal{D}\phi(x) \tilde{Z}_0[\phi] = 1. \quad (14.45)$$

Note that the expression (14.44) has precisely the form of the quantum mechanical version (1.491) of the thermodynamical Gibbs distribution (1.489):

$$w_n \equiv Z_{\text{QM}}^{-1}(t_b - t_a) e^{-iE_n(t_b - t_a)/\hbar}. \quad (14.46)$$

There exists a useful formula for harmonically fluctuating fields which are encountered in many physical contexts that can be derived immediately from this. Consider the correlation function of two exponentials of a free field $\phi(x)$. Inserting into Eq. (14.59) the special current

$$j_{12}(x) = a \int d^D x [a\phi(x - x_1) - b\phi(x - x_2)], \quad (14.47)$$

the partition function (14.27) reads

$$Z_0[j_{12}] = \text{Det}^{-1/2}(-iG_0) \int \mathcal{D}\phi(x) e^{ia\phi(x_1)} e^{-ib\phi(x_2)} e^{i \int d^D x [\mathcal{L}_0(\phi, \partial\phi)]}. \quad (14.48)$$

As such it coincides with the harmonic expectation value

$$\langle e^{ia\phi(x_1)} e^{-ib\phi(x_2)} \rangle. \quad (14.49)$$

Inserting (14.43) and performing the functional integral in (14.48) yields

$$\langle e^{ia\phi(x_1)} e^{-ib\phi(x_2)} \rangle = e^{-\frac{1}{2}[a^2 G(x_1, x_1) - 2abG(x_1, x_2) + b^2 G(x_2, x_2)]}. \quad (14.50)$$

In the brackets of the exponent we recognize the expectation values of pairs of fields

$$a^2 \langle \phi(x_1) \phi(x_1) \rangle - 2ab \langle \phi(x_1) \phi(x_2) \rangle + b^2 \langle \phi(x_2) \phi(x_2) \rangle, \quad (14.51)$$

such that we may also write (14.50) as

$$\langle e^{ia\phi(x_1)} e^{-ib\phi(x_2)} \rangle = \langle e^{ia\phi(x_1) - ib\phi(x_2)} \rangle = e^{-\frac{1}{2} \langle [a\phi(x_1) - b\phi(x_2)]^2 \rangle}. \quad (14.52)$$

Of course, this result may also be derived by using *field operators* and Wick's theorem along the lines of Subsection 7.17.1.

14.4 Interactions

Let us now include interactions. We have seen in Eq. (10.24) that the generating functional in the interaction picture [more precisely the functional $Z_D[j]$ of Eq. (10.22)] may simply be written as

$$Z[j] = e^{i \int d^D x \mathcal{L}^{\text{int}}(-i\delta/\delta j(x))} Z_0[j]. \quad (14.53)$$

This can immediately be Fourier-transformed to

$$\tilde{Z}[\phi] = \int \mathcal{D}j(x) e^{-i \int d^D x j(x) \phi(x)} \left[e^{i \int d^D x \mathcal{L}^{\text{int}}(\phi)(-i\delta/\delta j)} Z_0[j] \right]. \quad (14.54)$$

Removing the second exponential by a partial functional integration, we obtain

$$\begin{aligned} \tilde{Z}[\phi] &= e^{i \int d^D x \mathcal{L}^{\text{int}}(\phi)} \int \mathcal{D}j(x) e^{-i \int d^D x j(x) \phi(x)} Z_0[j] \\ &= e^{i \int d^D x \mathcal{L}^{\text{int}}(\phi, \partial\phi)} \mathcal{N} e^{i \int d^D x \frac{1}{2} [(\partial\phi)^2 - m^2 \phi^2]} \\ &= \frac{e^{i \int d^D x \mathcal{L}(\phi, \partial\phi)}}{\int \mathcal{D}\phi(x) e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)}}. \end{aligned} \quad (14.55)$$

The functional Fourier transform of this renders a generalization of (14.39) that includes interactions. In this way we have derived functional integral representation of the interacting theory:

$$\begin{aligned} Z[j] &= \mathcal{N} \int \mathcal{D}\phi(x) e^{i \int d^D x [\mathcal{L}(\phi, \partial\phi) + j(x)\phi(x)]} \\ &= \frac{\int \mathcal{D}\phi(x) e^{i \int d^D x [\mathcal{L}(\phi, \partial\phi) + j(x)\phi(x)]}}{\int \mathcal{D}\phi(x) e^{i \int d^D x \mathcal{L}_0(\phi, \partial\phi)(\phi)}}. \end{aligned} \quad (14.56)$$

This representation may be compared with the perturbation theoretic formula of operator quantum field theory

$$Z[j] = \langle 0 | T e^{i \int d^D x [\mathcal{L}^{\text{int}}(\phi) + j(x)\phi(x)]} | 0 \rangle, \quad (14.57)$$

where the symbol $\phi(x)$ denotes free-field operators, and the vacuum expectation value of products of these fields follow Wick's theorem. In the functional integral representations (14.54)–(14.56), on the other hand, $\phi(x)$ is a classical c -number field. All quantum properties of $Z[j]$ arise from the infinitely many integrals over $\phi(x)$, one at each spacetime point x , rather than from field operators.

Note that in formula (14.56), the full action appears in the exponent, whereas in (14.57), only the interacting part appears.

In contrast to $\tilde{Z}_0[\phi]$ of Eqs. (14.44) and (14.45), the amplitude for the interacting theory is no longer properly normalized. In fact, we know from the perturbative evaluation of (14.57) that it represents the sum of all vacuum diagrams displayed in (10.81). Since the denominator does not normalize $A[\phi]$ anyhow, it is convenient to drop it and work with the numerator only, using the unnormalized

$$Z[j] = \int \mathcal{D}\phi(x) e^{i \int d^D x [\mathcal{L}(\phi, \partial\phi) + j(x)\phi(x)]} \quad (14.58)$$

as the generating functional.

The normalization in (14.58) has an important advantage over the previous one in (14.56). In the euclidean formulation of the theory to be discussed in Section 14.5, it makes $Z[0]$ equal to the thermodynamic partition function of the system.

For free fields, $Z[0]$ is equal to the partition function of a set of harmonic oscillators of frequencies $\omega(\mathbf{k})$ for all momenta $\mathbf{k}$. This statement can be proved only in the lattice version of the theory. In the continuum limit the statement is nontrivial, since the determinants on the right-hand sides are infinite. However, we shall see in Section 14.7, Eqs. (14.123)–(14.133), that correct finite partition functions are obtained if the infinities are removed by the method of dimensional regularization, that was used in Section 11.5 to remove divergences from Feynman integrals.

Even though the operator formula (14.57) and the functional integral formula (14.58) are completely equivalent, there are important advantages of the latter. In some theories it may be difficult to find a canonically quantized set of free fields on which to construct an interaction representation for $Z[j]$ following Eq. (14.57). The photon field is an important example where it was quite hard to interpret the Hilbert space. In particular, we remind the reader of the problem that in the Gupta-Bleuler quantization scheme, the vacuum energy contains the quanta of two unphysical polarization states of the photon. Within the functional approach, this problem can easily be avoided as will be explained in Chapter 17.

A second and very important advantage is the possibility of deriving the Feynman rules, without any knowledge of the Hilbert space, directly from the representation (14.58). For this we simply take the non-quadratic piece of the action, which defines

the vertices of the perturbation expansion, outside the functional integral as in (14.53), i.e., we rewrite (14.58) as:

$$Z[j] = e^{i \int d^D x \mathcal{L}^{\text{int}}(-i\delta/\delta j(x))} \int \mathcal{D}\phi(x) e^{i \int d^D x [\mathcal{L}_0(\phi, \partial\phi) + j(x)\phi(x)]}. \quad (14.59)$$

Using (14.34), this reads more explicitly

$$Z[j] = e^{i \int d^D x \mathcal{L}^{\text{int}}(-i\delta/\delta j(x))} \int \mathcal{D}\phi(x) e^{[\frac{i}{2} \int d^D x d^D x' \phi(x) iG_0^{-1}(x, x') \phi(x') + j(x)\phi(x)]}. \quad (14.60)$$

A shift in the field variables to

$$\phi'(x) = \phi(x) + \int dy G_0(x, x') j(x'), \quad (14.61)$$

and a quadratic completion lead to

$$\begin{aligned} Z[j] &= e^{i \int d^D x \mathcal{L}^{\text{int}}(-i\delta/\delta j(x))} e^{-\frac{1}{2} \int d^D x d^D x' j(x) G_0(x, x') j(x')} \\ &\quad \times \int \mathcal{D}\phi'(x) e^{\frac{i}{2} \int d^D x d^D x' \phi'(x) iG_0^{-1}(x, x') \phi'(x')}. \end{aligned} \quad (14.62)$$

The functional integral over the shifted field $\phi'(x)$ can now be performed with the help of formula (14.25), inserting there $M(x, x') = -iG_0(x, x')$. The result is, recalling (14.36),

$$\int \mathcal{D}\phi'(x) e^{\frac{i}{2} \int d^D x d^D x' \phi'(x) iG_0^{-1}(x, x') \phi'(x')} = \text{Det}^{-1/2}(-iG_0), \quad (14.63)$$

such that we find

$$Z[j] = \text{Det}^{-1/2}(-iG_0) e^{i \int d^D x \mathcal{L}^{\text{int}}(-i\delta/\delta j(x))} e^{-\frac{1}{2} \int d^D x d^D x' j(x) G_0(x, x') j(x')}. \quad (14.64)$$

Expanding the prefactor in (14.60) in a power series yields all terms of the perturbation expansion (10.29). They correspond to the Wick contractions in Section 10.3.1, with the associated Feynman diagrams. The free-field propagators are the functional inverse of the operators between the fields in the quadratic part of the Lagrangian. If this is written as

$$\frac{i}{2} \int d^D x d^D x' \phi(x) D(x, x') \phi(x'), \quad (14.65)$$

then

$$G_0(x, x') = iD^{-1}(x, x'). \quad (14.66)$$

This formal advantage of obtaining perturbation expansions from the functional integral representations has far-reaching consequences. We have seen in Chapter 11 that the evaluation of the perturbation series proceeds most conveniently by Wick-rotating all energy integrations to make them run along the imaginary axes in the complex energy plane. In this way one avoids the singularities in the propagators

that would be encountered at the physical particle energies. In Section 10.7, on the other hand, these singularities were shown to be responsible for the fact that particles leave a scattering region and form asymptotic states. Hence, Wick-rotated perturbation expansions describe a theory which does not possess any particles states. In fact, they cannot be described by field operators creating particle states in a Hilbert space. Such states can be obtained from a simple modification of the above functional integral representation of the generating functional $Z[j]$. We simply perform the x -space version of the Wick-rotation that was illustrated before on page 495 in Fig. 7.2.

14.5 Euclidean Quantum Field Theory

In Eq. (7.136), we replaced the coordinates x^μ ($\mu = 0, 1, 2, 3$) in $D = 4$ spacetime dimensions by the *euclidean coordinates* $x_E^\mu = (x^1, \dots, x^3, x^4 = -ix^0)$. The same operation may be done to the time x^0 in any dimensions. Under this replacement, the action

$$\mathcal{A} \equiv \int d^D x \mathcal{L}(\phi, \partial_E \phi) \equiv \int d^D x \left\{ \left[\frac{1}{2}(\partial \phi)^2 - \frac{m^2}{2}\phi^2 \right] + \mathcal{L}^{\text{int}}(\phi) \right\} \quad (14.67)$$

goes over into i times the *euclidean action*

$$\mathcal{A}_E = \int d^D x_E \left\{ \left[\frac{1}{2}(\partial_E \phi)^2 + \frac{m^2}{2}\phi^2 \right] + \mathcal{L}^{\text{int}}(\phi) \right\}. \quad (14.68)$$

The euclidean versions of the Gaussian integral formulas (14.40) and (14.89) are

$$\int \mathcal{D}\phi(x) e^{-\frac{1}{2} \int d^D x d^D x' \phi(x) M(x, x') \phi(x')} = (\text{Det } M)^{-\frac{1}{2}}, \quad (14.69)$$

and

$$\int \mathcal{D}\phi^*(x) \mathcal{D}\phi(x) e^{-\int d^D x d^D x' \phi^*(x) M(x, x') \phi(x')} = (\text{Det } M)^{-1}, \quad (14.70)$$

for complex fields $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$, where $\mathcal{D}\phi^*(x) \mathcal{D}\phi(x) \equiv \mathcal{D}\phi_1(x) \mathcal{D}\phi_2(x)$.

The amplitude (14.55) becomes

$$w_E[\phi] = \frac{e^{-\int d^D x_E \mathcal{L}_E(\phi, \partial \phi)}}{\int \mathcal{D}\phi(x) e^{-\int d^D x_E \mathcal{L}_{E0}(\phi, \partial \phi)}}. \quad (14.71)$$

The normalized version of this,

$$w[\phi] = \frac{e^{-\int d^D x_E \mathcal{L}_E(\phi, \partial \phi)}}{\int \mathcal{D}\phi(x) e^{-\int d^D x_E \mathcal{L}_E(\phi, \partial \phi)}}, \quad (14.72)$$

represents the functional version of the proper quantum statistical Gibbs distribution corresponding to (14.46) [recall (1.489)]:

$$w_n = \frac{e^{-E_n/k_B T}}{\sum_n e^{-E_n/k_B T}}. \quad (14.73)$$

The functional integral representation for the unnormalized generating functional of all Wick-rotated Green functions corresponding to (14.58) is then

$$Z_E[j] = \int \mathcal{D}\phi(x) e^{-\int d^D x_E [\mathcal{L}_E(\phi, \partial_E \phi) - j(x)\phi(x)]}. \quad (14.74)$$

The euclidean action corresponds to an energy of a field configuration. The integrand plays the role of a Boltzmann factor and gives the relative probability for this configuration to occur in a thermodynamic ensemble.

We now understand the advantage of working with the unnormalized functional integral: At zero external source, $Z_E[j]$ corresponds precisely to the thermodynamic partition function of the system. This will be seen explicitly in the examples in Section 14.7.

14.6 Functional Integral Representation for Fermions

If we want to use the functional technique to also describe the statistical properties of fermions, some modifications are necessary. Then the fields must be taken to be anticommuting c -numbers. In mathematics, such objects form a so-called *Grassmann algebra* G . If ξ, ξ' are real elements of G , then

$$\theta\theta' = -\theta'\theta. \quad (14.75)$$

A trivial consequence of this condition is that the square of each Grassmann element vanishes, i.e., $\theta^2 = 0$. If $\theta = \theta_1 + i\theta_2$ is a complex element of G , then $\theta^2 = -\theta^*\theta = -2i\theta_1\theta_2$ is nonzero, but $(\theta^*\theta)^2 = (\theta\theta)^2 = 0$.

All properties of operator quantum field theory for fermions can be derived from functional integrals if we find an appropriate extension of the integral formulas in the previous sections to Grassmann variables. Integrals are linear functionals. For Grassmann variables, these are completely determined from the following basic integration rules, which for real θ are

$$\int \frac{d\theta}{\sqrt{2\pi}} \equiv 0, \quad \int \frac{d\theta}{\sqrt{2\pi}} \theta \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}} \theta^n \equiv 0, \quad n > 1. \quad (14.76)$$

For complex variable $\theta = (\theta_1 + i\theta_2)/\sqrt{2}$, these lead to

$$\int \frac{d\theta}{\sqrt{2\pi}} \equiv 0, \quad \int \frac{d\theta^*}{\sqrt{2\pi}} \theta \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}} \theta^* \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}} \frac{d\theta^*}{\sqrt{2\pi}} (\theta^*\theta)^n \equiv -\delta_{n1}, \quad (14.77)$$

with the definition $d\theta d\theta^* \equiv -id\theta_1 d\theta_2$.

Note that these integration rules make the linear operation of integration in (14.76) coincide with the linear operation of *differentiation*. A function $F(\theta)$ of a real Grassmann variable θ , is determined by only two parameters: the zeroth- and the first-order Taylor coefficients. Indeed, due to the property $\theta^2 = 0$, the Taylor

series has only two terms $F(\theta) = F_0 + F'\theta$, where $F_0 = F(0)$ and $F' \equiv dF(\theta)/d\theta$. But according to (14.76), also the integral gives F' :

$$\int \frac{d\theta}{\sqrt{2\pi}} F(\theta) = F'. \quad (14.78)$$

The coincidence of integration and differentiation has the important consequence that any changes in integration variables will not transform with the Jacobian, but rather with the inverse Jacobian:

$$\int \frac{d\theta}{\sqrt{2\pi}} = a \int \frac{d(a\theta)}{\sqrt{2\pi}}, \quad (14.79)$$

We shall use this transformation property below in Eq. (14.85).

As far as perturbation theory is concerned, it is sufficient to define only Gaussian functional integrals such as (14.40) and (14.89). In the discretized form, we may derive the formula

$$\prod_{\mathbf{n}} \left[\int_{-\infty}^{\infty} \frac{d\theta_{\mathbf{n}}}{\sqrt{2\pi i \epsilon^D}} \right] \exp \left(\frac{i}{2} \epsilon^{2D} \sum_{\mathbf{m}, \mathbf{n}} \theta_{\mathbf{m}} M_{\mathbf{mn}} \theta_{\mathbf{n}} \right) = \det^{1/2}(\epsilon^D M). \quad (14.80)$$

The right-hand side is the inverse of the bosonic result (14.40). In addition, there is an important difference: only the *antisymmetric* part of the functional matrix contributes.

If the matrix $M_{\mathbf{mn}}$ is Hermitian, complex Grassmann variables are necessary to produce a nonzero Gaussian integral. For complex variables we have

$$\prod_{\mathbf{n}} \left[\int \frac{d\theta_{\mathbf{n}} d\theta_{\mathbf{n}}^*}{\sqrt{2\pi i \epsilon^D} \sqrt{2\pi i \epsilon^D}} \right] \exp \left(i \epsilon^{2D} \sum_{\mathbf{m}, \mathbf{n}} \theta_{\mathbf{m}}^* M_{\mathbf{mn}} \theta_{\mathbf{n}} \right) = \det(\epsilon^D M), \quad (14.81)$$

the right-hand side being again the inverse of the corresponding bosonic result (14.89):

We first prove the latter formula. After bringing the matrix $M_{\mathbf{mn}}$ to a diagonal form via a unitary transformation, we obtain the product of integrals

$$\prod_{\mathbf{n}} \left[\int \frac{d\theta_{\mathbf{n}} d\theta_{\mathbf{n}}^*}{\sqrt{2\pi i \epsilon^D} \sqrt{2\pi i \epsilon^D}} \right] \exp \left(i \epsilon^{2D} \sum_{\mathbf{n}} \theta_{\mathbf{n}}^* M_{\mathbf{n}} \theta_{\mathbf{n}} \right). \quad (14.82)$$

Expanding the exponentials into a power series leaves only the first two terms, since $(\theta_{\mathbf{n}}^* \theta_{\mathbf{n}})^2 = 0$, so that the integral reduces to

$$\prod_{\mathbf{n}} \int \frac{d\theta_{\mathbf{n}} d\theta_{\mathbf{n}}^*}{\sqrt{2\pi i \epsilon^D} \sqrt{2\pi i \epsilon^D}} (1 + i \epsilon^{2D} \theta_{\mathbf{n}}^* M_{\mathbf{n}} \theta_{\mathbf{n}}). \quad (14.83)$$

Each of these integrals is performed via the formulas (14.77), and we obtain the product of eigenvalues $M_{\mathbf{n}}$, which is the determinant:

$$\prod_{\mathbf{n}} M_{\mathbf{n}} = \det M. \quad (14.84)$$

For real fermion fields, we observe that an arbitrary real antisymmetric matrix $M_{\mathbf{mn}}$ can always be brought to a canonical form $\mathbf{C}$, that is zero except for 2×2 matrices $c = i\sigma^2$ along the diagonal, by a real orthogonal transformation T . Thus $M = T^T \mathbf{C} T$. The matrix $\mathbf{C}$ has a unit determinant so that $\det T = \det^{1/2}(M)$. Let $\theta'_{\mathbf{m}} \equiv T_{\mathbf{mn}} \theta_{\mathbf{n}}$, then the measure of integration in (14.80) changes according to (14.79) as follows:

$$\prod_{\mathbf{n}} d\theta_{\mathbf{n}} = \det T \prod_{\mathbf{n}} d\theta'_{\mathbf{n}}. \quad (14.85)$$

Applying now the formulas (14.76), the Grassmannian functional integral (14.80) can be evaluated as follows:

$$\begin{aligned} \prod_{\mathbf{n}} \left[\int \frac{d\theta_{\mathbf{n}}}{\sqrt{2\pi i \epsilon^D}} \right] \exp \left(i \epsilon^{2D} \sum_{k,l} \theta_{\mathbf{k}} M_{\mathbf{kl}} \theta_{\mathbf{l}} \right) &= \det T \prod_{\mathbf{n}} \left[\int \frac{d\theta'_{\mathbf{n}}}{\sqrt{2\pi i \epsilon^D}} \right] \exp \left(\sum_{\mathbf{m},\mathbf{n}} \theta'_{\mathbf{m}} C_{\mathbf{mn}} \theta'_{\mathbf{n}} \right) \\ &= \det^{1/2}(i \epsilon^D M). \end{aligned} \quad (14.86)$$

The integrals over θ_n in one dimension decompose into a product of two-dimensional Grassmannian integrals involving the antisymmetric unit matrix $c = i\sigma_2$. They have the generic form

$$\prod_n \left[\int \frac{d\theta'_{2n}}{\sqrt{2\pi i \epsilon^D}} \right] \frac{d\theta'_{2n+1}}{\sqrt{2\pi i \epsilon^D}} (1 + i \epsilon^{2D} \theta'_{2n} \theta'_{2n+1}) = \epsilon^{2D}. \quad (14.87)$$

There is one such factor for every second lattice site, which changes $\det T = \det^{1/2} M$ into $\det^{1/2}(\epsilon^D M)$, thus proving (14.80). See [4].

In the continuum limit, the result of this discussion can be summarized in an extension of the Gaussian functional integral formulas (14.40) and (14.26) to

$$\int \mathcal{D}\phi(x) e^{\frac{i}{2} \int d^D x d^D x' \phi(x) M(x, x') \phi(x')} = \text{Det}^{\mp \frac{1}{2}} M, \quad (14.88)$$

where $M(x, x')$ is real symmetric or antisymmetric for bosons or fermions, respectively, and

$$\int \mathcal{D}\phi^*(x) \mathcal{D}\phi(x) e^{i \int d^D x d^D x' \phi^*(x) M(x, x') \phi(x')} = \text{Det}^{\mp 1} M, \quad (14.89)$$

where the matrix is Hermitian.

The functional integral formulation of fermions follows now closely that of bosons. For N relativistic real fermion fields χ_a , we can obtain an amplitude $\tilde{Z}[\chi]$ from the Fourier transform

$$\tilde{Z}[\chi] = \int \mathcal{D}j(x) Z[j] e^{-i \int d^D x j_a(x) \chi_a(x)}, \quad (14.90)$$

and find

$$\tilde{Z}[\chi] = \frac{e^{i \int d^D x \mathcal{L}(\chi, \partial\chi)}}{\left[\int \mathcal{D}\chi e^{i \int d^D x \mathcal{L}_0(\chi, \partial\chi)} \right]}. \quad (14.91)$$

The functional

$$Z[j] = \mathcal{N} \prod_a \left[\int \mathcal{D}\chi_a \right] e^{i \int d^D x \mathcal{L}(\chi, \partial\chi)}, \quad (14.92)$$

with a normalization factor

$$\mathcal{N}^{-1} = \prod_a \left[\int \mathcal{D}\chi_a \right] e^{i \int d^D x \mathcal{L}_0(\chi, \partial\chi)}, \quad (14.93)$$

provides us with a functional integral representation of the generating functional of all fermionic Green functions.

An obvious extension of this holds for complex fermion fields. In the case of a Dirac field, for example, where the sources j are commonly denoted by η , we obtain

$$Z[\eta, \bar{\eta}] = \mathcal{N} \int \mathcal{D}\psi \mathcal{D}\psi^* e^{i \int d^D x [\bar{\psi}(i\partial - m)\psi + \mathcal{L}^{\text{int}}(\psi) + \bar{\eta}\psi + \bar{\psi}\eta]} \quad (14.94)$$

with

$$\mathcal{N}^{-1} = \int \mathcal{D}\psi \mathcal{D}\psi^* e^{i \int d^D x \bar{\psi}(i\partial - m)\psi} = \text{Det } iG_0^{-1}(x, x') = \text{Det } (i\partial - m). \quad (14.95)$$

As in the boson case, we shall from now on work with the unnormalized functional without the factor $\mathcal{N}$,

$$Z[\eta, \bar{\eta}] = \int \mathcal{D}\psi e^{i \int d^D x [\bar{\psi}(i\partial - m)\psi + \mathcal{L}^{\text{int}}(\psi) + \bar{\eta}\psi + \bar{\psi}\eta]}, \quad (14.96)$$

which again has the advantage that the euclidean version of $Z[0, 0]$ becomes directly the thermodynamic partition function of the system.

The functional representations of the generating functionals can of course be continued to a euclidean form, as in Section 14.5, thereby replacing operator quantum physics by statistical physics. The corresponding Gaussian formulas for boson and fermion fields are the obvious generalization of Eqs. (14.88) and (14.89):

$$\int \mathcal{D}\phi(x) e^{-\frac{1}{2} \int d^D x d^D x' \phi(x) M(x, x') \phi(x')} = \text{Det } \mp^{\frac{1}{2}} M, \quad (14.97)$$

and

$$\int \mathcal{D}\phi(x) \mathcal{D}\phi^*(x) e^{-\int d^D x d^D x' \phi^*(x) M(x, x') \phi(x')} = \text{Det } \mp^1 M. \quad (14.98)$$

Here we have defined the measure of the euclidean functional integration in the same way as before in Eqs. (14.88) and (14.89), except without the factors i under the square roots. The euclidean version of the generating functional (14.94) can be used to obtain all Wick-rotated Green functions from functional derivatives $Z[\eta, \bar{\eta}]$.

As a side result of the above development we can state the following functional integral formulas known under the name *Hubbard-Stratonovich transformations*:

$$\begin{aligned} \int \mathcal{D}\varphi(\mathbf{x}, t) e^{\frac{i}{2} \int d^3x dt d^3x' dt' [\varphi(\mathbf{x}, t) A(\mathbf{x}, t; \mathbf{x}', t') \varphi(\mathbf{x}', t') + 2j(\mathbf{x}, t) \varphi(\mathbf{x}, t) \delta^3(\mathbf{x} - \mathbf{x}') \delta(t - t')]} \\ = e^{i(\pm \frac{i}{2} \text{Trlog} \left\{ \frac{1}{i} \right\} A) - \frac{i}{2} \int d^3x dt d^3x' dt' j(\mathbf{x}, t) A^{-1}(\mathbf{x}, t; \mathbf{x}', t') j(\mathbf{x}', t')}, \end{aligned} \quad (14.99)$$

$$\begin{aligned} \int \mathcal{D}\psi^*(\mathbf{x}, t) \mathcal{D}\psi(\mathbf{x}, t) e^{i \int d^3x dt d^3x' dt' \{ \psi^*(\mathbf{x}, t) A(\mathbf{x}, t; \mathbf{x}', t') \psi(\mathbf{x}', t') + [\eta^*(\mathbf{x}, t) \psi(\mathbf{x}) \delta^3(\mathbf{x} - \mathbf{x}') \delta(t - t') + \text{c.c.}] \}} \\ = e^{i(\pm i \text{Trlog} A) - i \int d^3x dt d^3x' dt' \eta^*(\mathbf{x}, t) A^{-1}(\mathbf{x}, t; \mathbf{x}', t') \eta(\mathbf{x}', t')}. \end{aligned} \quad (14.100)$$

These formulas will be needed repeatedly in the remainder of this text. They are the basis for the reformulation of many interacting quantum field theories in terms of *collective quantum fields*.

14.7 Relation Between $Z[j]$ and the Partition Function

The introduction of the unnormalized functional integral representation (14.58) for $Z[j]$ was motivated by the fact that, in the euclidean version (14.74), $Z[0]$ is equal to the thermodynamic partition function of the system, except for a trivial overall factor. Let us verify this for a free field theory in $D = 1$ dimension. Then $Z_E[0]$ of Eq. (14.74) becomes

$$Z_\omega = \int \mathcal{D}x \exp \left\{ - \int_0^\beta d\tau \left[\frac{1}{2} \dot{x}^2(\tau) + \frac{\omega^2}{2} x^2(\tau) \right] \right\}. \quad (14.101)$$

For $D = 1$, the fields $\phi(\tau)$ may be interpreted as paths $x(\tau)$ in imaginary time $\tau = -it$, and we have changed the notation accordingly. In the exponent, we recognize the euclidean version

$$\mathcal{A}_E = \int_0^\beta d\tau \left[\frac{1}{2} \dot{x}^2(\tau) + \frac{\omega^2}{2} x^2(\tau) \right] \quad (14.102)$$

of the action of the harmonic oscillator:

$$\mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{1}{2} \dot{x}^2(t) - \frac{\omega^2}{2} x^2(t) \right], \quad (14.103)$$

for $t_b - t_a = -i\hbar\beta = -i\hbar/k_B T$. Thus Z_ω in expression (14.114) is a quantum-statistical *path integral* for a harmonic oscillator. The measure of path integration is defined as a product of integrals on a lattice of points $\tau_n = n\epsilon$ with $n = 0, \dots, N+1$ on the τ -axis:

$$\int \mathcal{D}x(\tau) = \prod_{n=0}^N \int \frac{dx_n}{\sqrt{2\pi\epsilon}}, \quad (14.104)$$

where $x_n \equiv x(\tau_n)$ and $N + 1 = \hbar\beta/\epsilon$. For a finite τ -interval $\hbar\beta$, the paths have to satisfy periodic boundary conditions

$$x(\hbar\beta) = x(0), \quad (14.105)$$

as a reflection of the quantum-mechanical trace. On the τ -lattice, this implies $x_{N+1} = x_0$, and the action becomes

$$\mathcal{A}_E^N = \frac{1}{2}\epsilon \sum_{n=1}^{N+1} \left[\frac{(x_n - x_{n-1})^2}{\epsilon^2} + \omega^2 x_n^2 \right]. \quad (14.106)$$

This can be rewritten as

$$\mathcal{A}_E^N = \frac{1}{2\epsilon} \sum_{n=1}^{N+1} x_n (-\epsilon^2 \nabla \bar{\nabla} + \epsilon^2 \omega^2) x_n, \quad (14.107)$$

where $\nabla \bar{\nabla} x$ denotes the lattice version of $\ddot{x}$. It may be represented as an $(N + 1) \times (N + 1)$ -matrix

$$-\epsilon^2 \nabla \bar{\nabla} = \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 & -1 \\ -1 & 2 & -1 & \dots & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & & 0 & \dots & -1 & 2 & -1 \\ -1 & 0 & 0 & \dots & 0 & -1 & 2 \end{pmatrix}. \quad (14.108)$$

The Gaussian functional integral can now be evaluated using formula (14.40), and we obtain

$$Z_\omega = \det_{N+1} [-\epsilon^2 \nabla \bar{\nabla} + \epsilon \omega^2]^{-1/2}. \quad (14.109)$$

The determinant is calculated recursively,² and yields

$$Z_\omega = \frac{1}{2 \sinh(\hbar \tilde{\omega} \beta / 2)}, \quad (14.110)$$

where $\tilde{\omega}$ is the auxiliary frequency

$$\tilde{\omega} \equiv \frac{2}{\epsilon} \operatorname{arsinh} \frac{\omega \epsilon}{2}. \quad (14.111)$$

In the continuum limit $\epsilon \rightarrow 0$, the frequency $\tilde{\omega}$ goes against ω , and Z_ω becomes

$$Z_\omega = \frac{1}{2 \sinh(\hbar \omega \beta / 2)}. \quad (14.112)$$

This can be expanded as

$$Z_\omega = e^{-\hbar \omega / 2k_B T} + e^{-3\hbar \omega / 2k_B T} + e^{-5\hbar \omega / 2k_B T} + \dots, \quad (14.113)$$

²See the textbook [1] and Section 2.12 of the textbook [2].

which is the quantum statistical partition function of the harmonic oscillator, as we wanted to prove. The ground state has a nonzero energy, as observed in the operator discussion in Chapter 7.32.

For the quantum-mechanical version of the functional integral (14.114)

$$Z_\omega = \int \mathcal{D}x \exp \left\{ i \int_{t_a}^{t_b} dt \left[\frac{1}{2} \dot{x}^2(t) - \frac{\omega^2}{2} x^2(t) \right] \right\}, \quad (14.114)$$

we obtain, with the measure of functional integration analog to (14.104)

$$\int \mathcal{D}x(t) = \prod_{n=0}^N \int \frac{dx_n}{\sqrt{2\pi i \epsilon}}, \quad (14.115)$$

and the use of the Gaussian integral formula (14.40), the result

$$Z_\omega = \det_{N+1} [-\epsilon^2 \nabla \nabla - \epsilon \omega^2]^{-1/2}. \quad (14.116)$$

Thus we only have to replace $\omega \rightarrow i\omega$ in (14.111)–(14.112). In the continuum limit, we therefore obtain

$$Z_\omega = \frac{1}{2 \sin(\hbar \omega \beta / 2)}. \quad (14.117)$$

We end this section by mentioning that the path-integral representation of the partition function (14.114) with the integration measure (14.104) can be obtained from a euclidean phase space path integral³

$$Z_\omega = \int \int \mathcal{D}x(\tau) \frac{\mathcal{D}p(\tau)}{2\pi\hbar} \exp \left\{ \int_0^\beta d\tau \left[ip\dot{x} - \frac{1}{2}p^2 - \frac{\omega^2}{2}x^2 \right] \right\} \quad (14.118)$$

by going to a τ -lattice and integrating out the momentum variables. The momentum integrals give the factors $\sqrt{2\pi\epsilon}$ in the denominators of the measure (14.104). In the quantum-mechanical version of (14.118)

$$Z_\omega = \int \int \mathcal{D}x(t) \frac{\mathcal{D}p(t)}{2\pi\hbar} \exp \left\{ i \int_{t_a}^{t_b} dt \left[p\dot{x} - \frac{1}{2}p^2 - \frac{\omega^2}{2}x^2 \right] \right\}, \quad (14.119)$$

the p -integrals produce the denominators containing the factors $\sqrt{i}$ in the measure (14.104).

The measure of functional integration on the τ -lattice

$$\prod_{n=0}^N \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] \quad (14.120)$$

is the obvious generalization of the classical statistical weight in phase space

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \quad (14.121)$$

³For a detailed discussion of the measure see Chapters 2 and 7 in the textbook [2].

to fluctuating paths with many variables $x_n = x(\tau_n)$.

For completeness, we write down the free energy $F_\omega = -\beta \log Z_\omega$ associated with the partition function (14.112):

$$F_\omega = \frac{1}{\beta} \log[2 \sinh(\hbar\omega\beta/2)] = \frac{\hbar\omega}{2} + \frac{1}{\beta} \log(1 - e^{-\beta\hbar\omega}). \quad (14.122)$$

At zero temperatures, only the ground-state oscillations contribute.

The detailed time-sliced calculation of the partition functions has to be compared with the formal evaluation of the partition function (14.114) according to formula (14.69), which would yield

$$\begin{aligned} Z_\omega &= \int \mathcal{D}x(\tau) \exp \left\{ - \int_0^\beta d\tau \left[\frac{1}{2} \dot{x}^2(\tau) + \frac{\omega^2}{2} x^2(\tau) \right] \right\} \\ &= \text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2). \end{aligned} \quad (14.123)$$

In this continuum formulation, the right-hand side is at first meaningless. It differs from the results obtained by proper time-sliced calculations (14.109)–(14.112) by a temperature-dependent infinite overall factor. In order to see what this factor is, we note that for a periodic boundary condition (14.105), the eigenvectors of the matrix $-\partial_\tau^2 + \omega^2$ are $e^{-i\omega_m\tau}$ with eigenvalues $\omega_m^2 + \omega^2$. Since ω_m grows with m like m^2 , the functional determinant $\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)$ is strongly divergent. Indeed, the bosonic lattice result (14.112) can only be obtained in the limit $\epsilon \rightarrow 0$ after dividing out of the the lattice result (14.109) an equally divergent ω -independent functional determinant and calculating the ratio

$$\frac{\det_{N+1}[-\epsilon^2 \nabla \bar{\nabla} - \epsilon \omega^2]^{-1/2}}{\hbar\beta \det'_{N+1}[-\epsilon^2 \nabla \bar{\nabla} - \epsilon \omega^2]^{-1/2}} \xrightarrow{\epsilon \rightarrow 0} \frac{\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)}{\hbar\beta \text{Det}'^{-1/2}(-\partial_\tau^2)}. \quad (14.124)$$

The prime in the denominator indicates that the zero-frequency ω_0 must be omitted to obtain a finite result. The factor $1/\hbar\beta$ is the regularized contribution of the zero frequency. This follows from a simple integral consideration. An integral

$$\int_{-b/2}^{b/2} \frac{dx}{\sqrt{2\pi}} e^{-\omega^2 x^2/2} \quad (14.125)$$

gives $1/\omega$ only for finite $\omega (\gg 1/b)$. In the limit $\omega \rightarrow 0$, it gives $b/\sqrt{2\pi}$. In the path integral, the zero mode is associated with the fluctuations of the average of the path $x(\tau)$. To indicate this origin of the factor $\hbar\beta$ in the ratio (14.124), we may write (14.124) as

$$\frac{\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)}{\text{Det}_R^{-1/2}(-\partial_\tau^2)}, \quad (14.126)$$

where the subscript R indicates the above regularization.

Explicitly, the ratio (14.124) is calculated from the product of eigenvalues:

$$\frac{\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)}{\hbar\beta \text{Det}'^{-1/2}(-\partial_\tau^2)} = \frac{1}{\hbar\beta\omega} \prod_{m>0} \frac{\omega_m^2}{\omega_m^2 + \omega^2}. \quad (14.127)$$

The product can be found in the tables⁴:

$$\prod_{m \neq 0} \frac{\omega_m^2}{\omega_m^2 + \omega^2} = \frac{\hbar\beta\omega/2}{\sinh(\hbar\beta\omega/2)}, \quad (14.128)$$

so that (14.127) is equal to $1/2 \sinh(\hbar\beta\omega/2)$, and the properly renormalized partition function (14.123) yields the lattice result (14.112). In a lattice calculation, the determinant $\text{Det}_R^{-1/2}(-\partial_\tau^2)$ for $\beta \rightarrow \infty$ is equal to unity.

It is curious to see that a formal evaluation of the functional determinant via the analytic regularization procedure of Sections 7.12 and 11.5 is indifferent to this denominator. It produces precisely the same result from the formal expression (14.123) as from the proper lattice calculation. Recalling formula (11.134) and setting $D = 1$, we find

$$\begin{aligned} \text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2) &= \exp \left\{ -\frac{1}{2} \text{Tr} \log(-\partial_\tau^2 + \omega^2) \right\} \\ &= \exp \left\{ -\frac{1}{2} \beta \hbar \int \frac{d\omega'}{2\pi} \log(\omega'^2 + \omega^2) \right\} = e^{-\beta \frac{\hbar\omega}{2}}. \end{aligned} \quad (14.129)$$

The exponent gives precisely the free energy at zero temperatures in Eq. (14.122).

We now admit finite temperatures. For this purpose, we have to replace the integral over ω' by a sum over Matsubara frequencies (2.415), and evaluate

$$\frac{1}{\hbar\beta} \sum_m \log(\omega_m^2 + \omega^2) = \int \frac{d\omega'}{2\pi} \log(\omega'^2 + \omega^2) + \left(\frac{1}{\hbar\beta} \sum_m - \int \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + \omega^2). \quad (14.130)$$

In contrast to the first term whose evaluation required the analytic regularization, the second term is finite. It can be rewritten as

$$- \left(\frac{1}{\hbar\beta} \sum_m - \int \frac{d\omega_m}{2\pi} \right) \int_{\omega^2}^{\infty} d\omega'^2 \frac{1}{\omega_m^2 + \omega'^2}. \quad (14.131)$$

Recalling the summation formula (2.424), this becomes

$$\begin{aligned} - \int_{\omega^2}^{\infty} \frac{d\omega'^2}{2\omega'} \left[\left\{ \frac{\coth(\hbar\beta\omega'/2)}{\tanh(\hbar\beta\omega'/2)} \right\} - 1 \right] &= \pm \int_{\omega^2}^{\infty} \frac{d\omega'^2}{2\omega'} \frac{2}{e^{\beta\hbar\omega'} \mp 1} \\ &= k_B T 2 \log(1 \mp e^{-\beta\hbar\omega}). \end{aligned} \quad (14.132)$$

For later applications, we have treated also the case of fermionic Matsubara frequencies (the lower case). Together with the zero-temperature result (14.129), we find at any temperature

$$\begin{aligned} Z_\omega &= e^{-\beta F_\omega} = \text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2) = \exp \left\{ -\frac{1}{2} \text{Tr} \log(-\partial_\tau^2 + \omega^2) \right\} \\ &= \exp \left\{ - \left[\beta \frac{\hbar\omega}{2} + \log(1 - e^{-\beta\hbar\omega}) \right] \right\}, \end{aligned} \quad (14.133)$$

in agreement with (14.122).

⁴I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 1.431.2: $\sinh x = \prod_{m=1}^{\infty} (1 + x^2/m^2\pi^2)$.

14.8 Bosons and Fermions in a Single State

The discussion in the last section cannot be taken over to fermionic variables $x(\tau)$. For fermions the action (14.114) vanishes identically, as a consequence of the symmetry of the functional matrix $D(\tau, \tau') = (-\partial_\tau^2 + \omega^2)\delta(\tau - \tau')$. A fermionic version of the above path integral can only be introduced within the canonical formulation (14.119) of the harmonic path integral. With the help of a canonical transformation

$$a^\dagger = \sqrt{1/2\hbar\omega}(\omega x - ip), \quad a = \sqrt{1/2\hbar\omega}(\omega x + ip), \quad (14.134)$$

this may be transformed into the action

$$\mathcal{A}_{\omega \text{ QM}} = \int_{t_a}^{t_b} d\tau (a^* i \partial_t a - \omega a^* a). \quad (14.135)$$

A canonical quantization with commutation and anticommutation rules

$$\begin{aligned} [\hat{a}(t), \hat{a}^\dagger(t)]_\mp &= 1, \\ [\hat{a}^\dagger(t), \hat{a}^\dagger(t)]_\mp &= 0, \\ [\hat{a}(t), \hat{a}(t)]_\mp &= 0 \end{aligned} \quad (14.136)$$

produces a second-quantized Hilbert space of the type discussed in Chapter 2. Since $a^\dagger(t)$ and $a(t)$ carry no space variables. They describe Bose and Fermi particles at a single point.

The path-integral representation of the quantum-mechanical partition function of this system is

$$Z_{\omega \text{ QM}} \equiv \int \frac{\mathcal{D}a(t)\mathcal{D}a^*(t)}{2\pi} e^{i\mathcal{A}_{\omega \text{ QM}}}. \quad (14.137)$$

The measure of integration is

$$\int \int \frac{\mathcal{D}a^*\mathcal{D}a}{2\pi} \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\mathcal{D}a_1 \mathcal{D}a_2}{2\pi}, \quad (14.138)$$

where $a = (a_1 + ia_2)/\sqrt{2}$ and $a^\dagger = (a_1 - ia_2)/\sqrt{2}$ are directly obtained from the canonical measure of path integration in (14.118).

At a euclidean time $\tau = -it$, the action of the free nonrelativistic field becomes

$$\mathcal{A}_\omega = \int_0^{\hbar\beta} d\tau (a^* \partial_\tau a + \omega a^* a), \quad (14.139)$$

and the thermodynamic partition function has the path-integral representation

$$Z_\omega \equiv \int \frac{\mathcal{D}a(\tau)\mathcal{D}a^*(\tau)}{2\pi} e^{-\mathcal{A}_\omega}. \quad (14.140)$$

In this formulation, there is no problem of treating both bosons or fermions at the same time. We simply have to assume the fields $a(\tau), a^*(\tau)$ to be periodic or antiperiodic, respectively, in the imaginary-time interval $\hbar\beta$:

$$a(\hbar\beta) = \pm a(0), \quad (14.141)$$

or in the sliced form

$$a_{N+1} = \pm a_0. \quad (14.142)$$

Using formula (14.98), the partition function can be written as

$$\begin{aligned} Z_\omega &= \int \frac{\mathcal{D}a^* \mathcal{D}a}{2\pi} \exp \left[- \int_0^{\hbar\beta} d\tau (a^* \partial_\tau a + \omega a^* a) \right] \\ &= \text{Det}^{\mp 1/2} (\partial_\tau + \omega). \end{aligned} \quad (14.143)$$

Contact with the previous oscillator calculation is established by observing that in the determinant, the operator $\partial_\tau + \omega$ can be replaced by the conjugate operator $-\partial_\tau + \omega$, since all eigenvalues come in complex-conjugate pairs, except for the $m = 0$ - value, which is real. Hence the determinant of $\partial_\tau + \omega$ can be substituted everywhere by

$$\det (\partial_\tau + \omega) = \det (-\partial_\tau + \omega) = \sqrt{\det (-\partial_\tau^2 + \omega^2)}. \quad (14.144)$$

In the boson case, we thus reobtain the result (14.123). In both cases, we may therefore write

$$Z_\omega = \text{Det}^{\mp 1/2} (-\partial_\tau^2 + \omega^2). \quad (14.145)$$

The right-hand side was evaluated for bosons in Eqs. (14.129)–(14.133). In anticipation of the present result, we have calculated the Matsubara sums up to Eq. (14.132) for bosons and fermions, with the results

$$\begin{aligned} Z_\omega &= e^{-\beta F_\omega} = \text{Det}^{\mp 1/2} (-\partial_\tau^2 + \omega^2) = \exp \left\{ \mp \frac{1}{2} \text{Tr} \log (-\partial_\tau^2 + \omega^2) \right\} \\ &= \exp \left\{ \mp \left[\beta \frac{\hbar\omega}{2} + \log(1 \mp e^{-\beta\hbar\omega}) \right] \right\}. \end{aligned} \quad (14.146)$$

This can be written as

$$Z_\omega = \left\{ \frac{[\sinh(\hbar\beta\omega/2)]^{-1}}{\cosh(\hbar\beta\omega/2)} \right\} \quad \text{for} \quad \left\{ \begin{array}{l} \text{bosons,} \\ \text{fermions.} \end{array} \right\}. \quad (14.147)$$

For bosons, the physical interpretation of this expression was given after Eq. (14.110). The analog sum of Boltzmann factors for fermions is

$$Z_\omega = e^{\hbar\omega/2k_B T} + e^{-\hbar\omega/2k_B T}. \quad (14.148)$$

This shows that the fermionic system at a point has two states, one with no particle and one with a single particle, where the no-particle state has a *negative* vacuum energy, as observed in the operator discussion in Chapter 2.

14.9 Free Energy of Free Scalar Fields

The results of the last section are easily applied to fluctuating scalar fields. Consider the free-field partition function

$$Z_0 = \int \mathcal{D}\phi(x) e^{-\int d^D x \frac{1}{2} [(\partial\phi)^2 + m^2 \phi^2]}, \quad (14.149)$$

which is of the general form (14.74) for $j = 0$. If the fields are decomposed into their spatial Fourier components in a finite box of volume V ,

$$\phi(x) = \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \int [e^{i\mathbf{k}\mathbf{x}} \phi_{\mathbf{k}}(\tau) + \text{c.c.}], \quad (14.150)$$

the partition function becomes

$$Z_0 = \prod_{\mathbf{k}} \int \mathcal{D}\phi_{\mathbf{k}}(\tau) e^{-\int_0^{\hbar\beta} dt \frac{1}{2} \{ |\dot{\phi}_{\mathbf{k}}(\tau)|^2 + \mathbf{k}^2 |\phi_{\mathbf{k}}(\tau)|^2 + m^2 |\phi_{\mathbf{k}}(\tau)|^2 \}}. \quad (14.151)$$

For each $\mathbf{k}$, the functional integral is obviously the same as in (14.114), so that

$$Z_0 = \prod_{\mathbf{k}} Z_{\omega(\mathbf{k})}, \quad (14.152)$$

where $\omega(\mathbf{k}) \equiv \sqrt{\mathbf{k}^2 + m^2}$, and by (14.112)

$$Z_{\omega(\mathbf{k})} = \frac{1}{2 \sinh[\hbar\omega(\mathbf{k})\beta/2]}. \quad (14.153)$$

For a real field $\phi(x)$, the anticommuting alternative cannot be accommodated into the functional integral (14.149). We must first go to the field-theoretic analog of the path integral in phase space

$$Z_0 = \int \int \mathcal{D}\phi(x) \frac{\mathcal{D}\pi(x)}{2\pi\hbar} \times \exp \left\{ \int d^4x \left[i\pi(x) \partial_\mu \phi(x) - \frac{1}{2} \pi^2(x) - \frac{1}{2} [(\nabla \phi(x))^2 + m^2 \phi^2(x)] \right] \right\}, \quad (14.154)$$

where $\pi(x)$ are the canonical field momenta (7.1). After the Fourier decomposition (14.150) and a similar one for $\pi(x)$, we perform again a canonical transformation corresponding to (14.134),

$$a_{\mathbf{k}}^\dagger(\tau) = \frac{1}{\sqrt{2\hbar\omega}} [\omega(\mathbf{k}) \phi_{\mathbf{k}}(\tau) - i\pi_{\mathbf{k}}(\tau)], \quad a_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{2\hbar\omega}} [\omega(\mathbf{k}) \phi_{\mathbf{k}}(\tau) + i\pi_{\mathbf{k}}(\tau)], \quad (14.155)$$

and arrive at the analog of (14.143):

$$\begin{aligned} Z_\omega &= \prod_{\mathbf{k}} \int \frac{\mathcal{D}a_{\mathbf{k}}^* \mathcal{D}a_{\mathbf{k}}}{2\pi} \exp \left[- \int_0^{\hbar\beta} d\tau (a_{\mathbf{k}}^* \partial_\tau a_{\mathbf{k}} + \omega a_{\mathbf{k}}^* a_{\mathbf{k}}) \right] \\ &= \prod_{\mathbf{k}} \text{Det}^{\mp 1/2} (\partial_\tau + \omega(\mathbf{k})). \end{aligned} \quad (14.156)$$

This can be evaluated as in (14.147) to yield

$$Z_\omega = \prod_{\mathbf{k}} \left\{ \frac{\{2 \sinh[\hbar\beta\omega(\mathbf{k})/2]\}^{-1}}{2 \cosh[\hbar\beta\omega(\mathbf{k})/2]} \right\} \quad \text{for} \quad \left\{ \begin{array}{l} \text{bosons,} \\ \text{fermions.} \end{array} \right\}. \quad (14.157)$$

The associated free energies are

$$F_0 = -\beta \log Z_0 = \pm \sum_{\mathbf{k}} \left\{ \frac{\omega(\mathbf{k})}{2} + \log [1 \mp e^{-\beta \hbar \omega(\mathbf{k})}] \right\}. \quad (14.158)$$

For a complex field, the canonical transformation is superfluous. The field in the partition function

$$Z_0 = \int \mathcal{D}\phi(x) \mathcal{D}\phi^*(x) e^{-\int d^D x \frac{1}{2} (\partial \phi^* \partial \phi + m^2 \phi^* \phi)} \quad (14.159)$$

can directly be assumed to be of the bosonic or of the fermionic type. A direct application of the Gaussian formula (14.98) leads to

$$\begin{aligned} Z_\omega &= \prod_{\mathbf{k}} \text{Det} [-\partial_\tau^2 + \omega^2(\mathbf{k})]^{\mp 1} \\ &= \prod_{\mathbf{k}} \left\{ \frac{\{2 \sinh[\hbar \beta \omega(\mathbf{k})/2]\}^{-2}}{\{2 \cosh[\hbar \beta \omega(\mathbf{k})/2]\}^2} \right\} \quad \text{for} \quad \begin{cases} \text{bosons,} \\ \text{fermions.} \end{cases} \end{aligned} \quad (14.160)$$

with free energies twice as large as (14.158).

14.10 Interacting Nonrelativistic Fields

The quantization of nonrelativistic particles was amply discussed in Chapter 2 and applied to many-body Bose and Fermi systems in Chapter 3. Here we shall demonstrate that a completely equivalent formulation of the second-quantized nonrelativistic field theory is possible with the help of functional integrals.

Consider a many-fermion system described by an action

$$\begin{aligned} \mathcal{A} \equiv \mathcal{A}_0 + \mathcal{A}_{\text{int}} &= \int d^3x dt \psi^*(\mathbf{x}, t) [i\partial_t - \epsilon(-i\nabla)] \psi(\mathbf{x}, t) \\ &\quad - \frac{1}{2} \int d^3x dt d^3x' dt' \psi^*(\mathbf{x}', t') \psi^*(\mathbf{x}, t) V(\mathbf{x}, t; \mathbf{x}' t') \psi(\mathbf{x}, t) \psi(\mathbf{x}', t') \end{aligned} \quad (14.161)$$

with a translationally invariant two-body potential

$$V(\mathbf{x}, t; \mathbf{x}', t') = V(\mathbf{x} - \mathbf{x}', t - t'). \quad (14.162)$$

In the systems to be treated in this text we shall be concerned with a potential that is, in addition, instantaneous in time

$$V(\mathbf{x}, t; \mathbf{x}', t') = \delta(t - t') V(\mathbf{x} - \mathbf{x}'). \quad (14.163)$$

This property will greatly simplify the discussion.

The fundamental field $\psi(x)$ may describe bosons or fermions. The complete information on the physical properties of the system resides in the Green functions.

In the operator Heisenberg picture, these are given by the expectation values of the time-ordered products of the field operators

$$G(\mathbf{x}_1, t_1, \dots, \mathbf{x}_n, t_n; \mathbf{x}_{n'}, t_{n'}, \dots, \mathbf{x}_{1'}, t_{1'}) \quad (14.164)$$

$$= \langle 0 | \hat{T} \left(\hat{\psi}_H(\mathbf{x}_1, t_1) \cdots \hat{\psi}_H(\mathbf{x}_n, t_n) \hat{\psi}_H^\dagger(\mathbf{x}_{n'}, t_{n'}) \cdots \hat{\psi}_H^\dagger(\mathbf{x}_{1'}, t_{1'}) \right) | 0 \rangle.$$

The time-ordering operator $\hat{T}$ changes the position of the operators behind it in such a way that earlier times stand to the right of later times. To achieve the final ordering, a number of field transmutations are necessary. If F denotes the number of transmutations of Fermi fields, the final product receives a sign factor $(-1)^F$.

It is convenient to view all Green functions (14.164) as derivatives of the generating functional

$$Z[\eta^*, \eta] = \langle 0 | \hat{T} \exp \left\{ i \int d^3x dt \left[\hat{\psi}_H^\dagger(\mathbf{x}, t) \eta(\mathbf{x}, t) + \eta^*(\mathbf{x}, t) \hat{\psi}_H(\mathbf{x}, t) \right] \right\} | 0 \rangle, \quad (14.165)$$

namely

$$G(\mathbf{x}_1, t_1, \dots, \mathbf{x}_n, t_n; \mathbf{x}_{n'}, t_{n'}, \dots, \mathbf{x}_{1'}, t_{1'}) \quad (14.166)$$

$$= (-i)^{n+n'} \frac{\delta^{n+n'} Z[\eta^*, \eta]}{\delta \eta^*(\mathbf{x}_1, t_1) \cdots \delta \eta^*(\mathbf{x}_n, t_n) \delta \eta(\mathbf{x}_{n'}, t_{n'}) \cdots \delta \eta(\mathbf{x}_{1'}, t_{1'})} \Big|_{\eta=\eta^*=0}.$$

Physically, the generating functional (14.165) describes the probability amplitude for the vacuum to remain a vacuum in the presence of external sources $\eta^*(\mathbf{x}, t)$ and $\eta(\mathbf{x}, t)$.

The calculation of these Green functionals is usually performed in the interaction picture which can be summarized by the operator expression for Z :

$$Z[\eta^*, \eta] = N \langle 0 | T \exp \left\{ i \mathcal{A}_{\text{int}}[\psi^\dagger, \psi] + i \int d^3x dt \left[\psi^\dagger(\mathbf{x}, t) \eta(\mathbf{x}, t) + \text{h.c.} \right] \right\} | 0 \rangle. \quad (14.167)$$

In the interaction picture, the fields $\psi(\mathbf{x}, t)$ possess free-field propagators and the normalization constant N is determined by the condition [which is trivially true for (14.165)]:

$$Z[0, 0] = 1. \quad (14.168)$$

The standard perturbation theory is obtained by expanding $\exp\{i\mathcal{A}_{\text{int}}\}$ in (14.167) in a power series and bringing the resulting expression to normal order via Wick's expansion technique. The perturbation expansion of (14.167) often serves conveniently to *define* an interacting theory. Every term can be pictured graphically and has a physical interpretation as a virtual process.

Unfortunately, the perturbation series up to a certain order in the coupling constant is unable to describe several important physical phenomena. Examples are the formation of bound states in the vacuum, or the existence and properties of collective excitations in many-body systems. Those require the summation of infinite subsets

of diagrams to all orders. In many situations it is well-known which subsets have to be taken in order to account approximately for specific effects. What is not so clear is how such lowest approximations can be improved in a systematic manner. The point is that, as soon as a selective summation is performed, the original coupling constant has lost its meaning as an organizer of the expansion and there is need for a new systematics of diagrams. This will be presented in the sequel.

As soon as bound states or collective excitations are formed, it is very suggestive to use *them* as new quantum fields rather than the original fundamental particles ψ . The goal would then be to rewrite the expression (14.167) for $Z[\eta^*, \eta]$ in terms of new fields whose unperturbed propagator has the free energy spectrum of the *bound states* or collective excitations and whose $\mathcal{A}_{\text{int}}$ describes *their* mutual interactions. In the operator form (14.167), however, such changes of fields are hard to conceive.

14.10.1 Functional Formulation

In the functional integral approach, the generating functional (14.165) is given by [5]:

$$Z[\eta^*, \eta] = N \int \mathcal{D}\psi^*(\mathbf{x}, t) \mathcal{D}\psi(\mathbf{x}, t) \times \exp \left\{ i\mathcal{A}[\psi^*, \psi] + i \int d^3x dt [\psi^*(\mathbf{x}, t)\eta(\mathbf{x}, t) + \text{c.c.}] \right\}. \quad (14.169)$$

It is worth emphasizing that the field $\psi(\mathbf{x}, t)$ in the path-integral formulation is a complex number and *not* an operator. All quantum effects are accounted for by fluctuations; the path integral includes not only the classical field configurations but also all classically forbidden ones, i.e., all those which do not run through the valley of extremal action in the exponent.

By analogy with the development in Section 14.4 we take the interactions outside the integral and write the functional integral (14.169) as

$$Z[\eta^*, \eta] = \exp \left\{ i\mathcal{A}_{\text{int}} \left[\frac{1}{i} \frac{\delta}{\delta \eta}, \frac{1}{i} \frac{\delta}{\delta \eta^*} \right] \right\} Z_0[\eta^*, \eta], \quad (14.170)$$

where Z_0 is the generating functional of the free-field correlation functions, whose functional integral looks like (14.169), but with the action being only the free-particle expression

$$\mathcal{A}_0[\psi^*, \psi] = \int dx dt \psi^*(\mathbf{x}, t) [i\partial_t - \epsilon(-i\nabla)] \psi(\mathbf{x}, t), \quad (14.171)$$

rather than the full $\mathcal{A}[\psi^*, \psi] = \mathcal{A}_0[\psi^*, \psi] + \mathcal{A}_{\text{int}}[\psi^*, \psi]$ of Eq. (14.161) in the exponent. The functional integral is of the Gaussian type (14.89) with a matrix

$$A(\mathbf{x}, t; \mathbf{x}', t') = [i\partial_t - \epsilon(-i\nabla)] \delta^{(3)}(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (14.172)$$

This matrix is the inverse of the free propagator

$$A(\mathbf{x}, t; \mathbf{x}', t') = iG_0^{-1}(\mathbf{x}, t; \mathbf{x}', t') \quad (14.173)$$

where

$$G_0(\mathbf{x}, t; \mathbf{x}', t') = \int \frac{dE}{2\pi} \int \frac{d^3p}{(2\pi)^4} e^{-i[E(t-t') - \mathbf{p}(\mathbf{x}-\mathbf{x}')] } \frac{i}{E - \epsilon(\mathbf{p}) + i\eta}. \quad (14.174)$$

Inserting this into (14.100), we see that

$$Z_0[\eta^*, \eta] = N \exp \left[i \left(\pm i \text{Tr} \log iG_0^{-1} \right) - \int d^3x dt d^3x' dt' \eta^*(\mathbf{x}, t) G_0(\mathbf{x}, t; \mathbf{x}', t') \eta(\mathbf{x}', t') \right]. \quad (14.175)$$

We now fix N in accordance with the normalization (14.168) to

$$N = \exp [i (\pm i \text{Tr} \log iG_0)] \quad (14.176)$$

and arrive at

$$Z_0[\eta^*, \eta] = \exp \left[- \int d^3x dt d^3x' dt' \eta^*(\mathbf{x}, t) G_0(\mathbf{x}, t; \mathbf{x}', t') \eta(\mathbf{x}', t') \right]. \quad (14.177)$$

This coincides exactly with what would have been obtained from the operator expression (14.167) for $Z_0[\eta^*, \eta]$ (i.e., without $\mathcal{A}_{\text{int}}$).

Indeed, according to Wick's theorem [2, 5, 6], any time ordered product can be expanded as a sum of normal products with all possible contractions taken via Feynman propagators. The formula for an arbitrary functional of free fields ψ, ψ^* is

$$TF[\psi^*, \psi] = \exp \int d^3x dt d^3x' dt' \frac{\delta}{\delta \psi(\mathbf{x}, t)} G_0(\mathbf{x}, t; \mathbf{x}', t') \frac{\delta}{\delta \psi^*(\mathbf{x}', t')} : F[\psi^*, \psi] :. \quad (14.178)$$

Applying this to

$$\langle 0 | TF[\psi^*, \psi] | 0 \rangle = \langle 0 | T \exp \left[i \int d^3x dt (\psi^* \eta + \eta^* \psi) \right] | 0 \rangle \quad (14.179)$$

one finds:

$$\begin{aligned} Z_0[\eta^*, \eta] &= \exp \left[- \int d^3x dt d^3x' dt' \eta^*(\mathbf{x}, t) G_0(\mathbf{x}, t; \mathbf{x}', t') \eta(\mathbf{x}', t') \right] \\ &\times \langle 0 | : \exp \left[i \int d^3x dt (\psi^* \eta + \eta^* \psi) \right] : | 0 \rangle. \end{aligned} \quad (14.180)$$

The second factor is equal to unity, thus proving the equality of this operatorially defined $Z_0[\eta^*, \eta]$ with the path-integral expression (14.177). Because of (14.170), this equality holds also for the interacting generating functional $Z[\eta^*, \eta]$.

14.10.2 Grand-Canonical Ensembles at Zero Temperature

All these results are easily generalized from vacuum expectation values to thermodynamic averages at fixed temperatures T and chemical potential μ . The change

at $T = 0$ is trivial: The single particle energies in the action (14.161) have to be replaced by

$$\xi(-i\nabla) = \epsilon(-i\nabla) - \mu \quad (14.181)$$

and new boundary conditions have to be imposed upon all Green functions via an appropriate $i\epsilon$ prescription in $G_0(\mathbf{x}, t; \mathbf{x}', t')$ of (14.174) [see [2, 7]]:

$$^{T=0}G_0(\mathbf{x}, t; \mathbf{x}', t') = \int \frac{dE d^3p}{(2\pi)^4} e^{-iE(t-t') + i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \frac{i}{E - \xi(\mathbf{p}) + i\eta \operatorname{sgn} \xi(\mathbf{p})}. \quad (14.182)$$

Note that, as a consequence of the chemical potential, fermions with $\xi < 0$ inside the Fermi sea propagate backwards in time. Bosons, on the other hand, have in general $\xi > 0$ and, hence, always propagate forward in time.

In order to simplify the notation we shall often use four-vectors $p = (p^0, \mathbf{p})$ and write the measure of integration in (14.182) as

$$\int \frac{dE d^3p}{(2\pi)^4} = \int \frac{d^4p}{(2\pi)^4}. \quad (14.183)$$

Note that in a solid, the momentum integration is really restricted to a Brillouin zone. If the solid has a finite volume V , the integral over spacial momenta becomes a sum over momentum vectors,

$$\int \frac{d^3p}{(2\pi)^3} = \frac{1}{V} \sum_{\mathbf{p}}, \quad (14.184)$$

and the Green function (14.182) reads

$$^{T=0}G_0(\mathbf{x}, t; \mathbf{x}', t') \equiv \int \frac{dE}{2\pi} \frac{1}{V} \sum_{\mathbf{p}} e^{-ip(x-x')} \frac{i}{p^0 - \xi(\mathbf{p}) + i\eta \operatorname{sgn} \xi(\mathbf{p})}. \quad (14.185)$$

The resulting power series expansions for the generating functional at zero-temperature $^{T=0}Z[\eta^*, \eta]$ and nonzero coupling can be written down as before after performing a Wick rotation in the complex energy plane in all energy integrals occurring in the expansions of formulas (14.180) and (14.167) in powers of the sources $\eta(\mathbf{x}, t)$ and $\eta^*(\mathbf{x}, t)$. For this, one sets $E = p^0 \equiv i\omega$ and replaces

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi} \rightarrow i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}. \quad (14.186)$$

Then the Green function (14.182) becomes

$$^{T=0}G_0(\mathbf{x}, t; \mathbf{x}', t') = - \int \frac{d\omega}{2\pi} \frac{d^3p}{(2\pi)^3} e^{\omega(t-t') + i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \frac{1}{i\omega - \xi(\mathbf{p})}. \quad (14.187)$$

Note that with formulas (14.170) and (14.177) the generating functional $^{T=0}Z[\eta^*, \eta]$ is the grand-canonical partition function in the presence of sources [7].

Finally, we have to introduce arbitrary temperatures T . According to the standard rules of quantum field theory (for an elementary introduction see Chapter 2 in Ref. [2]), we must continue all times to imaginary values $t = i\tau$, restrict the imaginary time interval to the inverse temperature⁵ $\beta \equiv 1/T$, and impose periodic or antiperiodic boundary conditions upon the fields $\psi(\mathbf{x}, -i\tau)$ of bosons and fermions, respectively [2, 7]:

$$\psi(\mathbf{x}, -i\tau) = \pm \psi(\mathbf{x}, -i(\tau + 1/T)). \quad (14.188)$$

When there is no danger of confusion, we shall drop the factor $-i$ in front of the imaginary time in field arguments, for brevity. The same thing will be done with Green functions.

By virtue of (14.177), these boundary conditions wind up in all free Green functions, i.e., they have the property

$${}^T G_0(\mathbf{x}, \tau + 1/T; \mathbf{x}', \tau') \equiv \pm {}^T G_0(\mathbf{x}, -i\tau; \mathbf{x}', -i\tau'). \quad (14.189)$$

This property is enforced automatically by replacing the energy integrations $\int_{-\infty}^{\infty} d\omega/2\pi$ in (14.187) by a summation over the discrete Matsubara frequencies [by analogy with the momentum sum (14.184), the temporal “volume” being $\beta = 1/T$]

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rightarrow T \sum_{\omega_n}, \quad (14.190)$$

which are even or odd multiples of πT

$$\omega_n = \begin{cases} 2n \\ 2n+1 \end{cases} \pi T \quad \text{for} \quad \begin{cases} \text{bosons} \\ \text{fermions} \end{cases}. \quad (14.191)$$

The prefactor T of the sum over the discrete Matsubara frequencies accounts for the density of these frequencies yielding the correct $T \rightarrow 0$ -limit.

Thus we obtain the following expression for the imaginary-time Green function of a free nonrelativistic field at finite temperature (the so-called *free thermal Green function*)

$${}^T G_0(\mathbf{x}, \tau, \mathbf{x}', \tau') = -T \sum_{\omega_n} \int \frac{d^3 p}{(2\pi)^3} e^{-i\omega_n(\tau-\tau') + i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \frac{1}{i\omega_n - \xi(\mathbf{p})}. \quad (14.192)$$

Incorporating the Wick rotation in the sum notation we may write

$$T \sum_{p_0} = -iT \sum_{\omega_n} = -iT \sum_{p_4}, \quad (14.193)$$

where $p_4 = -ip_0 = \omega$. If temperature and volume are both finite, the Green function is written as

$${}^T G_0(\mathbf{x}, \tau, \mathbf{x}', \tau') = -\frac{T}{V} \sum_{p_0} \sum_{\mathbf{p}} e^{-i\omega_n(\tau-\tau') + i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \frac{1}{i\omega_n - \xi(\mathbf{p})}. \quad (14.194)$$

⁵We use natural units in this chapter, so that $k_B = 1, \hbar = 1$.

At equal space points and equal imaginary times, the sum can easily be evaluated. One must, however, specify the order in which $\tau \rightarrow \tau'$. Let η denote an infinitesimal positive number and consider the case $\tau' = \tau + \eta$, where the Green function is

$${}^T G_0(\mathbf{x}, \tau, \mathbf{x}, \tau + \eta) = -T \sum_{\omega_n} \int \frac{d^3 p}{(2\pi)^3} e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi(\mathbf{p})}. \quad (14.195)$$

Then the sum is found after converting it into a contour integral

$$T \sum_{\omega_n} e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi(\mathbf{p})} = \frac{T}{2\pi i} \int_C dz \frac{e^{\eta z}}{e^{z/T} \mp 1} \frac{1}{z - \xi}. \quad (14.196)$$

The upper sign holds for bosons, the lower for fermions. The contour of integration C encircles the imaginary z -axis in a positive sense, thereby enclosing all integer or half-integer valued poles of the integrand at the Matsubara frequencies $z = i\omega_m$ (see Fig. 2.8). The factor $e^{\eta z}$ ensures that the contour in the left half-plane does not contribute.

By deforming the contour C into C' and contracting C' to zero we pick up the pole at $z = \xi$ and find

$$T \sum_{\omega_n} e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi(\mathbf{p})} = \mp \frac{1}{e^{\xi(\mathbf{p})/T} \mp 1} = \mp \frac{1}{e^{\xi(\mathbf{p})/T} \mp 1} = \mp n(\xi(\mathbf{p})). \quad (14.197)$$

The phase $e^{\eta z}$ ensures that the contour in the left half-plane does not contribute. The function on the right is known as the *Bose or Fermi distribution function*.

By subtracting from (14.197) the sum with ξ replaced by $-\xi$, we obtain the important sum formula

$$T \sum_{\omega_n} \frac{1}{\omega_n^2 + \xi^2(\mathbf{p})} = \frac{1}{2\xi(\mathbf{p})} \coth^{\pm 1} \frac{\xi(\mathbf{p})}{T}. \quad (14.198)$$

In the opposite limit with $\tau' = \tau - \eta$, the phase factor in the sum would be $e^{-i\omega_m \eta}$ leading to a contour integral

$$-k_B T \sum_{\omega_m} e^{i\omega_m \eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \pm \frac{k_B T}{2\pi i} \int_C dz \frac{e^{-\eta z}}{e^{-z/k_B T} \mp 1} \frac{1}{z - \xi}, \quad (14.199)$$

and we would find $1 \pm n_{\xi(\mathbf{p})}$.

In the operator language, these limits correspond to the expectation values of free non-relativistic field operators

$$\begin{aligned} {}^T G_0(\mathbf{x}, \tau; \mathbf{x}, \tau + \eta) &= \langle 0 | \hat{T} \left(\hat{\psi}_H(\mathbf{x}, \tau) \hat{\psi}_H^\dagger(\mathbf{x}, \tau + \eta) \right) | 0 \rangle = \pm \langle 0 | \hat{\psi}_H^\dagger(\mathbf{x}, \tau) \hat{\psi}_H(\mathbf{x}, \tau) | 0 \rangle \\ {}^T G_0(\mathbf{x}, \tau; \mathbf{x}, \tau - \eta) &= \langle 0 | \hat{T} \left(\hat{\psi}_H(\mathbf{x}, \tau) \hat{\psi}_H^\dagger(\mathbf{x}, \tau - \eta) \right) | 0 \rangle = \langle 0 | \hat{\psi}_H(\mathbf{x}, \tau) \hat{\psi}_H^\dagger(\mathbf{x}, \tau) | 0 \rangle \\ &= 1 \pm \langle 0 | \hat{\psi}_H^\dagger(\mathbf{x}, \tau) \hat{\psi}_H(\mathbf{x}, \tau) | 0 \rangle. \end{aligned}$$

The function $n(\xi(\mathbf{p}))$ is the thermal expectation value of the number operator

$$\hat{N} = \hat{\psi}_H^\dagger(\mathbf{x}, \tau) \hat{\psi}_H(\mathbf{x}, \tau). \quad (14.200)$$

In the case of $T \neq 0$ ensembles, it is also useful to employ a four-vector notation. The four-vector

$$p_E \equiv (p_4, \mathbf{p}) = (\omega, \mathbf{p}) \quad (14.201)$$

is called the *euclidean four-momentum*. Correspondingly, we define the *euclidean spacetime coordinate*

$$x_E \equiv (-\tau, \mathbf{x}). \quad (14.202)$$

The exponential in (14.192) can be written as

$$p_E x_E = -\omega\tau + \mathbf{p}\mathbf{x}. \quad (14.203)$$

Collecting integral and sum in a single four-dimensional summation symbol, we shall write (14.192) as

$$^T G_0(x_E - x') \equiv -\frac{T}{V} \sum_{p_E} \exp[-ip_E(x_E - x'_E)] \frac{1}{ip_4 - \xi(\mathbf{p})}. \quad (14.204)$$

It is quite straightforward to derive the general $T \neq 0$ Green function from a path-integral formulation analogous to (14.169). For this we consider classical fields $\psi(\mathbf{x}, \tau)$ with the periodicity or anti-periodicity

$$\psi(\mathbf{x}, \tau) = \pm \psi(\mathbf{x}, \tau + 1/T). \quad (14.205)$$

They can be Fourier-decomposed as

$$\psi(\mathbf{x}, \tau) = \frac{T}{V} \sum_{\omega_n} \sum_{\mathbf{p}} e^{-i\omega_n\tau + i\mathbf{p}\mathbf{x}} a(\omega_n, \mathbf{p}) \equiv \frac{T}{V} \sum_{p_E} e^{-ip_E x_E} a(p_E) \quad (14.206)$$

with a sum over even or odd Matsubara frequencies ω_n . If a free action is now defined as

$$\mathcal{A}_0[\psi^*, \psi] = -i \int_{-1/2T}^{1/2T} d\tau \int d^3x \psi^*(\mathbf{x}, \tau) [-\partial_\tau - \xi(-i\nabla)] \psi(\mathbf{x}, \tau), \quad (14.207)$$

formula (14.100) renders [1, 8]

$$^T Z_0[\eta^*, \eta] = e^{\mp \text{Tr} \log A + \int_{-1/2T}^{1/2T} d\tau d\tau' \int d^3x d^3x' \eta^*(\mathbf{x}, \tau) A^{-1}(\mathbf{x}, \tau, \mathbf{x}', \tau') \eta(\mathbf{x}', \tau')}, \quad (14.208)$$

with the functional matrix

$$A(\mathbf{x}, \tau; \mathbf{x}', \tau') = [\partial_\tau + \xi(-i\nabla)] \delta^{(3)}(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \quad (14.209)$$

Its inverse A^{-1} is equal to the propagator (14.192), the Matsubara frequencies arising due to the finite- τ interval of euclidean space together with the periodic boundary condition (14.205).

Again, interactions are taken care of by multiplying ${}^T Z_0[\eta^* \eta]$ with the factor (14.170). In terms of the fields $\psi(\mathbf{x}, \tau)$, the exponent has the form:

$$\begin{aligned} \mathcal{A}_{\text{int}} &= \frac{1}{2} \int \int_{-1/2T}^{1/2T} d\tau d\tau' \\ &\times \int d^3x d^3x' \psi^*(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau') \psi(\mathbf{x}', \tau') \psi(\mathbf{x}, \tau) V(\mathbf{x}, -i\tau; \mathbf{x}', -i\tau'). \end{aligned} \quad (14.210)$$

In the case of a potential (14.163) that is instantaneous in time t , the potential of the euclidean formulation becomes instantaneous in τ :

$$V(\mathbf{x}, -i\tau; \mathbf{x}', -i\tau') = V(\mathbf{x} - \mathbf{x}') i\delta(\tau - \tau'). \quad (14.211)$$

In this case $\mathcal{A}_{\text{int}}$ can be written in terms of the interaction Hamiltonian as

$$\mathcal{A}_{\text{int}} = i \int_{-1/2T}^{1/2T} d\tau H_{\text{int}}(\tau). \quad (14.212)$$

Thus the grand-canonical partition function in the presence of external sources may be calculated from the path integral [8]:

$${}^T Z[\eta^*, \eta] = \int \mathcal{D}\psi^*(\mathbf{x}, \tau) \mathcal{D}\psi(\mathbf{x}, \tau) e^{i {}^T \mathcal{A} + \int_{-1/2T}^{1/2T} d\tau \int d^3x [\psi^*(\mathbf{x}, \tau) \eta(\mathbf{x}, \tau) + \text{c.c.}]}, \quad (14.213)$$

where the grand-canonical action is

$$\begin{aligned} i {}^T \mathcal{A}[\psi^*, \psi] &= - \int_{-1/2T}^{1/2T} d\tau \int d^3x \psi^*(\mathbf{x}, \tau) [\partial_\tau + \xi(-i\nabla)] \psi(\mathbf{x}, \tau) \\ &+ \frac{i}{2} \int_{-1/2T}^{1/2T} d\tau d\tau' \int d^3x d^3x' \psi^*(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau') \psi(\mathbf{x}, \tau') \psi(\mathbf{x}, \tau) V(\mathbf{x}, -i\tau; \mathbf{x}', -i\tau'). \end{aligned} \quad (14.214)$$

The Green functions of the fully interacting theory are obtained from the functional derivatives

$$\begin{aligned} G(\mathbf{x}_1, \tau_1, \dots, \mathbf{x}_n, \tau_n; \mathbf{x}_{n'}, \tau_{n'}, \dots, \mathbf{x}_{1'}, \tau_{1'}) \\ = (-i)^{n+n'} \frac{\delta^{n+n'} Z[\eta^*, \eta]}{\delta \eta^*(\mathbf{x}_1, \tau_1) \cdots \delta \eta^*(\mathbf{x}_n, \tau_n) \delta \eta(\mathbf{x}_{n'}, \tau_{n'}) \cdots \delta \eta(\mathbf{x}_{1'}, \tau_{1'})} \Big|_{\eta=\eta^* \equiv 0}. \end{aligned} \quad (14.215)$$

Explicitly, the right-hand side represent the functional integrals

$$N \int \mathcal{D}\psi^*(\mathbf{x}, t) \mathcal{D}\psi(\mathbf{x}, t) \hat{\psi}(\mathbf{x}_1, \tau_1) \cdots \hat{\psi}(\mathbf{x}_n, \tau_n) \hat{\psi}^*(\mathbf{x}_{n'}, \tau_{n'}) \cdots \hat{\psi}^*(\mathbf{x}_{1'}, \tau_{1'}) e^{i {}^T \mathcal{A}[\psi^*, \psi]}. \quad (14.216)$$

In the sequel, we shall always assume the normalization factor to be chosen in such a way that $Z[0, 0]$ is normalized to unity. Then the functional integrals (14.216) are obviously the *correlation function* of the fields:

$$\langle \hat{\psi}(\mathbf{x}_1, \tau_1) \cdots \hat{\psi}(\mathbf{x}_n, \tau_n) \hat{\psi}^*(\mathbf{x}_{n'}, \tau_{n'}) \cdots \hat{\psi}^*(\mathbf{x}_{1'}, \tau_{1'}) \rangle. \quad (14.217)$$

In contrast to Section 1.2, the bra and ket symbols denote now a thermal average of the classical fields.

If the generating functional of the interacting theory is evaluated in a perturbation expansion using formula (14.170), the periodic boundary conditions for the free Green functions (14.189) will go over to the fully interacting Green functions (14.215).

The functional integral expression (14.213) for the generating functional have a great advantage in comparison to the equivalent operator formulation based on (14.180) and (14.170). They share with ordinary integrals the extreme flexibility with respect to changes in the field variables.

Summarizing we have seen that the functional (14.213) defines the most general type of theory involving two-body forces. It contains all information on a physical system in the vacuum as well as in thermodynamic ensembles. The vacuum theory is obtained by setting $T = 0$ and $\mu = 0$, and by continuing the result back from T to physical times. Conversely, the functional (14.169) in the vacuum can be generalized to ensembles in a straight-forward manner by first continuing the times t to imaginary values $-i\tau$ via a Wick rotation in all energy integrals and then going to periodic functions in τ .

There is a complete correspondence between the real-time generating functional (14.169) and the thermodynamic imaginary-time expression (14.213). For this reason it will be sufficient to exhibit all techniques only in one version, for which we shall choose (14.169). Note, however, that due to the singular nature of the propagators (14.174) in real energy-momentum, the thermodynamic formulation specifies the way how to avoid singularities.

14.11 Interacting Relativistic Fields

Let us see how this formalism works for relativistic boson and fermion systems. Consider a Lagrangian of Klein-Gordon and Dirac particles consisting of a sum

$$\mathcal{L}(\psi, \bar{\psi}, \varphi) = \mathcal{L}_0 + \mathcal{L}_{\text{int}}. \quad (14.218)$$

As in the case of nonrelativistic fields, all time ordered Green's functions can be obtained from the derivatives with respect to the external sources of the generating functional

$$Z[\eta, \bar{\eta}, j] = \text{const} \times \langle 0 | T e^{i \int dx (\mathcal{L}_{\text{int}} + \bar{\eta}\psi + \bar{\psi}\eta + j\varphi)} | 0 \rangle. \quad (14.219)$$

The fields in the exponent follow free equations of motion and $|0\rangle$ is the free-field vacuum. The constant is conventionally chosen to make $Z[0, 0, 0] = 1$, i. e.

$$\text{const} = \left[\langle 0 | T e^{i \int dx \mathcal{L}_{\text{int}}(\psi, \bar{\psi}, \varphi)} | 0 \rangle \right]^{-1}. \quad (14.220)$$

This normalization may always be enforced at the very end of any calculation such that $Z[\eta, \bar{\eta}, j]$ is only interesting as far as its functional dependence is concerned. Any constant prefactor is irrelevant.

It is then straight-forward to show that $Z[\eta, \bar{\eta}, j]$ can alternatively be computed via the Feynman path-integral formula

$$Z[\eta, \bar{\eta}, j] = \text{const} \times \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}\varphi e^{i \int dx [\mathcal{L}_0(\psi, \bar{\psi}, \varphi) + \mathcal{L}_{\text{int}} + \bar{\eta}\psi + \bar{\psi}\eta + j\varphi]}. \quad (14.221)$$

Here the fields are no more operators but classical functions (with the mental reservation that classical Fermi fields are anticommuting objects). Notice that contrary to the operator formula (14.219) the *full* action appears in the exponent.

For simplicity, we demonstrate the equivalence only for one real scalar field $\varphi(x)$. The extension to other fields is immediate [9, 10, 51]. Note that it is sufficient to give the proof for free fields, where

$$\begin{aligned} Z_0[j] &= \langle 0 | T e^{i \int dx j(x) \varphi(x)} | 0 \rangle \\ &= \text{const} \times \int \mathcal{D}\varphi e^{i \int dx [\frac{1}{2} \varphi(x) (-\square_x - \mu^2) \varphi(x) + j(x) \varphi(x)]}. \end{aligned} \quad (14.222)$$

For if it holds there, a simple multiplication on both sides of (14.222) by the differential operator

$$e^{i \int dx \mathcal{L}_{\text{int}}(\frac{1}{i} \frac{\delta}{\delta j(x)})} \quad (14.223)$$

would extend it to the interacting functionals (14.219) or (14.221). But (14.222) follows directly from Wick's theorem, according to which any time-ordered product of a free field can be expanded into a sum of normal products with all possible time ordered contractions. This statement can be summarized in operator form valid for any functional $F[\varphi]$ of a free field $\varphi(x)$:

$$TF[\varphi] = e^{\frac{1}{2} \int dx dy \frac{\delta}{\delta \varphi(x)} D(x-y) \frac{\delta}{\delta \varphi(y)}} : F[\varphi] :, \quad (14.224)$$

where $D(x-y)$ is the free-field propagator

$$D(x-y) = \frac{i}{-\square_x - \mu^2 + i\epsilon} \delta(x-y) = \int \frac{d^4 q}{(2\pi)^4} e^{-iq(x-y)} \frac{i}{q^2 - \mu^2 + i\epsilon}. \quad (14.225)$$

Applying this to (14.224) gives

$$\begin{aligned} Z_0 &= e^{\frac{1}{2} \int dx dy \frac{\delta}{\delta \varphi(x)} D(x-y) \frac{\delta}{\delta \varphi(y)}} \langle 0 | : e^{i \int dx j(x) \hat{\varphi}(x)} : | 0 \rangle \\ &= e^{-\frac{1}{2} \int dx dy j(x) D(x-y) j(y)} \langle 0 | : e^{i \int dx j(x) \hat{\varphi}(x)} : | 0 \rangle \\ &= e^{-\frac{1}{2} \int dx dy j(x) D(x-y) j(y)}. \end{aligned} \quad (14.226)$$

The last part of the equation follows from the vanishing of all normal products of $\varphi(x)$ between vacuum states.

Exactly the same result is obtained by performing the functional integral in (14.222) and by using the functional integral formula (14.99). The matrix A is equal to $A(x, y) = (-\square_x - \mu^2) \delta(x-y)$, and its inverse yields the propagator $D(x-y)$:

$$A^{-1}(x, y) = \frac{1}{-\square_x - \mu^2 + i\epsilon} \delta(x-y) = -iD(x-y), \quad (14.227)$$

yielding again (14.226).

The generating functional of a free Dirac field theory reads

$$\begin{aligned} Z_0[\eta, \bar{\eta}] &= \langle 0 | T e^{i \int (\bar{\eta} \hat{\psi} + \hat{\bar{\psi}} \eta) dx} | 0 \rangle \\ &= \text{const} \times \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{i \int dx [\mathcal{L}_0(\psi, \bar{\psi}) + \bar{\eta} \psi + \bar{\psi} \eta]}. \end{aligned} \quad (14.228)$$

where $\mathcal{L}_0(x)$ is the free-field Lagrangian

$$\mathcal{L}_0(x) = \bar{\psi}(x) (i\gamma^\mu \partial_\mu - M) \psi(x) = \bar{\psi}(x) A(x, y) \psi(y), \quad (14.229)$$

By analogy with the bosonic expression (14.226) we obtain for Dirac particles

$$\begin{aligned} Z_0[\bar{\eta}, \eta] &= e^{\frac{1}{2} \int dx dy \frac{\delta}{\delta \bar{\psi}(x)} G_0(x-y) \frac{\delta}{\delta \psi(y)}} \langle 0 | : e^{i \int dx (\bar{\eta} \hat{\psi} + \hat{\bar{\psi}} \eta) \eta} : | 0 \rangle \\ &= e^{-\frac{1}{2} \int dx dy \bar{\eta}(x) G_0(x-y) \eta(y)} \langle 0 | : e^{i \int dx (\bar{\eta} \hat{\psi} + \hat{\bar{\psi}} \eta) \eta} : | 0 \rangle \\ &= e^{-\frac{1}{2} \int dx dy \bar{\eta}(x) G_0(x-y) \eta(y)}, \end{aligned} \quad (14.230)$$

where $G_0(x-y)$ is the free fermion propagator, related to the functional inverse of the matrix $A(x, y)$ by

$$A^{-1}(x, y) = \frac{1}{i\gamma^\mu \partial_\mu - M + i\epsilon} \delta(x-y) = -iG_0(x-y). \quad (14.231)$$

Note that it is Wick's expansion which supplies the free part of the Lagrangian when going from the operator form (14.224) to the functional version (14.221).

14.12 Plasma Oscillation

The functional formulation of second-quantized many-body systems allows us to treat efficiently various collective phenomena. As a first example we shall consider a many-electron system that interacts only via long-range Coulomb forces. The Coulomb forces give rise to collective modes called plasmons.

The other extremely important example caused by attractive short-range interactions will be treated in the next chapter.

14.12.1 Plasmon Fields

Let us give a first application of the functional method by transforming the grand partition function (14.213) to plasmon coordinates.

For this, we make use of the Hubbard-Stratonovich transformation (14.99) and observe that a two-body interaction (14.161) in the generating functional (14.213) can always be produced (following Maxwell's original ideas in electromagnetism) by an auxiliary field $\varphi(x)$ as follows:

$$\begin{aligned} &\exp \left[-\frac{i}{2} \int dx dx' \psi^*(x) \psi^*(x') \psi(x) \psi(x') V(x, x') \right] \\ &= \text{const} \times \int \mathcal{D}\varphi \left\{ \frac{i}{2} \int dx dx' [\varphi(x) V^{-1}(x, x') \varphi(x') - 2\varphi(x) \psi^*(x) \psi(x) \delta(x-x')] \right\}. \end{aligned} \quad (14.232)$$

To abbreviate the notation, we have used a four-vector notation in which

$$x \equiv (\mathbf{x}, t), \quad dx \equiv d^3x dt, \quad \delta(x) \equiv \delta^3(\mathbf{x})\delta(t).$$

The symbol $V^{-1}(x, x')$ denotes the functional inverse of the matrix $V(x, x')$, i.e., the solution of the equation

$$\int dx' V^{-1}(x, x') V(x', x'') = \delta(x - x''). \quad (14.233)$$

The constant prefactor in (14.232) is $[\det V]^{-1/2}$. Absorbing this into the always omitted normalization factor N of the functional integral, the grand-canonical partition function $\Omega = Z$ becomes

$$Z[\eta^*, \eta] = \int \mathcal{D}\psi^* \mathcal{D}\psi D\varphi \exp \left[i\mathcal{A} + i \int dx (\eta^*(x)\psi(x) + \psi^*(x)\eta(x)) \right], \quad (14.234)$$

where the new action is

$$\begin{aligned} \mathcal{A}[\psi^*, \psi, \varphi] = \int dx dx' \bigg\{ & \psi^*(x) [i\partial_t - \xi(-i\nabla) - \varphi(x)] \delta(x - x') \psi(x') \\ & + \frac{1}{2} \varphi(x) V^{-1}(x, x') \varphi(x') \bigg\}. \end{aligned} \quad (14.235)$$

Note that the effect of using formula (14.99) in the generating functional amounts to the addition of the complete square in φ in the exponent:

$$\begin{aligned} \frac{1}{2} \int dx dx' \bigg[& \varphi(x) - \int dy V(x, y) \psi^*(y) \psi(y) \bigg] V^{-1}(x, x') \\ & \times \bigg[\varphi(x') - \int dy' V(x', y') \psi^*(y') \psi(y') \bigg], \end{aligned} \quad (14.236)$$

together with the additional integration over $\mathcal{D}\varphi$. This procedure of going from (14.161) to (14.235) is probably simpler mnemonically than via the formula (14.99). The fact that the functional Z remains unchanged by this addition is obvious, since the integral $D\varphi$ produces only the irrelevant constant $[\det V]^{-1/2}$.

The physical significance of the new field $\varphi(x)$ is easy to understand: $\varphi(x)$ is directly related to the particle density. At the classical level this is seen immediately by extremizing the action (14.235) with respect to variations $\delta\varphi(x)$:

$$\frac{\delta\mathcal{A}}{\delta\varphi(x)} = \varphi(x) - \int dy V(x, y) \psi^*(y) \psi(y) = 0. \quad (14.237)$$

Quantum mechanically, there will be fluctuations around the field configuration $\varphi(x)$ determined by Eq. (14.237), causing a difference between the Green functions involving the fields $\varphi(x)$ versus those involving the associated composite field operators $\int dy V(x, y) \psi^*(y) \psi(y)$. Due to the Gaussian nature of the $D\varphi$ integration, the

difference between the two is quite simple. for example, one can easily see that the propagators of the two fields differ merely by the direct interaction:

$$\begin{aligned} \langle T(\varphi(x)\varphi(x')) \rangle & \quad (14.238) \\ &= V(x-x') + \left\langle T \left[\int dy V(x,y)\psi(y) \right] \left[\int dy' V(x',y')\psi^*(y')\psi(y') \right] \right\rangle. \end{aligned}$$

For the proof, the reader is referred to Appendix 14A. Note that for a potential V which is dominantly caused by a single fundamental-particle exchange, the field $\varphi(x)$ coincides with the field of this particle: If, for example, $V(x,y)$ represents the Coulomb interaction

$$V(x,x') = \frac{e^2}{|\mathbf{x} - \mathbf{x}'|} \delta(t-t'), \quad (14.239)$$

then Eq. (14.237) amounts to

$$\varphi(\mathbf{x}, t) = -\frac{4\pi e^2}{\nabla^2} \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t), \quad (14.240)$$

revealing the auxiliary field as the electric potential.

If the particles $\psi(x)$ have spin indices, the potential will, in this example, be thought of as spin conserving at every vertex, and Eq. (14.237) must be read as spin contracted: $\varphi(x) \equiv \int d^4y V(x,y) \psi^{*\alpha}(y) \psi_\alpha(y)$. This restriction is initially applied only for convenience, and can easily be dropped later. Nothing in our procedure depends on this particular property of V and φ . In fact, V could arise from the exchange of many different fundamental particles and their multiparticle configurations (for example $\pi, \pi\pi, \sigma, \varphi$, etc. in nuclei) so that the spin dependence is the rule rather than the exception.

The important point is now that the entire theory can be rewritten as a field theory of only the auxiliary field $\varphi(x)$. For this we integrate out ψ^* and ψ in Eq. (14.234), and make use of formula (14.100) to obtain

$$Z[\eta^*, \eta] \equiv \Omega[\eta^*, \eta] = Ne^{i\mathcal{A}}, \quad (14.241)$$

where the new action is

$$\mathcal{A}[\varphi] = \pm \text{Tr} \log (iG_\varphi^{-1}) + \frac{1}{2} \int dx dx' \eta^*(x) G_\varphi(x, x') \eta(x'), \quad (14.242)$$

with G_φ being the Green function of the fundamental particles in an external classical field $\varphi(x)$:

$$[i\partial_t - \chi(-i\nabla) - \varphi(x)] G_\varphi(x, x') = i\delta(x - x'). \quad (14.243)$$

The field $\varphi(x)$ is called a plasmon field. The new plasmon action can easily be interpreted graphically. For this, one expands G_φ in powers of φ :

$$G_\varphi(x, x') = G_0(x - x') - i \int dx_1 G_0(x - x_1) \varphi(x_1 - x') + \dots \quad (14.244)$$

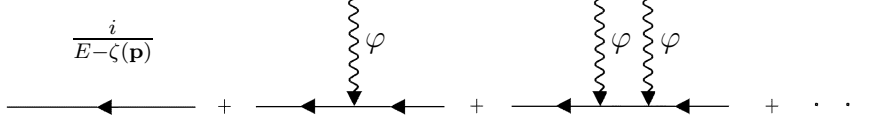


FIGURE 14.1 The last pure-current term of collective action (14.242). The original fundamental particle (straight line) can enter and leave the diagrams only via external currents, emitting an arbitrary number of plasmons (wiggly lines) on its way.

Hence the couplings to the external currents η^*, η in (14.242) amount to radiating one, two, etc. φ fields from every external line of fundamental particles (see Fig. 14.1).

A functional expansion of the $\text{Tr} \log$ expression in powers of φ gives

$$\begin{aligned} \pm i \text{Tr} \log(iG_\varphi^{-1}) &= \pm i \text{Tr} \log(iG_0^{-1}) \pm i \text{Tr} \log(1 + iG_0\varphi) \\ &= \pm i \text{Tr} \log(iG_0^{-1}) \mp i \text{Tr} \sum_{n=1}^{\infty} (-iG_0\varphi)^n \frac{1}{n}. \end{aligned} \quad (14.245)$$

The first term leads to an irrelevant multiplicative factor in (14.241). The n th term corresponds to a loop of the original fundamental particle emitting $n\varphi$ lines (see Fig. 14.2).

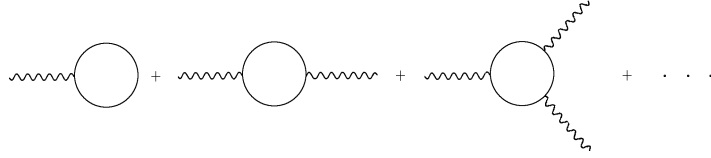


FIGURE 14.2 Non-polynomial self-interaction terms of plasmons arising from the $\text{Tr} \log$ in (14.242). The n th term presents a single-loop diagram emitting n plasmons.

Let us now use the action (14.242) to construct a quantum field theory of plasmons. For this we may include the quadratic term

$$\pm i \text{Tr}(G_0\varphi)^2 \frac{1}{2} \quad (14.246)$$

into the free part of φ in (14.242) and treat the remainder perturbatively. The free propagator of the plasmon becomes

$$\{0|T\varphi(x)\varphi(x')|0\} \equiv (2s+1)G_0(x', x). \quad (14.247)$$

This corresponds to an inclusion into the V propagator of all ring graphs (see Fig. 14.3). It is worth pointing out that the propagator in momentum space $G^{\text{pl}}(k)$ contains actually two important physical informations. From the derivation at fixed temperature it appears in the transformed action (14.242) as a function of discrete

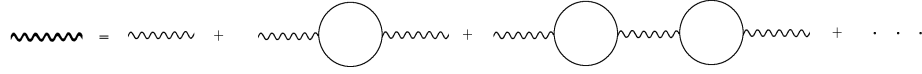


FIGURE 14.3 Free plasmon propagator containing an infinite sequence of single-loop corrections (“bubblewise summation”).

euclidean frequencies $\nu_n = 2\pi nT$ only. In this way it serves to set up a time-independent fixed- T description of the system. The calculation (14.247), however, renders it as a function in the whole complex energy plane. It is this function which determines by analytic continuation the *time-dependent* collective phenomena for *real* times⁶.

With the propagator (14.247) and the interactions given by (14.245), the original theory of fundamental fields ψ^*, ψ has been transformed into a theory of φ fields whose bare propagator accounts for the original potential which has absorbed ringwise an infinite sequence of fundamental loops.

This transformation is exact. Nothing in our procedure depends on the statistics of the fundamental particles nor on the shape of the potential. Such properties are important when it comes to *solving* the theory perturbatively. Only under appropriate physical circumstances will the field φ represent important collective excitations with weak residual interactions. Then the new formulation is of great use in understanding the dynamics of the system. As an illustration consider a dilute fermion gas of very low temperature. Then the function $\xi(-i\nabla)$ is $\epsilon(-i\nabla) - \mu$ with $\epsilon(-i\nabla) = -\nabla^2/2m$.

14.12.2 Physical Consequences

Let the potential be translationally invariant and instantaneous:

$$V(x, x') = \delta(t - t')V(\mathbf{x} - \mathbf{x}'). \quad (14.248)$$

Then the plasmon propagator (14.247) reads in momentum space

$$G_{\text{pl}}(\nu, \mathbf{k}) = V(\mathbf{k}) \frac{1}{1 - V(\mathbf{k})\pi(\nu, \mathbf{k})} \quad (14.249)$$

where the single electron loop symbolizes the analytic expression⁷

$$\pi(\nu, \mathbf{k}) = 2 \frac{T}{V} \sum_p \frac{1}{i\omega - \mathbf{p}^2/2m + \mu} \frac{1}{i(\omega + \nu) - (\mathbf{p} + \mathbf{k})^2/2m + \mu}. \quad (14.250)$$

⁶See the discussion in Chapter 9 of the last of Ref. [7] and G. Baym and N.D. Mermin, J. Math. Phys. **2**, 232 (1961).

⁷The factor 2 stems from the trace over the electron spin.

The frequencies ω and ν are odd and even multiples of πT . In order to calculate the sum we introduce a convergence factor $e^{i\omega\eta}$, and rewrite (14.250) as

$$\pi(\nu, \mathbf{k}) = 2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{\xi(\mathbf{p} + \mathbf{k}) - \xi(\mathbf{p}) - i\nu} \quad (14.251)$$

$$\times T \sum_{\omega_n} e^{i\omega_n\eta} \left[\frac{1}{i(\omega_n + \nu) - \xi(\mathbf{p} + \mathbf{k})} - \frac{1}{i\omega_n - \xi(\mathbf{p})} \right].$$

Using the summation formula (14.197), this becomes

$$\pi(\nu, \mathbf{k}) = 2 \int \frac{d^3p}{(2\pi)^3} \frac{n(\mathbf{p} + \mathbf{k}) - n(\mathbf{p})}{\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p}) - i\nu}, \quad (14.252)$$

or, after some rearrangement,

$$\pi(\nu, \mathbf{k}) = -2 \int \frac{d^3p}{(2\pi)^3} n(\mathbf{p}) \left[\frac{1}{\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p}) - i\nu} + \frac{1}{\epsilon(\mathbf{p} - \mathbf{k}) - \epsilon(\mathbf{p}) + i\nu} \right]. \quad (14.253)$$

Let us study this function for real physical frequencies $\omega = i\nu$ where we rewrite it as

$$\pi(\omega, \mathbf{k}) = -2 \int \frac{d^3p}{(2\pi)^3} n(\mathbf{p}) \left[\frac{1}{\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p}) - \omega} + \frac{1}{\epsilon(\mathbf{p} - \mathbf{k}) - \epsilon(\mathbf{p}) + \omega} \right], \quad (14.254)$$

which can be brought to the form

$$\pi(\omega, \mathbf{k}) = 2 \frac{k^2}{m\omega^2} \int \frac{d^3p}{(2\pi)^3} n(\mathbf{p}) \frac{1}{(\omega - \mathbf{p} \cdot \mathbf{k}/m + i\eta)^2 - (k^2/2M)^2}. \quad (14.255)$$

For $|\omega| > p_F k/m + k^2/2m$, the integrand is real and we can expand

$$\pi(\omega, \mathbf{k}) = 2 \frac{k^2}{m\omega^2} \int \frac{d^3p}{(2\pi)^3} n(\mathbf{p}) \left[1 + \frac{2\mathbf{p} \cdot \mathbf{k}}{m\omega} + 3 \left(\frac{\mathbf{p} \cdot \mathbf{k}}{m\omega} \right)^2 \right. \\ \left. + \left(\frac{\mathbf{p} \cdot \mathbf{k}}{m\omega} \right)^3 + \frac{80(\mathbf{p} \cdot \mathbf{k})^4 + m^2\omega^2 k^4}{16m^2\omega^4} + \dots \right]. \quad (14.256)$$

Zero Temperature

For zero temperature, the chemical potential coincides with the radius of the Fermi sphere $\mu = p_F$, and all levels below the Fermi momentum are occupied, so that the Fermi distribution function is $n(\mathbf{p}) = \Theta(p - p_F)$. Then the integral in (14.256) can be performed trivially using the integral

$$2 \int \frac{d^3p}{(2\pi)^3} n_{T=0}(\mathbf{p}) = \frac{N}{V} = n = \frac{p_F^3}{3\pi^2}, \quad (14.257)$$

and we obtain

$$\pi(\omega, \mathbf{k}) = \frac{k^2}{\omega^2} \frac{n}{m} \left[1 + \frac{3}{5} \left(\frac{p_F k}{m\omega} \right)^2 + \frac{1}{5} \left(\frac{p_F k}{m\omega} \right)^4 + \frac{1}{16} \frac{k^4}{m^2 \omega^2} + \dots \right]. \quad (14.258)$$

Inserting this into (14.249) we find, for long wavelengths, the Green function

$$G^{\text{pl}}(\nu, \mathbf{k}) \approx V(\mathbf{k}) \left[1 - \frac{V(\mathbf{k})}{\omega^2} \frac{n}{m} + \dots \right]^{-1}. \quad (14.259)$$

Thus the original propagator is modified by a factor

$$\epsilon(\omega, \mathbf{k}) = 1 - \frac{4\pi e^2}{\omega^2} \frac{n}{m} + \dots. \quad (14.260)$$

The dielectric constant vanishes at the frequency

$$\omega = \omega_{\text{pl}} = \sqrt{\frac{4\pi e^2}{m}}, \quad (14.261)$$

which is the famous plasma frequency of the electron gas. At this frequency, the plasma propagator (14.249) has a pole on the real- ω axis, implying the existence of an undamped excitation of the system.

For an electron gas we insert the Coulomb interaction (14.240), and obtain

$$G^{\text{pl}}(\nu, \mathbf{k}) \approx \frac{4\pi e^2}{\mathbf{k}^2} \left[1 - \frac{4\pi e^2}{m\omega^2} n + \dots \right]^{-1}. \quad (14.262)$$

Thus the original Coulomb propagator is modified by a factor

$$\epsilon(\omega, \mathbf{k}) = 1 - \frac{4\pi e^2}{m\omega^2} n + \dots, \quad (14.263)$$

which is simply the dielectric constant.

The zero temperature limit can also be calculated exactly starting from the expression (14.256), written in the form

$$\pi(\omega, \mathbf{k}) = -2 \int \frac{d^3 p}{(2\pi)^3} \Theta(p - p_F) \left[\frac{1}{\mathbf{p} \cdot \mathbf{k} + k^2/2m - \omega} + (\omega \rightarrow -\omega) \right]. \quad (14.264)$$

Performing the integral yields

$$\begin{aligned} \pi(\omega, \mathbf{k}) = & -\frac{mp_F}{2\pi^2} \left\{ 1 - \frac{1}{2kp_F} \left[p_F^2 - \left(\frac{k}{2} + \frac{m\omega}{k} \right)^2 + p_F^2 \right] \log \frac{k^2 + 2m\omega - 2kp_F}{k^2 + 2m\omega + 2kp_F} \right\} \\ & + (\omega \rightarrow -\omega). \end{aligned} \quad (14.265)$$

The lowest terms of a Taylor expansion in powers of k agree with (14.258).

Short-Range Potential

Let us also find the real poles of $G_{\text{pl}}(\nu, \mathbf{k})$ for a short-range potential where the singularity at $\mathbf{k} = 0$ is absent. Then a rotationally invariant $[V(\mathbf{k})]^{-1}$ has the long-wavelength expansion

$$[V(\mathbf{k})]^{-1} = [V(\mathbf{0})]^{-1} + a\mathbf{k}^2 + \dots, \quad (14.266)$$

as long as $[V(\mathbf{0})]^{-1}$ is finite and positive, i.e., for a well behaved overall repulsive potential satisfying $V(\mathbf{0}) = \int d^3x V(\mathbf{x}) > 0$. Then the Green function (14.249) becomes

$$G_{\text{pl}}(\omega, \mathbf{k}) = \omega^2 \left\{ \omega^2 [V(\mathbf{0})]^{-1} + a\omega^2 k^2 - k^2 \frac{n}{m} \left[1 + \frac{3}{5} \left(\frac{p_F k}{m\omega} \right)^2 + \dots \right] \right\}^{-1}. \quad (14.267)$$

This has a pole at $\omega = \pm c_0 k$ where

$$c_0 = V(\mathbf{0}) \frac{n}{m}. \quad (14.268)$$

This is the spectrum of zero sound with the velocity c_0 .

In the neighbourhood of the positive-energy pole, the propagator has the form

$$G^{\text{pl}}(k_0, k) \approx V(\mathbf{0}) \times \frac{|\mathbf{k}|}{\omega - c_0 |\mathbf{k}|}. \quad (14.269)$$

Nonzero Temperature

In order to discuss the case of nonzero temperature it is convenient to add and subtract a term $-n(\mathbf{p} + \mathbf{k})n(\mathbf{k})$ in the numerator of (14.252), and rewrite it as

$$\pi(\nu, \mathbf{k}) = 2 \int \frac{d^3p}{(2\pi)^3} \frac{n(\mathbf{p} + \mathbf{k}) [1 - n(\mathbf{p})] - n(\mathbf{p}) [1 - n(\mathbf{p} + \mathbf{k})]}{\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p}) - i\nu}, \quad (14.270)$$

which can be rearranged to

$$\pi(\nu, \mathbf{k}) = -4 \int \frac{d^3p}{(2\pi)^3} n(\mathbf{p}) [1 - n(\mathbf{p} + \mathbf{k})] \frac{\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p})}{[\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p})]^2 + \nu^2}. \quad (14.271)$$

In the high-temperature limit the Fermi distribution becomes Boltzmannian, $n(\mathbf{p}) \approx e^{-\beta(\mathbf{p}^2/2 - \mu)}$, and we evaluate again most easily expression (14.256) as follows:

$$\pi(\omega, \mathbf{k}) = -2 \int_0^\infty d\sigma \int \frac{d^3p}{(2\pi)^3} e^{-\beta(\mathbf{p}^2/2 - \mu) - \sigma[\epsilon(\mathbf{p} + \mathbf{k}) - \epsilon(\mathbf{p}) - \omega]} + (\omega \rightarrow -\omega). \quad (14.272)$$

The right-hand side is equal to

$$-\int_0^\infty d\sigma \int_{-1}^1 \frac{d \cos \theta}{2} \int \frac{d^3p}{(2\pi)^3} e^{-\beta(\mathbf{p}^2/2 - \mu) - \sigma[(pk \cos \theta/m + k^2/2m) - \omega]} + (\omega \rightarrow -\omega). \quad (14.273)$$

Performing the angular integral yields

$$-\frac{m^2}{k^2} \int_0^\infty \frac{d\sigma}{2\pi^2} \int \frac{d^3p}{(2\pi)^3} e^{-\beta(\mathbf{p}^2/2 - \mu) + \sigma\omega} \frac{1}{p^2} (pk \cosh pk - \sinh pk) + (\omega \rightarrow -\omega). \quad (14.274)$$

14.13 Pair Fields

The introduction of a scalar field $\varphi(x)$ was historically the first way, invented by Maxwell, to convert the Coulomb interaction in a theory (14.232) into a local field theory. The resulting plasmon action depends only on the *local field* φ . There exists an alternative way of converting the interaction between four fermions in (14.232) into a new field theory. That is based on introducing a *bilocal scalar* field which has been very successful to understand the properties of electrons in of superconductors. It is a collective field complementary to the plasmon field. Generically it will be called a *pair field*. It describes the dominant low-energy collective excitations in systems such as type II superconductors, superfluid ^3He , excitonic insulators, etc. The pair field is originally a bilocal field and will be denoted by $\Delta(\mathbf{x}t; \mathbf{x}'t')$, with two space arguments and two time arguments. It is introduced into the generating functional by rewriting the exponential of the interaction term in (14.232) in the partition function (14.169) as a functional integral

$$\exp \left[-\frac{i}{2} \int dxdx' \psi^*(x) \psi^*(x') \psi(x') \psi(x) V(x, x') \right] = \text{const} \times \int \mathcal{D}\Delta(x, x') \mathcal{D}\Delta^*(x, x') \\ \times e^{\frac{i}{2} \int dxdx' \left\{ |\Delta(x, x')|^2 \frac{1}{V(x, x')} - \Delta^*(x, x') \psi(x) \psi(x') - \psi^*(x) \psi^*(x') \Delta(x, x') \right\}}. \quad (14.275)$$

In contrast to the similar-looking plasmon expression (14.232), the inverse $1/V(x, x')$ in (14.275) is understood as a numeric division for each x, y , not as a functional inverse. Hence the grand-canonical potential becomes

$$Z[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi \mathcal{D}\Delta^* \mathcal{D}\Delta e^{i\mathcal{A}[\psi^*, \psi, \Delta^*, \Delta] + i \int dx (\psi^*(x) \eta(x) + \text{c.c.})}, \quad (14.276)$$

with the action

$$\mathcal{A}[\psi^*, \psi, \Delta^*, \Delta] = \int dxdx' \left\{ \psi^*(x) [i\partial_t - \xi(-i\nabla)] \delta(x - x') \psi(x') \right. \\ \left. - \frac{1}{2} \Delta^*(x, x') \psi(x) \psi(x') - \frac{1}{2} \psi^*(x) \psi^*(x') \Delta(x, x') + \frac{1}{2} |\Delta(x, x')|^2 \frac{1}{V(x, x')} \right\}, \quad (14.277)$$

where $\xi_{\mathbf{p}} \equiv \varepsilon_{\mathbf{p}} - \mu$ is the grand-canonical single particle energy (2.256). This new action arises from the original one in (14.169) by adding to it the complete square

$$\frac{i}{2} \int dxdx' |\Delta(x, x') - V(x', x) \psi(x') \psi(x)|^2 \frac{1}{V(x, x')}, \quad (14.278)$$

which removes the fourth-order interaction term and gives, upon functional integration over $\int \mathcal{D}\Delta^* \mathcal{D}\Delta$, merely an irrelevant constant factor to the generating functional.

At the classical level, the field $\Delta(x, x')$ is nothing but a convenient abbreviation for the composite field $V(x, x') \psi(x) \psi(x')$. This follows from the equation of motion obtained by extremizing the new action with respect to $\delta\Delta^*(x, x')$. This yields

$$\frac{\delta\mathcal{A}}{\delta\Delta^*(x, x')} = \frac{1}{2V(x, x')} [\Delta(x, x') - V(x, x') \psi(x) \psi(x')] \equiv 0. \quad (14.279)$$

Quantum mechanically, there are Gaussian fluctuations around this solution which are discussed in Appendix 14B.

Taking care of the spin components of the Fermi field, we can rewrite the first line in the expression (14.278), which are quadratic in the fundamental fields $\psi(x)$, in a matrix form as

$$\begin{aligned} & \frac{1}{2} f^*(x) A(x, x') f(x') \\ &= \frac{1}{2} f^\dagger(x) \begin{pmatrix} [i\partial_t - \xi(-i\nabla)] \delta(x - x') & -\Delta(x, x') \\ -\Delta^*(x, x') & \mp [i\partial_t + \xi(i\nabla)] \delta(x - x') \end{pmatrix} f(x'), \end{aligned} \quad (14.280)$$

where $f(x)$ denotes the fundamental field doublet

$$f(x) = \begin{pmatrix} \psi(x) \\ \psi^*(x) \end{pmatrix} \quad (14.281)$$

and $f^\dagger \equiv f^{*T}$, as usual. Here the field $f^*(x)$ is not independent of $f(x)$. Indeed, there is an identity

$$f^\dagger A f = f^T \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} A f. \quad (14.282)$$

Therefore, the real-field formula (14.99) must be used to evaluate the functional integral for the generating functional

$$Z[\eta^*, \eta] = \int \mathcal{D}\Delta^* \mathcal{D}\Delta e^{i\mathcal{A}[\Delta^*, \Delta] - \frac{1}{2} \int dx \int dx' j^\dagger(x) G_\Delta(x, x') j(x')}, \quad (14.283)$$

where $j(x)$ collects the external source $\eta(x)$ and its complex conjugate, $j(x) \equiv \begin{pmatrix} \eta(x) \\ \eta^*(x) \end{pmatrix}$. Then the collective action (14.278) reads

$$\mathcal{A}[\Delta^*, \Delta] = \pm \frac{i}{2} \text{Tr} \log [i\mathbf{G}_\Delta^{-1}(x, x')] + \frac{1}{2} \int dx dx' |\Delta(x, x')|^2 \frac{1}{V(x, x')}. \quad (14.284)$$

The 2×2 matrix $\mathbf{G}_\Delta$ denotes the propagator iA^{-1} which satisfies the functional equation

$$\int dx'' \begin{pmatrix} [i\partial_t - \xi(-i\nabla)] \delta(x - x'') & -\Delta(x, x'') \\ -\Delta^*(x, x'') & \mp [i\partial_t + \xi(i\nabla)] \delta(x - x'') \end{pmatrix} \mathbf{G}_\Delta(x'', x') = i\delta(x - x'). \quad (14.285)$$

Writing $\mathbf{G}_\Delta$ as a matrix $\begin{pmatrix} G & G_\Delta \\ G_\Delta^\dagger & \tilde{G} \end{pmatrix}$, the mean-field equations associated with this action are precisely the equations used by Gorkov to study the behavior of type II superconductors [12]. With $Z[\eta^*, \eta]$ being the *full* partition function of the system, the fluctuations of the collective field $\Delta(x, x')$ can now be incorporated, at least in principle, thereby yielding corrections to these equations.

Let us set the sources in the generating functional $Z[\eta^*, \eta]$ equal to zero and investigate the behavior of the collective quantum field Δ . In particular, we want to develop Feynman rules for a perturbative treatment of the fluctuations of $\Delta(x, x')$. As a first step we expand the Green function $\mathbf{G}_\Delta$ in powers of Δ as

$$\mathbf{G}_\Delta = \mathbf{G}_0 - i\mathbf{G}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \mathbf{G}_0 - \mathbf{G}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \mathbf{G}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \mathbf{G}_0 + \dots \quad (14.286)$$

with

$$\mathbf{G}_0(x, x') = \begin{pmatrix} \frac{i}{i\partial_t - \xi(-i\nabla)} \delta(x - x') & 0 \\ 0 & \mp \frac{i}{i\partial_t + \xi(i\nabla)} \delta(x - x') \end{pmatrix}. \quad (14.287)$$

We shall see later that this expansion is applicable only close to the critical temperature T_c . Inserting this expansion into (14.283), the source term can be interpreted graphically by the absorption and emission of lines $\Delta(k)$ and $\Delta^*(k)$, respectively, from virtual zig-zag configurations of the underlying particles $\psi(k), \psi^*(k)$ (see Fig. 14.4)

$$\Delta^*(\nu', \mathbf{q}') \quad \frac{i}{\omega - \xi(\mathbf{p})} \quad \frac{i}{\nu' - \omega - \xi(\mathbf{q}' - \mathbf{p})} \quad \frac{i}{\nu - \nu' + \omega - \xi(\mathbf{q} - \mathbf{q}' + \mathbf{p})} \quad \Delta(\nu, \mathbf{q}) \quad + \dots \quad (14.286)$$

FIGURE 14.4 Fundamental particles (fat lines) entering any diagram only via the external currents in the last term of (14.283), absorbing n pairs from the right (the past) and emitting the same number from the left (the future).

The functional submatrices in $\mathbf{G}_0$ have the Fourier representation

$$G_0(x, x') = \frac{T}{V} \sum_p \frac{i}{p^0 - \xi_{\mathbf{p}}} e^{-i(p^0 t - \mathbf{p}\mathbf{x})}, \quad (14.289)$$

$$\tilde{G}_0(x, x') = \pm \frac{T}{V} \sum_p \frac{i}{-p^0 - \xi_{-\mathbf{p}}} e^{-i(p^0 t - \mathbf{p}\mathbf{x})}, \quad (14.290)$$

where we have used the notation $\xi_{\mathbf{p}}$ for the Fourier components $\xi(\mathbf{p})$ of $\xi(-i\nabla)$.

The first matrix coincides with the operator Green function

$$G_0(x - x') = \langle 0 | T \psi(x) \psi^\dagger(x') | 0 \rangle. \quad (14.291)$$

The second one corresponds to

$$\begin{aligned} \tilde{G}_0(x - x') &= \langle 0 | T \psi^\dagger(x) \psi(x') | 0 \rangle = \pm \langle 0 | T (\psi(x') \psi^\dagger(x)) | 0 \rangle \\ &= \pm G_0(x' - x) \equiv \pm [G_0(x, x')]^T, \end{aligned} \quad (14.292)$$

where T denotes the transposition in the functional sense (i.e., x and x' are interchanged). After a Wick rotation of the energy integration contour, the Fourier components of the Green functions at fixed energy read

$$G_0(\mathbf{x} - \mathbf{x}', \omega) = - \sum_{\mathbf{p}} \frac{1}{i\omega - \xi_{\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x} - \mathbf{x}')} \quad (14.293)$$

$$\tilde{G}_0(\mathbf{x} - \mathbf{x}', \omega) = \mp \sum_{\mathbf{p}} \frac{1}{-i\omega - \xi_{-\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x} - \mathbf{x}')} = \mp G_0(\mathbf{x}' - \mathbf{x}, -\omega). \quad (14.294)$$

The $\text{Tr} \log$ term in Eq. (14.284) can be interpreted graphically just as easily by expanding as in (14.286):

$$\pm \frac{i}{2} \text{Tr} \log (i\mathbf{G}_{\Delta}^{-1}) = \pm \frac{i}{2} \text{Tr} \log (i\mathbf{G}_0^{-1}) \mp \frac{i}{2} \text{Tr} \left[-i\mathbf{G}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \Delta^* \right]^n \frac{1}{n}. \quad (14.295)$$

The first term only changes the irrelevant normalization N of Z . To the remaining sum only even powers can contribute so that we can rewrite

$$\begin{aligned} \mathcal{A}[\Delta^*, \Delta] &= \mp i \sum_{n=1}^{\infty} \frac{(-)^n}{2n} \text{Tr} \left[\left(\frac{i}{i\partial_t - \xi(-i\nabla)} \delta \right) \Delta \left(\frac{\mp i}{i\partial_t + \xi(i\nabla)} \delta \right) \Delta^* \right]^n \\ &\quad + \frac{1}{2} \int dx dx' |\Delta(x, x')|^2 \frac{1}{V(x, x')} \\ &= \sum_{n=1}^{\infty} \mathcal{A}_n[\Delta^*, \Delta] + \frac{1}{2} \int dx dx' |\Delta(x, x')|^2 \frac{1}{V(x, x')}. \end{aligned} \quad (14.296)$$

This form of the action allows an immediate quantization of the collective field Δ . The graphical rules are slightly more involved technically than in the plasmon case since the pair field is bilocal. Consider at first the *free* collective fields which can be obtained from the quadratic part of the action:

$$\mathcal{A}_2[\Delta^*, \Delta] = -\frac{i}{2} \text{Tr} \left[\left(\frac{i}{i\partial_t - \xi(-i\nabla)} \delta \right) \Delta \left(\frac{i}{i\partial_t + \xi(i\nabla)} \delta \right) \Delta^* \right]. \quad (14.297)$$

Variation with respect to Δ displays the equations of motion

$$\Delta(x, x') = iV(x, x') \left[\left(\frac{i}{i\partial_t - \xi(-i\nabla)} \delta \right) \Delta \left(\frac{i}{i\partial_t + \xi(i\nabla)} \delta \right) \right]. \quad (14.298)$$

This equation coincides exactly with the Bethe-Salpeter equation [13] in the ladder approximation. Originally, this was set up for two-body bound-state vertex functions, usually denoted in momentum space by

$$\Gamma(p, p') = \int dx dx' \exp[i(px + p'x')] \Delta(x, x'). \quad (14.299)$$

Thus the free excitations of the field $\Delta(x, x')$ consist of bound pairs of the original fundamental particles. The field $\Delta(x, x')$ will consequently be called pair field. If

we introduce total and relative momenta q and $P = (p - p')/2$, then (14.298) can be written as⁸

$$\begin{aligned} \Gamma(P|q) = & -i \int \frac{d^4 P'}{(2\pi)^4} V(P - P') \frac{i}{q_0/2 + P'_0 - \xi_{\mathbf{q}/2+\mathbf{P}'} + i\eta \operatorname{sgn} \xi} \\ & \times \Gamma(P'|q) \frac{i}{q_0/2 - P'_0 - \xi_{\mathbf{q}/2-\mathbf{P}'} + i\eta \operatorname{sgn} \xi}. \end{aligned} \quad (14.300)$$

Graphically this formula can be represented as follows: The Bethe-Salpeter *wave*

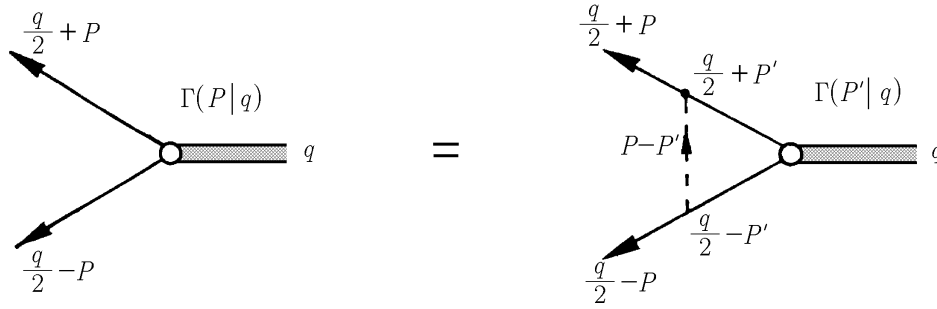


FIGURE 14.5 Free pair field following the Bethe-Salpeter equation as pictured in this diagram.

function is related to the vertex $\Gamma(P|q)$ by

$$\begin{aligned} \Phi(P|q) = & N \frac{i}{q_0/2 + P_0 - \xi_{\mathbf{q}/2+\mathbf{P}} + i\eta \operatorname{sgn} \xi} \\ & \times \frac{i}{q_0/2 - P_0 - \xi_{\mathbf{q}/2-\mathbf{P}} + i\eta \operatorname{sgn} \xi} \Gamma(P|q). \end{aligned} \quad (14.301)$$

It satisfies

$$G_0(q/2 + P) G_0(q/2 - P) \Phi(P|q) = -i \int \frac{dP'}{(2\pi)^4} V(P, P') \Phi(P'|q), \quad (14.302)$$

thus coinciding, up to a normalization, with the Fourier transform of the two-body state wave functions

$$\psi(\mathbf{x}, t; \mathbf{x}', t') = \langle 0|T(\psi(\mathbf{x}, t)\psi(\mathbf{x}', t'))|B(q)\rangle. \quad (14.303)$$

If the potential is instantaneous, then (14.298) shows $\Delta(x, x')$ to be factorizable according to

$$\Delta(x, x') = \delta(t - t') \Delta(\mathbf{x}, \mathbf{x}'; t) \quad (14.304)$$

so that $\Gamma(P|q)$ becomes independent of P_0 .

⁸Here q abbreviates the four-vector $q^\mu = (q^0, \mathbf{q})$ with $q_0 = E$.

Consider now the system at $T = 0$ in the vacuum. Then $\mu = 0$ and $\xi_{\mathbf{p}} = \varepsilon_{\mathbf{p}} > 0$. One can perform the P_0 integral in (14.300) with the result

$$\Gamma(\mathbf{P}|q) = \int \frac{d^3 P'}{(2\pi)^4} V(\mathbf{P} - \mathbf{P}') \frac{1}{q_0 - \varepsilon_{\mathbf{q}/2+\mathbf{P}'} - \varepsilon_{\mathbf{q}/2-\mathbf{P}'} + i\eta} \Gamma(\mathbf{P}'|q). \quad (14.305)$$

Now the equal-time Bethe-Salpeter wave function

$$\begin{aligned} \psi(\mathbf{x}, \mathbf{x}'; t) \equiv & N \int \frac{d^3 \mathbf{P} d q_0 d^3 \mathbf{q}}{(2\pi)^7} \exp \left[-i \left(q_0 t - \mathbf{q} \cdot \frac{\mathbf{x} + \mathbf{x}'}{2} - \mathbf{P} \cdot (\mathbf{x} - \mathbf{x}') \right) \right] \\ & \times \frac{1}{q_0 - \varepsilon_{\mathbf{q}/2+\mathbf{P}} - \varepsilon_{\mathbf{q}/2-\mathbf{P}} + i\eta} \Gamma(\mathbf{P}|q) \end{aligned} \quad (14.306)$$

satisfies

$$\left[i\partial_t - \epsilon_{(-i\nabla)} - \epsilon_{(-i\nabla')} \right] \psi(\mathbf{x}, \mathbf{x}'; t) = V(\mathbf{x} - \mathbf{x}') \psi(\mathbf{x}, \mathbf{x}'; t), \quad (14.307)$$

which is simply the Schrödinger equation of the two-body system. Thus, in the instantaneous case, the free collective excitations in $\Delta(x, x')$ are the bound states derived from the Schrödinger equation.

In a thermal ensemble, the energies in (14.300) have to be summed over the Matsubara frequencies only. First, we write the Schrödinger equation as

$$\Gamma(\mathbf{P}|q) = - \int \frac{d^3 \mathbf{P}'}{(2\pi)^3} V(\mathbf{P} - \mathbf{P}') l(\mathbf{P}'|q) \Gamma(\mathbf{P}'|q) \quad (14.308)$$

with

$$\begin{aligned} l(\mathbf{P}|q) &= -i \sum_{P_0} G_0(q/2 + P) \tilde{G}_0(P - q/2) \\ &= -i \sum_{P_0} \frac{i}{q_0/2 + P_0 - \xi_{\mathbf{q}/2+\mathbf{P}} + i\eta \operatorname{sgn} \xi} \frac{i}{q_0/2 - P_0 - \xi_{\mathbf{q}/2-\mathbf{P}} + i\eta \operatorname{sgn} \xi}. \end{aligned} \quad (14.309)$$

After a Wick rotation and setting $q_0 \equiv i\nu$, the replacement of the energy integration by a Matsubara sum leads to

$$\begin{aligned} l(\mathbf{P}|q) &= -T \sum_{\omega_n} \frac{1}{i(\omega_n + \nu/2) - \xi_{\mathbf{q}/2+\mathbf{P}}} \frac{1}{i(\omega_n - \nu/2) + \xi_{\mathbf{q}/2-\mathbf{P}}} \\ &= T \sum_{\omega_n} \frac{1}{i\nu - \xi_{\mathbf{q}/2+\mathbf{P}} - \xi_{\mathbf{q}/2-\mathbf{P}}} \\ &\quad \times \left[\frac{1}{i(\omega_n + \nu/2) - \xi_{\mathbf{q}/2+\mathbf{P}}} - \frac{1}{i(\omega_n - \nu/2) + \xi_{\mathbf{q}/2-\mathbf{P}}} \right] \\ &= -\frac{\pm [n_{\mathbf{q}/2+\mathbf{P}} + n_{\mathbf{q}/2-\mathbf{P}}]}{i\nu - \xi_{\mathbf{q}/2+\mathbf{P}} - \xi_{\mathbf{q}/2-\mathbf{P}}}. \end{aligned} \quad (14.310)$$

Here we have used the frequency sum [see (14.197)]

$$T \sum_{\omega_n} \frac{1}{i\omega_n - \xi_{\mathbf{p}}} = \mp \frac{1}{e^{\xi_{\mathbf{p}}/T} \mp 1} \equiv \mp n_{\mathbf{p}}. \quad (14.311)$$

with $n_{\mathbf{p}}$ being the occupation number of the state of energy $\xi_{\mathbf{p}}$. Using the identity $n_{\mathbf{p}} \rightarrow \mp 1 - n_{\mathbf{p}}$, the expression in brackets can be rewritten as $-N(\mathbf{P}, \mathbf{q})$ where

$$\begin{aligned} N(\mathbf{P}|q) &\equiv 1 \pm (n_{\mathbf{q}/2+\mathbf{P}} + n_{\mathbf{q}/2-\mathbf{P}}) \\ &= \frac{1}{2} \left(\tanh \mp 1 \frac{\xi_{\mathbf{q}/2+\mathbf{P}}}{2T} + \tanh \mp 1 \frac{\xi_{\mathbf{q}/2-\mathbf{P}}}{2T} \right), \end{aligned} \quad (14.312)$$

so that

$$l(\mathbf{P}|q) = - \frac{N(\mathbf{P}|q)}{i\nu - \xi_{\mathbf{q}/2+\mathbf{P}} - \xi_{\mathbf{q}/2-\mathbf{P}}}. \quad (14.313)$$

Defining again a Schrödinger type wave function for $T \neq 0$ as in (14.306), the bound-state problem can be brought to the form (14.305) but with a momentum dependent potential $V(\mathbf{P} - \mathbf{P}') \times N(\mathbf{P}'|q)$. Thus the Bethe-Salpeter equation at any temperature reads

$$\Gamma(\mathbf{P}|q) = \int \frac{d^3 P'}{(2\pi)^4} V(\mathbf{P} - \mathbf{P}') N(\mathbf{P}'|q) \frac{1}{q_0 - \varepsilon_{\mathbf{q}/2+\mathbf{P}'} - \varepsilon_{\mathbf{q}/2-\mathbf{P}'} + i\eta} \Gamma(\mathbf{P}'|q). \quad (14.314)$$

We are now ready to construct the propagator of the pair field $\Delta(x, x')$ for $T = 0$. In many cases, this is most simply done by considering Eq. (14.300) with a potential $\lambda V(P, P')$ rather than V , and asking for all eigenvalues λ_n at *fixed* q . Let $\Gamma_n(P|q)$ be a complete set of vertex functions for this q . Then one can write the propagator as

$$\overline{\Delta(P|q)} \Delta^\dagger(P'|q') = -i \sum_n \frac{\Gamma_n(P|q) \Gamma_n^*(P'|q)}{\lambda - \lambda_n(q)} \Big|_{\lambda=1} (2\pi)^4 \delta^{(4)}(q - q') \quad (14.315)$$

where a hook denotes, as usual, the Wick contraction of the fields. Obviously the vertex functions have to be normalized in a specific way, as discussed in Appendix 14A.

An expansion of (14.315) in powers of $[\lambda/\lambda_n(q)]^n$ exhibits the propagator of Δ as a ladder sum of exchanges as shown in Fig. 14.6.

$$\text{[Diagram: A shaded rectangle representing the propagator]} = \text{[Diagram: A single horizontal line with two vertical segments]} + \text{[Diagram: A horizontal line with two vertical segments and a loop]} + \text{[Diagram: A horizontal line with two vertical segments and two loops]} + \dots \quad (14.316)$$

FIGURE 14.6 Free pair propagator, amounting to a sum of all ladders of fundamental potential exchanges. This is revealed explicitly by the expansion of (14.315) in powers of $(\lambda/\lambda_n(q))$.

For an instantaneous interaction, either side is independent of P_0, P'_0 . Then the propagator can be shown to coincide directly with the scattering matrix T of the Schrödinger equation (14.307) and the associated integral equation in momentum space (14.305) [see Eq. (14A.13)].

$$\overline{\Delta} \Delta^\dagger = iT \equiv iV + iV \frac{1}{E - H} V. \quad (14.317)$$

Consider now the higher interactions $\mathcal{A}_n, n \geq 3$ of Eq. (14.296). They correspond to zig-zag loops shown in Fig. 14.7. These have to be calculated with every possible $\Gamma_n(P|q), \Gamma_m^*(P|q)$ entering or leaving, respectively. Due to the P dependence at

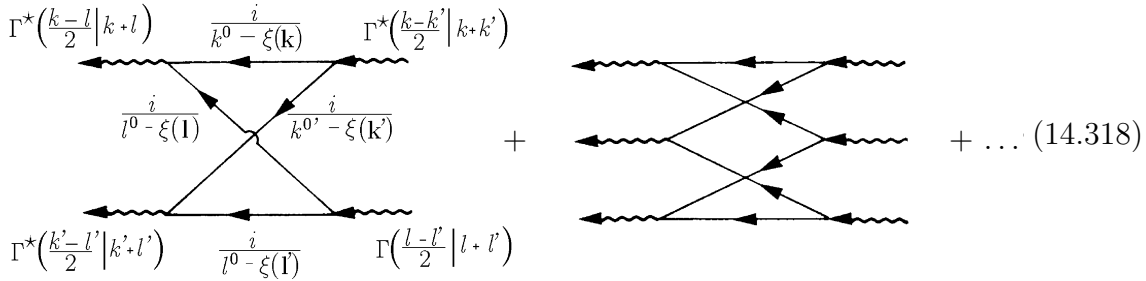


FIGURE 14.7 Self-interaction terms of the non-polynomial pair action (14.296) amounting to the calculation of all single zig-zag loop diagrams absorbing and emitting n pair fields.

every vertex, the loop integrals become very involved. A slight simplification arises for instantaneous potentials. Then the frequency sums can be performed. Only in the special case of a completely local action, the full P -dependence disappears and the integrals can be calculated. See Section IV.2 in Ref. [4].

14.14 Competition of Plasmon and Pair Fields

The Hubbard-Stratonovich transformation has a well-established place in many-body theory [8, 9, 4]. After it had been successfully applied in 1957 by Bardeen, Cooper, and Schrieffer to explain the phenomenon of superconductivity by with the so-called BCS theory [50], Nambu and Jona-Lasinio [14] discovered that the same mechanism which explains the formation of an energy gap and Cooper pairs of electrons in a metal can be used to understand the surprising properties of quark masses in the physics of strongly interacting particles. This aspect of particle physics will be explained in Chapter 26.

In many-body theory, the use of the Hubbard-Stratonovich transformation has led to a good understanding of important collective physical phenomena such as plasma oscillations and other charge-density type of waves, for example paramagnons in superfluid He^3 . It has put heuristic calculations such as the Gorkov's derivation [12] of the Ginzburg-Landau equations [15] on a reliable theoretical ground [4]. In

addition, it is in spirit close to the density functional theory [16] via the Hohenberg-Kohn and Kohn-Sham theorems [17].

In Sections 14.12 and 14.13 we have used the Hubbard-Stratonovich transformation to rewrite the many-body action in two ways. One was theory of a local plasmon field $\varphi(x)$, the other a theory of a bilocal scalar pair field $\Delta(x, x')$. In the theory of collective excitation, either of the two transformations has been helpful to understand either the behavior of electron gases or that of superconductors. In the first case, one is able to deal efficiently with the oscillations of charge distributions in the gas. In the second case one is able to see how the electrons in a superconductor become bound to Cooper pairs, and how the binding gives rise to a frictionless flow of the doubly charged bosonic pairs through the metal. In general, however, there exists a competition between the two mechanisms.

The transformation was cherished by theoreticians since it allows them to re-express a four-particle interaction *exactly* in terms of a collective field variable whose fluctuations can in principle be described by higher loop diagrams. The only bitter pill is that any approximative treatment of a many-body system can describe interesting physics only if calculations can be restricted to a few low-order diagrams. If this is not the case, the transformation fails.

The trouble arises in all those many-body systems in which different collective effects compete with similar relevance. Historically, an important example is the fermionic superfluid He^3 . While BCS superconductivity is described easily via the Hubbard-Stratonovich transformation which turns the four-electron interaction into a field theory of Cooper pairs, the same approach did initially not succeed in a liquid of He^3 -atoms. Due to the strongly repulsive core of an atom, the forces in the attractive p -wave are not sufficient to bind the Cooper pairs. Only by taking into account the existence of another collective field that arises in the competing paramagnon channel was it possible to explain the formation of weakly-bound Cooper pairs [18].

It is important to learn how to deal with this kind of mixture. The answer is found with the help of Variational Perturbation Theory (VPT), which has been discussed in Chapter 3 (see the pages 177 and 216). The key is to abandon the *fluctuating collective quantum fields* introduced by means of the Hubbard-Stratonovich transformation. Instead one must turn to a variety of *collective classical fields*. After a perturbative calculation of the effective action, one obtains a functional that depends on these classical fields. The dependence can be optimized, usually by extremizing their influence upon the effective action. In this way one is able to obtain exponentially fast converging results.

It is the purpose of this section to point out how to circumvent the fatal focussing of the Hubbard-Stratonovich transformation on a specific channel and to take into account the competition between several competing channels.

14.15 Ambiguity in the Selection of Important Channels

The basic weakness of the Hubbard-Stratonovich transformation lies in the different possibilities of decomposing the fourth order interaction by a quadratic completion with the help of an auxiliary field. The first is based on the introduction of a scalar plasmon field $\varphi(x)$ and the use of the quadratic-completion formula (14.232). The other uses the introduction of a bilocal pair field $\Delta(x, x')$ in combination with the quadratic-completion formula (14.275). The trouble with both approaches is that, when introducing an auxiliary field $\varphi(x)$ or $\Delta(x, x')$ and summing over all fluctuations of one of the fields, the effects of the other is automatically included. At first sight, this may appear as an advantage. Unfortunately, this is an illusion. In either case, even the lowest-order fluctuation effect of the other is extremely hard to calculate. That can be seen most simply in the simplest models of quantum field theory such as the Gross-Neveu model (to be discussed in Chapter 23). There the propagator of the quantum field $\Delta(x, x')$ is a very complicated object. So it is practically impossible to recover the effects OF $\varphi(x)$ from the loop calculations with these propagators. As a consequence, the use of a specific quantum field theory must be abandoned whenever collective effects of different channels are important.

To be specific let us assume the fundamental interaction to be of the *local* form

$$\mathcal{A}_{\text{int}}^{\text{loc}} = \frac{g}{2} \int_x \psi_\alpha^* \psi_\beta^* \psi_\beta \psi_\alpha = g \int_x \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow, \quad (14.319)$$

where the subscripts $\uparrow, \downarrow$ denote the spin directions of the fermion fields. For brevity, we have absorbed the spacetime arguments x in the spin subscripts and written the symbol $\int_x$ for an integral over spacetime and a sum over the spin indices of the fermion field.

We now introduce auxiliary *classical* collective fields which are no longer assumed to undergo functional fluctuations, and we replace the exponential in the interacting version of the generating functional (14.276),

$$Z[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{i\mathcal{A}_0[\psi^*, \psi] + i\mathcal{A}_{\text{int}}^{\text{loc}} + i \int dx (\psi^*(x) \eta(x) + \text{c.c.})}, \quad (14.320)$$

identically by [34]

$$\begin{aligned} e^{i\mathcal{A}_{\text{int}}^{\text{loc}}} &= \exp\left\{i g \int_x \psi_{\uparrow, x}^* \psi_{\downarrow, x}^* \psi_{\downarrow, x} \psi_{\uparrow, x}\right\} = \exp\left\{-\frac{i}{2} \int_x f_x^T \mathcal{M}_x f_x\right\} \times \exp\{i\mathcal{A}_{\text{int}}^{\text{new}}\} \quad (14.321) \\ &= \exp\left\{-\frac{i}{2} \int_x \left(\psi_\beta \Delta_{\beta\alpha}^* \psi_\alpha + \psi_\alpha^* \Delta_{\alpha\beta} \psi_\beta^* + \psi_\beta^* \rho_{\beta\alpha} \psi_\alpha + \psi_\alpha^* \rho_{\alpha\beta} \psi_\beta\right)\right\} \times \exp\{i\mathcal{A}_{\text{int}}^{\text{new}}\}. \end{aligned}$$

Here $f(x)$ is here the doubled spinor field (14.281) with spin index:

$$f(x) = \begin{pmatrix} \psi_\alpha(x) \\ \psi_\alpha^*(x) \end{pmatrix}, \quad (14.322)$$

and f_x^T denotes the transposed fundamental field doublet $f_x^T = (\psi_\alpha, \psi_\alpha^*)$. The new interaction reads

$$\mathcal{A}_{\text{int}}^{\text{new}} = \mathcal{A}_{\text{int}}^{\text{loc}} + \frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x = \int_x \left[\frac{g}{2} \psi_\alpha^* \psi_\beta^* \psi_\beta \psi_\alpha + \frac{1}{2} \left(\psi_\beta \Delta_{\beta\alpha}^* \psi_\alpha + \psi_\alpha^* \Delta_{\alpha\beta} \psi_\beta^* \right) + \psi_\alpha^* \rho_{\alpha\beta} \psi_\beta \right]. \quad (14.323)$$

We now define a further free action by the quadratic form

$$\mathcal{A}_0^{\text{new}} \equiv \mathcal{A}_0 - \frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x = \frac{1}{2} f_x^\dagger A_{x,x'}^{\Delta,\rho} f_{x'}. \quad (14.324)$$

with the functional matrix $A_{x,x'}^{\Delta,\rho}$ being now equal to

$$\begin{pmatrix} [i\partial_t - \xi(-i\nabla)]\delta_{\alpha\beta} + \rho_{\alpha\beta} & \Delta_{\alpha\beta} \\ \Delta_{\alpha\beta}^* & [i\partial_t + \xi(i\nabla)]\delta_{\alpha\beta} - \rho_{\alpha\beta} \end{pmatrix}. \quad (14.325)$$

The physical properties of the theory associated with the action $\mathcal{A}_0 + \mathcal{A}_{\text{int}}^{\text{loc}}$ can now be derived as follows: first we calculate the generating functional of the new quadratic action $\mathcal{A}_0^{\text{new}}$ via the functional integral

$$Z_0^{\text{new}}[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{i\mathcal{A}_0^{\text{new}} + i \int dx (\psi^*(x) \eta(x) + \text{c.c.})}. \quad (14.326)$$

From its functional derivatives with respect to the sources η_α and $\eta_\alpha^\dagger$ we find the new free propagators G_Δ and G_ρ . To higher orders, we expand the exponential $e^{i\mathcal{A}_{\text{int}}^{\text{new}}}$ in a power series and evaluate all expectation values $(i^n/n!) \langle [\mathcal{A}_{\text{int}}^{\text{new}}]^n \rangle_0^{\text{new}}$ with the help of Wick's theorem. They are expanded into sums of products of the free particle propagators G_Δ and G_ρ . The sum of all diagrams up to a certain order g^N defines an effective collective action $\mathcal{A}_{\text{eff}}^N$ as a function of the collective classical fields $\Delta_{\alpha\beta}, \Delta_{\beta\alpha}^*, \rho_{\alpha\beta}$,

Obviously, if the expansion is carried to infinite order, the result must be independent of the auxiliary collective fields since they were introduced and removed in (14.322) without changing the theory. However, any calculation can only be carried up to a finite order, and that will *depend* on these fields. We therefore expect the best approximation to arise from the extremum of the effective action [6, 21, 54].

The lowest-order effective collective action is obtained from the trace of the logarithm of the matrix (14.325):

$$\mathcal{A}_{\Delta,\rho}^0 = -\frac{i}{2} \text{Tr} \log [i\mathbf{G}_{\Delta,\rho}^{-1}]. \quad (14.327)$$

The 2×2 matrix $\mathbf{G}_{\Delta,\rho}$ denotes the propagator $i[A_{x,x'}^{\Delta,\rho}]^{-1}$.

To first order in perturbation theory we must calculate the expectation value $\langle \mathcal{A}_{\text{int}} \rangle$ of the interaction (14.324). This is done with the help of Wick contractions in the three channels, Hartree, Fock, and Bogoliubov:

$$\langle \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow \rangle = \langle \psi_\uparrow^* \psi_\uparrow \rangle \langle \psi_\downarrow^* \psi_\downarrow \rangle - \langle \psi_\uparrow^* \psi_\downarrow \rangle \langle \psi_\downarrow^* \psi_\uparrow \rangle + \langle \psi_\uparrow^* \psi_\downarrow^* \rangle \langle \psi_\downarrow \psi_\uparrow \rangle. \quad (14.328)$$

For this purpose we now introduce the expectation values

$$\tilde{\Delta}_{\alpha\beta}^* \equiv g \langle \psi_\alpha^* \psi_\beta^* \rangle, \quad \tilde{\Delta}_{\beta\alpha} \equiv g \langle \psi_\beta \psi_\alpha \rangle = [\tilde{\Delta}_{\alpha\beta}^*]^*, \quad (14.329)$$

$$\tilde{\rho}_{\alpha\beta} \equiv g \langle \psi_\alpha^* \psi_\beta \rangle, \quad \tilde{\rho}_{\alpha\beta}^\dagger \equiv [\tilde{\rho}_{\beta\alpha}]^*, \quad (14.330)$$

and rewrite $\langle \mathcal{A}_{\text{int}}^{\text{new}} \rangle$ as

$$\langle \mathcal{A}_{\text{int}}^{\text{new}} \rangle = \frac{1}{g} \int_x (\tilde{\Delta}_{\downarrow\uparrow}^* \tilde{\Delta}_{\downarrow\uparrow} - \tilde{\rho}_{\uparrow\downarrow} \tilde{\rho}_{\downarrow\uparrow} + \tilde{\rho}_{\uparrow\uparrow} \tilde{\rho}_{\downarrow\downarrow}) - \frac{1}{2g} \int_x (\tilde{\Delta}_{\beta\alpha} \Delta_{\beta\alpha}^* + \tilde{\Delta}_{\alpha\beta}^* \Delta_{\beta\alpha} + 2\tilde{\rho}_{\alpha\beta} \rho_{\alpha\beta}).$$

Due to the locality of $\tilde{\Delta}_{\alpha\beta}$, the diagonal matrix elements vanish, and $\tilde{\Delta}_{\alpha\beta}$ has the form $c_{\alpha\beta} \tilde{\Delta}$, where $c_{\alpha\beta}$ is i times the Pauli matrix $\sigma_{\alpha\beta}^2$. In the absence of a magnetic field, the expectation values $\tilde{\rho}_{\alpha\beta}$ may have certain symmetries:

$$\tilde{\rho}_{\uparrow\uparrow} \equiv \tilde{\rho} = \rho_{\downarrow\downarrow}, \quad \tilde{\rho}_{\uparrow\downarrow} = \rho_{\downarrow\uparrow} \equiv 0, \quad (14.331)$$

so that (14.331) simplifies to

$$\langle \mathcal{A}_{\text{int}}^{\text{new}} \rangle = \frac{1}{g} \int_x [(|\tilde{\Delta}|^2 + \tilde{\rho}^2) - (\tilde{\Delta} \Delta^* + \tilde{\Delta}^* \Delta + 2\tilde{\rho} \rho)]. \quad (14.332)$$

The total first-order collective classical action $\mathcal{A}_{\Delta,\rho}^1$ is given by the sum

$$\mathcal{A}_{\Delta,\rho}^1 = \mathcal{A}_{\Delta,\rho}^0 + \langle \mathcal{A}_{\text{int}}^{\text{new}} \rangle. \quad (14.333)$$

Now we observe that the functional derivatives of the zeroth-order action $\mathcal{A}_{\Delta,\rho}^0$ are the free-field propagators G_Δ and G_ρ

$$\frac{\delta}{\delta \Delta_{\alpha\beta}} \mathcal{A}_{\Delta,\rho}^0 = [G_\Delta]_{\alpha\beta}, \quad \frac{\delta}{\delta \rho_{\alpha\beta}} \mathcal{A}_{\Delta,\rho}^0 = [G_\rho]_{\alpha\beta}. \quad (14.334)$$

Then we can extremize $\mathcal{A}_{\Delta,\rho}^1$ with respect to the collective fields Δ and ρ , and find that to this order these fields satisfy the gap-like equations

$$\tilde{\Delta}_x = g[G_\Delta]_{x,x}, \quad \tilde{\rho}_x = g[G_\rho]_{x,x}. \quad (14.335)$$

If the fields satisfy (14.335), the extremal action has the value

$$\mathcal{A}_{\Delta,\rho}^1 = \mathcal{A}_{\Delta,\rho}^0 - \frac{1}{g} \int_x (|\Delta|^2 + \rho^2). \quad (14.336)$$

Note how the theory differs, at this level, from the collective quantum field theory derived via the Hubbard-Stratonovich transformation. If we assume that ρ vanishes identically, the extremum of the one-loop action $\mathcal{A}_{\Delta,\rho}^1$ gives the same result as of the mean-field collective quantum field action (14.284), which reads for the present attractive δ -function in (14.319):

$$\mathcal{A}_{\Delta,0}^1 = \mathcal{A}_{\Delta,0}^0 - \frac{1}{g} \int_x |\Delta|^2. \quad (14.337)$$

On the other hand, if we extremize the action $\mathcal{A}_{\Delta,\rho}^1$ at $\Delta = 0$, we find the extremum from the expression

$$\mathcal{A}_{0,\rho}^1 = \mathcal{A}_{0,\rho}^0 - \frac{1}{g} \int_x \rho^2. \quad (14.338)$$

The extremum of the first-order combined collective classical action (14.336) agrees with the good-old Hartree-Fock-Bogoliubov theory.

The essential difference between this and the new approach arises in two issues:

- First, by being able to carry the expansion to higher orders: If the collective quantum field theory is based on the Hubbard-Stratonovich transformation, the higher-order diagrams must be calculated with the help of the propagators of the collective field such as $\langle \Delta_x \Delta_{x'} \rangle$. These are extremely complicated functions. For this reason, any loop diagram formed with them is practically impossible to integrate. In contrast to that, the higher-order diagrams in the present theory need to be calculated using only ordinary particle propagators G_Δ and G_ρ of Eq. (14.334) and the interaction (14.324). Even that becomes, of course, tedious for higher orders in g . At least, there is a simple rule to find the contributions of the quadratic terms $\frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x$ in (14.322), given the diagrams *without* these terms. One calculates the diagrams from only the four-particle interaction, and collects the contributions up to order g^N in an effective action $\tilde{\mathcal{A}}_{\Delta,\rho}^N$. Then one replaces $\tilde{\mathcal{A}}_{\Delta,\rho}^N$ by $\tilde{\mathcal{A}}_{\Delta-\epsilon g \Delta, \rho-\epsilon g \rho}^N$ and re-expands everything in powers of g up to the order g^N , forming a new series $\sum_{i=0}^N g^i \tilde{\mathcal{A}}_{\Delta,\rho}^i$. Finally one sets ϵ equal to $1/g$ [23] and obtains the desired collective classic action $\mathcal{A}_{\Delta,\rho}^N$ as an expansion extending (14.336) to:

$$\mathcal{A}_{\Delta,\rho}^N = \sum_{i=0}^N \tilde{\mathcal{A}}_{\Delta,\rho}^i - (1/g) \int_x (|\Delta|^2 + \rho^2). \quad (14.339)$$

Note that this action must merely be extremized. There are no more quantum fluctuations in the *classical collective fields* Δ, ρ . Thus, at the extremum, the action (14.339) provides us directly with the desired grand-canonical potential.

- The second essential difference with respect to the Hubbard-Stratonovich transformation approach is the following: It becomes possible to study a rich variety of competing collective fields without the danger of double-counting Feynman diagrams. One simply generalizes the matrix $\mathcal{M}_x$ subtracted from $\mathcal{A}_{\text{int}}^{\text{loc}}$ to define $\mathcal{A}_{\text{int}}^{\text{new}}$ in different ways. For instance, we may subtract and add a vector field $\psi^\dagger \sigma^a \psi S^a$ containing the Pauli matrices σ^a and study paramagnon fluctuations, thus generalizing the assumption (14.331) and allowing a spontaneous magnetization in the ground state. Or one may do the same thing with a term $\psi^\dagger \sigma^a \nabla^i \psi A_{ia} + \text{c.c.}$ added to the previous term. In this way we derive the Ginzburg-Landau theory of superfluid He^3 as in [4, 24].

An important property of the proposed procedure is that it yields good results even in the limit of infinitely strong coupling. It was precisely this property which led to the successful calculation of critical exponents of all ϕ^4 -theories in the textbook [21] since critical phenomena arise in the limit in which the unrenormalized coupling constant goes to infinity [57]. This is in contrast to another possibility. For example that of carrying the variational approach to higher order via the so-called *higher effective actions* [26]. These were discussed in Chapter 13. There one extremizes the Legendre transforms of the generating functionals of bilocal correlation functions, which sums up all two-particle irreducible diagrams. That does *not* give physically meaningful results [27] in the strong-coupling limit, even for simple quantum-mechanical models, as we have shown in Section 13.12.

The mother of this approach is Variational Perturbation Theory (VPT). Its origin was a variational approach developed for quantum mechanics some years ago by Feynman and the author [53]. in the textbook [21] to quantum field theory. It converts *divergent* perturbation expansions of quantum mechanical systems into exponentially fast *converging* expansions for any coupling strength [54].

What we have shown in this section is that this powerful theory can easily be transferred to many-body theory, if we identify a variety of relevant *collective classical fields*, rather than a fluctuating collective *quantum field* suggested by the Hubbard-Stratonovich Transformation. To lowest order in the coupling constant this starts out with the standard Hartree-Fock-Bogoliubov approximation, and allows to go to higher orders with arbitrarily high accuracy.

14.16 Gauge Fields and Gauge Fixing

The functional integral formalism developed in the previous sections does not immediately apply to electromagnetism and any other gauge fields. There are subtleties which we are now going to discuss. These will lead to an explanation of the mistake in the vacuum energy observed in Eq. (7.506) when quantizing the electromagnetic field via Gupta-Bleuler formalism. Consider a set of external electromagnetic currents described by the current density $j^\mu(x)$. Since charge is conserved, these satisfy

$$\partial_\mu j^\mu(x) = 0. \quad (14.340)$$

The currents are sources of electromagnetic fields $F_{\mu\nu}$ determined from the field equation (12.49),

$$\partial_\nu F^{\nu\mu}(x) = j^\mu(x), \quad (14.341)$$

if we employ natural units with $c = 1$. The action reads

$$\begin{aligned} \mathcal{A} &= \int d^4x \left[-\frac{1}{4} F_{\mu\nu}^2(x) - j^\mu(x) A_\mu(x) \right] \\ &= \int d^4x \left\{ \frac{1}{2} [\mathbf{E}^2(x) - \mathbf{B}^2(x)] - \left[\rho\phi(x) - \frac{1}{c} \mathbf{j} \cdot \mathbf{A}(x) \right] \right\}. \end{aligned} \quad (14.342)$$

The field strengths are the four-dimensional curls of the vector potential $A^\mu(x)$:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \quad (14.343)$$

that satisfy, for single-valued fields A_μ , the Bianchi identity

$$\epsilon_{\mu\nu\lambda\kappa} \partial_\nu F_{\lambda\kappa} = 0. \quad (14.344)$$

The decomposition (14.343) is not unique. If we add to $A_\mu(x)$ the gradient of an arbitrary function $\Lambda(x)$,

$$A_\mu(x) \rightarrow A_\mu^\Lambda(x) = A_\mu(x) + \partial_\mu \Lambda(x), \quad (14.345)$$

then Λ does not appear in the field strengths, assuming that it satisfies

$$(\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) \Lambda(x) = 0, \quad (14.346)$$

i.e., the derivatives in front of $\Lambda(x)$ commute. In the theory of partial differential equations, this is referred to as the *Schwarz integrability condition* for the function $\Lambda(x)$. In general, a function $\Lambda(x)$ which satisfies (14.346) in a simply-connected domain can be defined uniquely in this domain. Only if $\Lambda(x)$ fulfills this condition, the transformation (14.345) is called a *local gauge transformation*.

If the domain is multiply connected, there is more than one path along which to continue the function $\Lambda(x)$ from one spatial point to another and $\Lambda(x)$ becomes multi-valued. This happens, for example, if (14.346) is nonzero on a closed line in three-dimensional space, in which case the set of paths between two given points decomposes into equivalence classes, depending on how often the closed line is encircled. Each of these paths allows another continuation of $\Lambda(x)$. By (14.346), such functions are *not* allowed in gauge transformations (14.345).

Let us now see how we can construct the generating functional of fluctuating free electromagnetic fields in the presence of external currents $j_\mu(x)$. As in (14.58), we would like to calculate a functional integral, now in the unnormalized version corresponding to (14.58):

$$Z_0[j] = \int \mathcal{D}A^\mu(x) e^{i \int d^3x (-F_{\mu\nu}^2/4 - j_\mu A^\mu)}. \quad (14.347)$$

The $F_{\mu\nu}^2$ -terms in the exponents can be partially integrated and rewritten as

$$-\frac{1}{4} \int d^4x F_{\mu\nu}^2 = \frac{1}{2} \int d^4x A^\mu (\partial^2 g_{\mu\nu} - \partial_\mu \partial_\nu) A^\nu. \quad (14.348)$$

Hence we can identify the functional matrix $D(x, x')$ in (14.34) as

$$D_{\mu\nu}(x, x') = (\partial^2 g_{\mu\nu} - \partial_\mu \partial_\nu) \delta^{(4)}(x - x'). \quad (14.349)$$

Recalling (14.88) it appears, at first, as though the generating functional (14.347) should simply be equal to

$$Z_0[j] = (\text{Det } G_{0\mu\nu})^{1/2} e^{-\frac{1}{2} \int d^4x d^4x' j_\mu(x) G_{0\mu\nu}(x, x') j_\nu(x')}, \quad (14.350)$$

where, by analogy with (14.35), we get

$$G_{0\mu\nu}(x, x') = iD_{\mu\nu}^{-1}(x, x'). \quad (14.351)$$

We have divided out a normalization factor $\mathcal{N} = (\text{Det } G_{0\mu\nu})^{-1/2}$, assuming that we are dealing with an unnormalized version of $Z_0[j]$. Unfortunately, however, the expression (14.350) is meaningless, since the inverse of the functional matrix (14.349) does not exist. In order to see this explicitly we diagonalize the functional part (i.e., the x, y -part) of $G_{0\mu\nu}(x, x')$ by considering the Fourier transform

$$D_{\mu\nu}(q) = -q^2 g_{\mu\nu} + q_\mu q_\nu. \quad (14.352)$$

For every momentum q , this matrix has obviously an eigenvector with zero eigenvalue, namely q_μ . This prevents us from inverting the matrix $D_{\mu\nu}(q)$. Correspondingly, when trying to form the inverse determinant of the functional matrix $D_{\mu\nu}$ in (14.350), we encounter an infinite product of infinities, one for every momentum q .

The difficulty can be resolved using the fact that the action (14.342) is gauge invariant. For $F_{\mu\nu}$ this is trivially true; for the source term $j^\mu(x)A_\mu(x)$ this is a consequence of current conservation. Indeed, if we change A_μ according to (14.345), the source term is changed by $\int d^4x j^\mu(x)\partial_\mu\Lambda(x)$. With the help of a partial integration, this is equal to $-\int d^4x \partial_\mu j_\mu(x)\Lambda(x)$, and this expression vanishes due to current conservation (14.340).

Because of this invariance, not all degrees of freedom, which are integrated over in the functional integral (14.347), are associated with a Gaussian integral. The fluctuations corresponding to pure gauge transformations leave the exponent invariant. Since a path integral is a product of infinitely many integrals from minus to plus infinity, the gauge invariance of the integral produces an infinite product of infinite factors. This is precisely the origin of the infinity that occurs in the functional determinant.

This infinity must be controlled by restricting the functional integrals to field fluctuations via some specific gauge condition. For example, the restriction is achieved by inserting into the integral *gauge-fixing functionals*. Several examples have been used:

$$\begin{aligned} F_1[A] &= \delta[\partial_\mu A^\mu(x)], & (\text{Lorenz gauge}) \\ F_2[A] &= \delta[\nabla \cdot \mathbf{A}(x)], & (\text{Coulomb gauge}) \\ F_3[A] &= \delta[A^0(x)], & (\text{Hamiltonian gauge}) \\ F_3[A] &= \delta[A^3(x)], & (\text{axial gauge}) \\ F_4[A] &= \exp \left\{ -\frac{i}{2\alpha} \int d^4x [\partial_\mu A^\mu(x)]^2 \right\}, & (\text{generalized Lorenz gauge}) \\ F_5[A] &= \int \mathcal{D}\zeta e^{-i \int d^4x \zeta H\zeta/2} \delta[\partial_\mu A^\mu - \zeta] \times \text{Det}^{-1/2} H. & (\text{'t Hooft gauge}) \end{aligned} \quad (14.353)$$

The first is a δ -functional enforcing the Lorenz gauge at each spacetime point: $\partial_\mu A^\mu(x) = 0$. The second enforces the Coulomb gauge, the third corresponds to the axial gauge, and the fourth is a generalized form of the Lorenz gauge used

by Feynman and which also serves to derive the Feynman diagrams of the Gupta-Bleuler quantization formalism, thereby correcting the mistake in the vacuum energy. The fifth, finally, is a generalization of the fourth used by 't Hooft that arises by rewriting the fourth as a path integral $F_4[A] = \int \mathcal{D}\zeta e^{-i \int d^4x \zeta^2 / 2\alpha} \delta[\partial_\mu A^\mu - \zeta]$ and generalizing the constant $1/\alpha$ to a functional matrix $A(x, x')$. If we insert any of these gauge-fixing functionals $F_i[A]$ into the path integral, then gauge-transform the vector potential $A_\mu(x)$ à la (14.345), and integrate functionally over all $\Lambda(x)$, the integral receives a finite contribution from that gauge function $\Lambda(x)$ which enforces the desired gauge. The result is a gauge-invariant functional of $A^\mu(x)$:

$$\Phi[A] = \int \mathcal{D}\Lambda F[A^\Lambda] = \int \mathcal{D}\Lambda F[A + \partial\Lambda]. \quad (14.354)$$

Explicitly, we find for the above cases (14.353), the normalization functionals:

$$\Phi_1[A] = \int \mathcal{D}\Lambda F_1[A^\Lambda] = \int \mathcal{D}\Lambda \delta[\partial_\mu A^\mu(x) + \partial^2 \Lambda], \quad (14.355)$$

$$\Phi_2[A] = \int \mathcal{D}\Lambda F_2[A^\Lambda] = \int \mathcal{D}\Lambda \delta[\nabla \cdot \mathbf{A}(x) + \nabla^2 \Lambda], \quad (14.356)$$

$$\Phi_3[A] = \int \mathcal{D}\Lambda F_3[A^\Lambda] = \int \mathcal{D}\Lambda \delta[\nabla A^0(x) + \partial^0 \Lambda], \quad (14.357)$$

$$\Phi_4[A] = \int \mathcal{D}\Lambda F_4[A^\Lambda] = \int \mathcal{D}\Lambda \exp \left\{ -\frac{i}{2\alpha} \int d^4x [\partial_\mu A^\mu + \partial^2 \Lambda]^2 \right\}, \quad (14.358)$$

$$\begin{aligned} \Phi_5[A] = \int \mathcal{D}\Lambda F_5[A^\Lambda] = \int \mathcal{D}\Lambda \int \mathcal{D}\zeta \exp \left\{ -\frac{i}{2} \int d^4x \zeta H \zeta \right\} \delta[\partial_\mu A^\mu + \partial^2 \Lambda - \zeta] \\ \times \text{Det}^{-1/2} H \times \text{Det}(\partial^2). \end{aligned} \quad (14.359)$$

If we form the ratios $F_i[A]/\Phi_i[A]$, we obtain gauge fixing functionals which all yield unity when integrated over all gauge transformations. If any of these are inserted into the functional integral (14.347), they will all remove the gauge degree of freedom, and lead to a finite functional integral which is the same for each choice of $F_i[A]$.

Let us calculate the functionals $\Phi_i[A]$ explicitly. For $\Phi_{1,2,3}[A]$ we simply observe a trivial identity for δ -functions

$$\delta(ax) = a^{-1} \delta(x). \quad (14.360)$$

This is proved by multiplying both sides with a smooth function $f(x)$ and integrating over x . The functional generalization of this is

$$\delta[\mathcal{O}A] = \text{Det}^{-1} \mathcal{O} \delta[A], \quad (14.361)$$

where $\mathcal{O}$ is an arbitrary differential operator acting on the field $A^\mu(x)$. From this we find immediately the normalization functionals:

$$\Phi_1[A] = \text{Det}^{-1}(\partial^2), \quad (14.362)$$

$$\Phi_2[A] = \text{Det}^{-1}(\nabla^2), \quad (14.363)$$

$$\Phi_3[A] = \text{Det}^{-1}(\partial^0). \quad (14.364)$$

The fourth functional $\Phi_4[A]$ is simply a Gaussian functional integral. The additive term $\partial_\mu A^\mu(x)$ can be removed by a trivial shift of the integration variable $\Lambda(x) \rightarrow \Lambda'(x) = \Lambda(x) - \partial_\mu A^\mu(x)/\partial^2$, under which the measure of integration remains invariant, $\mathcal{D}\Lambda = \mathcal{D}\Lambda'$. Using formula (14.25) we obtain

$$\Phi_4[A] = \text{Det}^{-1}(\partial^2/\sqrt{\alpha}). \quad (14.365)$$

The functional determinants Φ_i^{-1} are called *Faddeev-Popov determinants* [49].

The Faddeev-Popov determinants in the four examples happen to be *independent* of $A^\mu(x)$, so that we shall write them as Φ_i without arguments. This independence is a very useful property. Complications arising for A -dependent functionals $\Phi[A]$ will be illustrated below in an example.

We now study the consequences of inserting the gauge-fixing factors $F_i[A]/\Phi_i$ into the functional integrands (14.347). For $F_4[A]/\Phi_4$, the generating functional becomes

$$Z_0[j] = (\text{Det } G_{0\mu\nu})^{1/2} \text{Det}^{1/2}(\partial^4/\alpha) \int \mathcal{D}A_\mu(x) e^{i \int d^4x \left[-\frac{1}{4} F_{\mu\nu}^2 - \frac{1}{\alpha} (\partial^\mu A_\mu)^2 - j^\mu A_\mu \right]}. \quad (14.366)$$

The free-field action in the exponent can be written in the form

$$\mathcal{A} = \int d^4x \frac{1}{2} \left[-(\partial_\mu A_\nu)^2 + \left(1 - \frac{1}{\alpha}\right) (\partial^\mu A_\mu)^2 \right]. \quad (14.367)$$

The associated Euler-Lagrange equation is

$$\partial^2 A^\mu - \left(1 - \frac{1}{\alpha}\right) \partial^\mu (\partial A) = 0, \quad (14.368)$$

which is precisely the field equation (7.381) of the covariant quantization scheme. With the additional term in the action, the matrix (14.352) becomes

$$D_{\mu\nu}(q) = -q^2 \left[g_{\mu\nu} - \left(1 - \frac{1}{\alpha}\right) \frac{q_\mu q_\nu}{q^2} \right]. \quad (14.369)$$

This can be decomposed into projection matrices with respect to the subspaces transverse and longitudinal to the four-vector q^μ ,

$$P_{\mu\nu}^l(q) = \frac{q_\mu q_\nu}{q^2}, \quad P_{\mu\nu}^t(q) = g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}, \quad (14.370)$$

as

$$D_{\mu\nu}(q) = -q^2 \left[P_{\mu\nu}^t(q) + \frac{1}{\alpha} P_{\mu\nu}^l(q) \right]. \quad (14.371)$$

It is easy to verify that the matrices are really projections, since they satisfy

$$P_{\mu\nu}^l P^{\mu\nu}{}_\lambda = P_{\mu\nu}^t, \quad P_{\mu\nu}^l P^{\mu\nu}{}_\lambda = P_{\mu\lambda}^l, \quad P_{\mu\nu}^t P^{\mu\nu}{}_\lambda = 0. \quad (14.372)$$

Similar projections appeared before in the three-dimensional subspace [see (4.334) and (4.336)], where the projections were indicated by capital subscripts T , L .

Due to the relations (14.372), there is no problem in inverting $D_{\mu\nu}(q)$, and we find the free photon propagator in momentum space

$$\begin{aligned} G_{0\mu\nu}(q) &= iD_{\mu\nu}^{-1}(q) = -\frac{i}{q^2}[P_{\mu\nu}^t(q) + \alpha P_{\mu\nu}^l(q)] \\ &= -\frac{i}{q^2}\left[g_{\mu\nu} - (1 - \alpha)\frac{q_\mu q_\nu}{q^2}\right]. \end{aligned} \quad (14.373)$$

For $\alpha = 0$, this is the propagator $G_{\mu\nu}$ derived in the Gupta-Bleuler canonical field quantization in Eq. (7.510), there obtained from canonical quantization rules with a certain filling of the vacuum with unphysical states.

Taking into account the Faddeev-Popov determinant Φ_4^{-1} of (14.365), we obtain for the generating functional (14.366):

$$Z[j] = [\text{Det}(-iG_{0\mu\nu})]^{1/2} \text{Det}^{1/2}(\partial^4/\alpha) e^{-\frac{1}{2} \int d^4x d^4x' j^\mu(x) G_{0\mu\nu}(x, x') j^\nu(x')}. \quad (14.374)$$

Let us calculate the functional determinant $\text{Det} G_{0\mu\nu}$. For this we take q^μ in the momentum representation (14.373) along the 0-direction, and see that there are three spacelike eigenvectors of eigenvalues iq^2 , and one timelike eigenvector of eigenvalue $i\alpha/q^2$. The total determinant is therefore

$$\text{Det}(-iG_{0\mu\nu}) = \frac{1}{\text{Det}(-\partial^2)^2 \text{Det}(\partial^4/\alpha)}. \quad (14.375)$$

The two prefactors of (14.374) together yield a factor

$$[\text{Det}(-iG_{0\mu\nu})]^{1/2} \text{Det}^{1/2}(\partial^4/\alpha) \propto \frac{1}{\text{Det}(-\partial^2)}. \quad (14.376)$$

Recalling the discussion of Eqs. (14.129)–(14.133), we see that the associated free energy is

$$F_0 = -\beta \log Z_0 = 2 \sum_{\mathbf{k}} \left\{ \frac{\omega(\mathbf{k})}{2} + \log [1 - e^{-\beta \hbar \omega(\mathbf{k})}] \right\}. \quad (14.377)$$

It contains precisely the energy of the two physical transverse photons. The unphysical polarizations have been eliminated by the Faddeev-Popov determinant in (14.374).

We now understand why the Gupta-Bleuler formalism failed to get the correct vacuum energy in Eq. (7.506). It has no knowledge of the Faddeev-Popov determinant.

Taking into account current conservation, the exponent in (14.374) reduces to

$$j^\mu(x) G_{0\mu\nu}(x, x') j^\nu(x') = j^\mu(x) \frac{i}{\partial^2} j_\mu(x), \quad (14.378)$$

so that the generating functional becomes

$$Z[j] = \text{const} \times \text{Det}^{-1}(-\partial^2) e^{-\frac{1}{2} \int d^4x d^4x' j^\mu(x) (i/\partial^2) j_\mu(x')}, \quad (14.379)$$

where const is an infinite product of identical constant factors.

Let us see what happens in the other gauges (14.353). The results in the Lorenz gauge are immediately obtained by going to the limit $\alpha \rightarrow 0$ in the previous calculation. In this limit, the functional Φ_4 coincides with Φ_1 , up to a trivial factor.

The Hamiltonian and the axial gauges are quite similar, so we may only discuss one of them. In the Hamiltonian gauge, where the Faddeev-Popov determinant is given by (14.364), the generating functional (14.374) becomes

$$Z[j] = (\text{Det } G_{0\mu\nu})^{1/2} \text{Det}(\partial_0) e^{-\frac{1}{2} \int d^4x d^4x' j^i(x) G_{0ij}(x, x') j^j(x')}, \quad (14.380)$$

where the matrix $G_{0ij}(q)$ has only spatial entries, and is equal to

$$G_{0ij}(q) = iD_{ij}^{-1}(q) \quad (14.381)$$

with

$$D_{ij}(q) = q^2 \delta_{ij} + q_i q_j \quad (14.382)$$

being the spatial part of the 4×4 -matrix (14.352). With the help of 3×3 -projection matrices

$$P_{ij}^T(q) = \delta_{ij} - q_i q_j / \mathbf{q}^2 \quad (14.383)$$

$$P_{ij}^L(q) = q_i q_j / \mathbf{q}^2, \quad (14.384)$$

this can be decomposed as follows:

$$D_{ij}(q) = q^2 P_{ij}^T(q) + q^0{}^2 P_{ij}^L(q). \quad (14.385)$$

The inverse of this is

$$D_{ij}^{-1}(q) = \frac{1}{q^2} P_{ij}^T(q) + \frac{1}{q^0{}^2} P_{ij}^L(q) = \frac{1}{q^2} \left(\delta_{ij} - \frac{q_i q_j}{q^0{}^2} \right). \quad (14.386)$$

In the exponent of (14.380) we have to evaluate $iD_{ij}^{-1}(q)$ between two conserved currents, and find

$$j^{i*}(q) G_{0ij}(q) j^j(q) = -\frac{i}{q^2} \left[\mathbf{j}^*(q) \cdot \mathbf{j}(q) - \frac{1}{q^0{}^2} \mathbf{q} \cdot \mathbf{j}^*(q) \mathbf{q} \cdot \mathbf{j}(q) \right]. \quad (14.387)$$

Inserting the momentum space version of the local current conservation law $\partial_\mu j^\mu(x) = 0$:

$$\mathbf{q} \cdot \mathbf{j}(q) = q^0 j^0(q), \quad (14.388)$$

we obtain

$$j^{i*}(q) G_{0ij}(q) j^j(q) = \frac{i}{q^2} j^{\mu*}(q) j_\mu(q). \quad (14.389)$$

Let us calculate the functional determinant $\text{Det } G_{0\mu\nu}$ in this gauge. From (14.386) we see that $G_{0\mu\nu}$ has two eigenvectors of eigenvalue i/q^2 , and one eigenvector of eigenvalue $-i/q^{02}$. Hence:

$$\text{Det } G_{0\mu\nu} = \frac{1}{\text{Det } (-i\partial^2)^2 \text{Det } (i\partial_0^2)}. \quad (14.390)$$

The two prefactors in (14.380) together are therefore proportional to

$$(\text{Det } G_{0\mu\nu})^{1/2} \text{Det } (\partial_0) \propto \frac{1}{\text{Det } (-i\partial^2)}, \quad (14.391)$$

which is the same as (14.376). Thus the generating functional (14.380) agrees with the previous one in (14.379).

Let us also show that the Coulomb gauge leads to the same result. We rewrite the exponent in (14.379) in momentum space as

$$\int d^4x j^\mu(x) \frac{1}{-\partial^2} j_\mu(x) = \int \frac{d^4q}{(2\pi)^4} \left[c^2 \rho(q) \frac{1}{q^2} \rho(q) - c^2 \mathbf{j}(q) \frac{1}{q^2} \mathbf{j}(q) \right]. \quad (14.392)$$

Here we keep explicitly the light velocity c in all formulas since we want to rederive the interaction equivalent to Eq. (12.85) where c is not set equal to unity. Writing the denominator as $q^2 = q_0^2 - \mathbf{q}^2$ and $j^2(q) = \mathbf{j}_L^2(q) + \mathbf{j}_T^2(q)$ with $\mathbf{j}_L(q) = \mathbf{q} \cdot \mathbf{j}(q)/|\mathbf{q}|$ and $\mathbf{j}_T(q) \cdot \mathbf{j}_L(q) = 0$, we can bring (14.392) to the form

$$\int \frac{d^4q}{(2\pi)^4} \left[c^2 \rho(q) \frac{1}{q_0^2 - \mathbf{q}^2} \rho(q) - \mathbf{j}_L(q) \frac{1}{q_0^2 - \mathbf{q}^2} \mathbf{j}_L(q) - \mathbf{j}_T(q) \frac{1}{q_0^2 - \mathbf{q}^2} \mathbf{j}_T(q) \right]. \quad (14.393)$$

Now we use the current conservation law $cq_0\rho(q) = \mathbf{q} \cdot \mathbf{j}(q)$ to rewrite (14.393) as

$$\int \frac{d^4q}{(2\pi)^4} \left[c^2 \rho(q) \frac{1}{q^2 - \mathbf{q}^2} \rho(q) - c^2 \frac{q_0^2}{\mathbf{q}^2} \rho(q) \frac{1}{q_0^2 - \mathbf{q}^2} \rho(q) - \mathbf{j}_T(q) \frac{1}{q_0^2 - \mathbf{q}^2} \mathbf{j}_T(q) \right]. \quad (14.394)$$

The first two terms can be combined to

$$\mathcal{A}_L^{\text{int}} = - \int \frac{d^4q}{(2\pi)^4} c^2 \rho(q) \frac{1}{\mathbf{q}^2} \rho(q). \quad (14.395)$$

Undoing the Fourier transformation and multiplying this by e^2/c^2 we find as a first term in the interaction (12.84) the Coulomb term which is the longitudinal part of the interaction (12.83):

$$\begin{aligned} \mathcal{A}_L^{\text{int}} &= -\frac{1}{2} \int d^4x \mathbf{E}_L^2(x) = \frac{e^2}{2} \int d^4x \rho(x) \frac{1}{\nabla^2} \rho(x) \\ &= -\frac{e^2}{8\pi} \int dt \int d^3x d^3x' \rho(\mathbf{x}, t) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}', t). \end{aligned} \quad (14.396)$$

The third term in (14.394) involves only the transverse current

$$\mathcal{A}_T^{\text{int}} = - \int \frac{d^4 q}{(2\pi)^4} \mathbf{j}_T^*(q) \frac{1}{q^2} \mathbf{j}_T(q). \quad (14.397)$$

It is the result of the transverse fields in the Lagrangian (12.54):

$$\mathcal{A}_T^{\text{int}} = \frac{1}{4\pi} \int d^4 x \{ [\mathbf{E}_T^2(x) - \mathbf{B}^2(x)] + \frac{1}{c} \mathbf{j}(x) \mathbf{A}_T(x) \}. \quad (14.398)$$

It is found by integrating out the vector potential. Using Eq. (5.56), the transverse interaction (14.397) can be rewritten as

$$\mathcal{A}_T^{\text{int}} = \int \frac{d^4 q}{(2\pi)^4} \left[j_\mu^*(q) \frac{1}{q^2} j^\mu(q) + \frac{1}{\mathbf{q}^2} |j_0(q)|^2 \right] = \mathcal{A}_{\text{tot}}^{\text{int}} - \mathcal{A}_L^{\text{int}}. \quad (14.399)$$

The transverse part of the electromagnetic action of a four-dimensional current $j^\mu(q)$ is the difference between the total covariant Biot-Savart interaction plus the instantaneous Coulomb interaction.

14.17 Nontrivial Gauge and Faddeev-Popov Ghosts

The Faddeev-Popov determinants in the above examples were all independent of the fields. As such they were irrelevant for the calculation of any Green function. This, however, is not always true.

As an example, consider the following nontrivial gauge-fixing functional (see also [55])

$$F[A] = \delta[(\partial A)^2 + gA^2]. \quad (14.400)$$

As in Eqs. (14.355)–(14.359), we calculate

$$\Phi[A] = \int \mathcal{D}\Lambda F[A^\Lambda] = \int \mathcal{D}\Lambda \delta[\partial A + gA^2 + \partial^2 \Lambda + 2gA\partial\Lambda + g(\partial\Lambda)^2]. \quad (14.401)$$

This path integral can trivially be performed by analogy with the ordinary integral

$$\int dx \delta(ax + bx^2) = \frac{1}{a}, \quad (14.402)$$

and yields the result

$$\Phi[A] = \text{Det} (\partial^2 + 2gA_\mu \partial^\mu)^{-1}. \quad (14.403)$$

The generating functional is therefore

$$Z[j] = \int \mathcal{D}A^\mu \text{Det} (\partial^2 + 2gA^\mu \partial_\mu) \delta[\partial_\mu A^\mu + gA^2] \exp \left[i \int d^4 x \left(-\frac{1}{4} F_{\mu\nu}^2 - j_\mu A^\mu \right) \right]. \quad (14.404)$$

Contrary to the previous gauges, the functional determinant is no longer a trivial overall factor, but it depends now functionally on the field A^μ . It can therefore no longer be brought outside the functional integral.

There is a simple way of including its effect within the usual field-theoretic formalism. One introduces an auxiliary *Faddeev-Popov ghost field*. We may consider the determinant as the result of a fluctuating complex fermion field c with a complex-conjugate c^* , and write

$$\text{Det}(\partial^2 + 2gA^\mu\partial_\mu) = \int \mathcal{D}c^*\mathcal{D}c e^{-i\int d^4x(\partial c^*\partial c - 2gA^\mu c^*\partial_\mu c)}. \quad (14.405)$$

Note that the Fermi fields are necessary to produce the determinant in the numerator; a Bose field would have put it into the denominator. A complex field is taken to make the determinant appear directly rather than the square-root of it.

The ghost fields interact with the photon fields. This interaction is necessary in order to compensate the interactions induced by the constraint $\delta[\partial A^\mu + gA^2]$ in the functional integral.

It is possible to exhibit the associated cancellations order by order in perturbation theory. For this we have to bring the integrand to a form in which all fields appear in the exponent. This can be achieved for the δ -functional by observing that the same representation (14.404) would be true with any other choice of gauge, say

$$\delta[\partial_\mu A^\mu(x) + gA^2(x) - \lambda(x)], \quad (14.406)$$

since this would lead to the same Faddeev-Popov ghost term (14.405). Therefore we can average over all possible functions $\lambda(x)$ with a Gaussian weight and replace (14.406) just as well by

$$\int \mathcal{D}\lambda e^{-\frac{i}{2}\int d^4x\lambda^2(x)} \delta[\partial_\mu A^\mu(x) + gA^2(x) - \lambda(x)]. \quad (14.407)$$

Now the generating functional has the form

$$Z[j] = \int \mathcal{D}A^\mu \int \mathcal{D}c^*\mathcal{D}c e^{i\int d^4x(\mathcal{L} - j^\mu A_\mu)} \quad (14.408)$$

with a Lagrangian

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}^2 - \frac{1}{2\alpha}(\partial A + gA^2)^2 - \partial_\mu c^* \partial^\mu c + 2gA^\mu c^* \partial_\mu c. \quad (14.409)$$

The photon and ghost propagators are

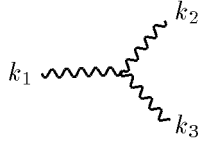
$$\text{wavy line } q \quad \overline{A_\mu(x)A_\nu(0)} = -\int \frac{d^4k}{(2\pi)^4} e^{-ikx} \frac{i}{k^2} \left[g_{\mu\nu} - (1-\alpha) \frac{k_\mu k_\nu}{k^2} \right], \quad (14.410)$$

$$\text{straight line } q \quad \overline{c^*(x)c(0)} = -\int \frac{d^4q}{(2\pi)^4} e^{-iqx} \frac{i}{q^2}. \quad (14.411)$$

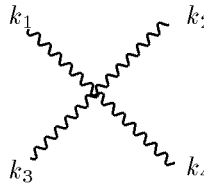
Contrary to the previous gauges, there are now photon-ghost and photon-photon interaction terms

$$-\frac{g}{\alpha}\partial_\mu A^\mu A^2 - \frac{g^2}{2\alpha}(A_\mu^2)^2 + 2gA^\mu c^* \partial_\mu c \quad (14.412)$$

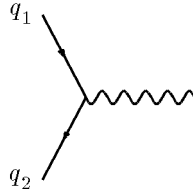
with the corresponding vertices



$$= \frac{2g}{\alpha} (g_{\mu_1\mu_2} k_{3\mu_3} + g_{\mu_2\mu_3} k_{1\mu_1} + g_{\mu_3\mu_1} k_{2\mu_2}) \quad (14.413)$$



$$= -\frac{4ig^2}{\alpha} (g_{\mu_1\mu_2} g_{\mu_3\mu_4} + g_{\mu_1\mu_3} g_{\mu_2\mu_4} + g_{\mu_1\mu_4} g_{\mu_2\mu_3}) \quad (14.414)$$



$$= -g(q_1 + q_2)_\mu. \quad (14.415)$$

It can be shown that the Faddeev-Popov ghost Lagrangian has the property of canceling all these unphysical contributions order by order in perturbation theory. We leave it as an exercise to show, for example, that there is no contribution of the ghosts to photon-photon scattering up to, say, second order in g , and that self-energy corrections to the photon propagator due to photon and ghost loops cancel exactly.

In the context of quantum electrodynamics, there is little sense in using a gauge fixing term (14.400). The present discussion is, however, a useful warm-up exercise to gauge-fixing procedures in nonabelian gauge theories, where the Faddeev-Popov determinant will always be field dependent.

Of course, also the previous field-independent Faddeev-Popov determinants can be generated from fermionic ghost fields. The determinant Φ_4^{-1} in (14.365), for example, can be generated from a complex ghost field $c(x)$ and its complex conjugate c^* by a functional integral

$$\Phi_4^{-1} = \int \mathcal{D}c^* \mathcal{D}c e^{i \int d^4x \partial c^* \partial c / \sqrt{\alpha}}. \quad (14.416)$$

It should be pointed out that the signs of the kinetic term of these c -field Lagrangians are opposite to those of a normal field. If these fields were associated with particles, their anticommutation rules would carry the wrong sign and the states would have a negative norm. Such states are commonly referred to as *ghosts*, and

this is the reason for the name of the fields c, c^* . Note that the determinant cannot be generated by a real fermion field via a functional integral

$$\Phi_4^{-1} \stackrel{?}{=} \int \mathcal{D}c e^{-i \int d^4x \partial^2 c \partial^2 c / \alpha}. \quad (14.417)$$

The reason is that the differential operator ∂^4 is a *symmetric* functional matrix, so that the exponent vanishes after diagonalization by an orthogonal transformation.

In the language of ghost fields, the mistake in calculating the vacuum energy in Eq. (7.506), that arose when quantizing the electromagnetic field via the Gupta-Bleuler formalism, can be phrased as follows. When fixing the gauge in the action (7.376) by adding an Lagrangian density $\mathcal{L}_{\text{GF}}$ (10.86), we must also add a ghost Lagrangian density

$$\mathcal{L}_{\text{ghost}} = \partial c^* \partial c / \sqrt{\alpha}. \quad (14.418)$$

The ghost fields have to be quantized canonically, and the physical states must satisfy, beside the Gupta-Bleuler subsidiary condition in Eq. (7.502), the condition of being a vacuum to the ghost fields:

$$c|\psi_{\text{phys}}\rangle = 0. \quad (14.419)$$

The Faddeev-Popov formalism is extremely useful offering many other possibilities of fixing a gauge and performing the functional integral for the generating functional over all A^μ -components.

14.18 Functional Formulation of Quantum Electrodynamics

For quantum electrodynamics, the functional integral from which we can derive all time-ordered vacuum expectation values reads [1, 3, 5]:

$$Z[j, \eta, \bar{\eta}] = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A^\mu \mathcal{D}D e^{i\mathcal{A} - i \int d^4x [\bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x)] - i \int d^4x j_\mu(x)A^\mu(x)}, \quad (14.420)$$

where $\mathcal{A}$ is the sum of the free-field action (12.86) and the minimal interaction (12.87), which we shall write here as

$$\mathcal{A} = \int d^4x \left[\bar{\psi} \left(i\partial\!\!\!/ - \frac{e}{c}A - m \right) \psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - D\partial^\mu A_\mu + D^2/2 \right]. \quad (14.421)$$

The Dirac field appears only quadratically in the action. It is therefore possible to integrate it out using the Gaussian integral formula (14.95), and we obtain

$$Z[j, \eta, \bar{\eta}] = \text{Det}(i\partial\!\!\!/ - M) \int \mathcal{D}A^\mu \mathcal{D}D e^{i\mathcal{A}' - \int d^4x d^4x' \bar{\eta}(x)G_0(x, x')\eta(x')\psi(x) - i \int d^4x j_\mu(x)A^\mu(x)}, \quad (14.422)$$

where $\mathcal{A}'$ is the action

$$\mathcal{A} = \int d^4x \left[-\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - D\partial^\mu A_\mu + D^2/2 \right] + \mathcal{A}^{\text{eff}}[A]. \quad (14.423)$$

The effects of the electron are collected in the effective action

$$e^{i\Delta\mathcal{A}^{\text{eff}}} = \exp [\text{Tr} \log (i\partial - e\mathcal{A} - M) - \text{Tr} \log (i\partial - M)], \quad (14.424)$$

where $\text{Tr}\mathcal{O}$ combines the functional trace of the operator $\mathcal{O}$ and the matrix trace in the 4×4 space of Dirac matrices. We have performed a subtraction of the infinite vacuum energy caused by the filled-negative energy states. The subtraction is compensated by the determinant in the prefactor of Eq. (14.422).

14.18.1 Decay Rate of Dirac Vacuum in Electromagnetic Fields

An important application of the functional formulation (14.422) of quantum electrodynamics was made by Heisenberg and Euler [32, 33]. They observed that in a constant external electric field the vacuum becomes unstable. There exists a finite probability of creating an electron-positron pair. This process has to overcome a large energy barrier $2Mc^2$, but if the pair is separated sufficiently far, the total energy of the pair can be made arbitrarily low, so that the process will occur with nonzero probability. The rate can be derived from the result (6.254). For a large total time Δt , the time dependence of an unstable vacuum state will have the form $e^{-i(E_0 - i\Gamma/2)\Delta t}$, where E_0 is the vacuum energy, Γ the desired decay rate, and Δt the total time over which the amplitude is calculated. If $\mathcal{L}^{\text{eff}}$ is the effective Lagrangian density causing the decay, and $\mathcal{A}^{\text{eff}}$ the associated action, we identify

$$\frac{\Gamma}{V} = 2 \text{Im} \frac{\mathcal{A}^{\text{eff}}}{V\Delta t} = 2 \text{Im} \mathcal{L}^{\text{eff}}. \quad (14.425)$$

We now make use of the fact that, due to the invariance under charge conjugation, the right-hand side of (14.424) can depend only on M^2 . Thus we also have

$$\begin{aligned} \exp [\text{Tr} \log (i\partial - e\mathcal{A} - M)] &= \exp [\text{Tr} \log (i\partial - e\mathcal{A} + M)] \\ &= \exp \left\{ \frac{1}{2} [\text{Tr} \log (i\partial - e\mathcal{A} - M) (i\partial - e\mathcal{A} + M)] \right\}, \end{aligned} \quad (14.426)$$

and may use the product relation (6.107) to calculate (14.424) from half the trace log of the Pauli operator in Eq. (6.241) to find the effective action

$$i\Delta\mathcal{A}^{\text{eff}} = \frac{1}{2} \text{Tr} \log \left\{ [i\partial - eA(x)]^2 - \frac{e}{2} \sigma^{\mu\nu} F_{\mu\nu} - M^2 \right\} - \frac{1}{2} \text{Tr} \log \left\{ -\partial^2 - M^2 \right\}. \quad (14.427)$$

We now use the integral identity

$$\log \frac{a}{b} = - \int_0^\infty \frac{d\tau}{\tau} [e^{ia\tau} - e^{ib\tau}] \quad (14.428)$$

and relation (6.206) to rewrite (14.427) as

$$i\Delta\mathcal{A}^{\text{eff}} = - \frac{1}{2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2 - i\epsilon)} \text{tr} \langle x | e^{i\tau \{ [i\partial - eA(x)]^2 + \frac{e}{2} \sigma^{\mu\nu} F_{\mu\nu}^e \}} - e^{-i\tau\partial^2} | x \rangle. \quad (14.429)$$

Recalling (6.189) and (6.206), the first, unsubtracted, term can be re-expressed as

$$i\Delta\mathcal{A}_1^{\text{eff}} = -\frac{1}{2} \int_0^\infty \frac{d\tau}{\tau} \text{tr} \langle x | e^{-i\tau\hat{H}} | x \rangle = -\frac{1}{2} \int_0^\infty \frac{d\tau}{\tau} \text{tr} \langle x, \tau | x 0 \rangle. \quad (14.430)$$

Inserting (6.254), and subtracting the field-free second term in (14.429), we obtain the contribution to the effective Lagrangian density

$$\Delta\mathcal{L}^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eE\tau}{\tanh eE\tau} - 1 \right) e^{-i\tau(M^2-i\eta)}. \quad (14.431)$$

The integral over τ is logarithmically divergent at $\tau = 0$. We can separate the divergent term by a further subtraction, splitting

$$\Delta\mathcal{L}^{\text{eff}} = \Delta\mathcal{L}_{\text{div}}^{\text{eff}} + \Delta\mathcal{L}_R^{\text{eff}} \quad (14.432)$$

into a convergent integral

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eE\tau}{\tanh eE\tau} - 1 - \frac{e^2 E^2 \tau^2}{3} \right) e^{-i\tau(M^2-i\eta)}, \quad (14.433)$$

and a divergent one

$$\Delta\mathcal{L}_{\text{div}}^{\text{eff}} = \frac{e^2}{2} E^2 \frac{1}{3(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2-i\eta)}. \quad (14.434)$$

The latter is proportional to the electric part of the original Maxwell Lagrangian density in (4.237). It can therefore be removed by *renormalization*. We add (14.434) to the Maxwell Lagrangian density, and define a renormalized charge e_R by the equation

$$\frac{1}{e_R^2} = \frac{1}{e^2} + \frac{1}{12\pi^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2-i\eta)} \equiv \frac{1}{Z_3 e^2}, \quad (14.435)$$

to obtain the modified electric Lagrangian density

$$\mathcal{L}_E = \frac{e^2}{2e_R^2} E^2. \quad (14.436)$$

Now we redefine the electric fields by introducing *renormalized fields*

$$E_R \equiv \frac{e}{e_R} E, \quad (14.437)$$

and identify these with the physical fields. In terms of these, (14.436) takes again the usual Maxwell form

$$\mathcal{L}_E = \frac{1}{2} E_R^2. \quad (14.438)$$

The finite effective Lagrangian density (14.433) possesses an imaginary part which by Eq. (14.425) determines the decay rate of the vacuum per unit volume

$$\frac{\Gamma}{V} = \text{Im} \frac{1}{(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eE\tau}{\tanh eE\tau} - 1 - \frac{e^2 E^2 \tau^2}{3} \right) e^{-i\tau(M^2 - i\eta)}. \quad (14.439)$$

For comparison we mention that, for a charged boson field, the expression (14.424) is replaced by

$$e^{i\Delta\mathcal{A}^{\text{eff}}} = \exp \left[-\text{Tr} \log \{ [i\partial - eA(x)]^2 - M^2 \} + \text{Tr} \log (-\partial^2 - M^2) \right]. \quad (14.440)$$

Hence the last factor $4 \cosh eE\tau$ in (6.254) is simply replaced by -2 , and the unsubtracted effective action (14.439) becomes

$$i\Delta\mathcal{A}_u^{\text{eff}} = \int_0^\infty \frac{d\tau}{\tau} \langle x, \tau | x 0 \rangle = -\frac{i}{4(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \frac{eE\tau}{\sinh eE\tau} e^{-i\tau(M^2 - i\eta)}, \quad (14.441)$$

implying a twice subtracted effective Lagrangian density

$$\Delta\mathcal{L}_R^{\text{eff}} = -\frac{1}{4(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eE\tau}{\sinh eE\tau} - 1 + \frac{e^2 E^2 \tau^2}{6} \right) e^{-i\tau(M^2 - i\eta)}, \quad (14.442)$$

and a charge renormalization

$$\frac{1}{e_R^2} = \frac{1}{e^2} - \frac{1}{6\pi^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2 - i\eta)} \equiv \frac{1}{Z_3 e^2}. \quad (14.443)$$

The decay rate per unit volume is

$$\frac{\Gamma_{\text{KG}}}{V} = \text{Im} \frac{1}{4(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eE\tau}{\sinh eE\tau} - 1 + \frac{e^2 E^2 \tau^2}{6} \right) e^{-i\tau(M^2 - i\eta)}. \quad (14.444)$$

The integrands in (14.439) and (14.444) are even in τ , so that the integrals for the decay rate can be extended symmetrically to run over the entire τ -axis. After this, the contour of integration can be closed in the lower half-plane and the integral can be evaluated by Cauchy's residue theorem. To find the pole terms we expand the integrand for fermions in Eq. (14.439) as

$$\frac{eE\tau}{\tanh eE\tau} - 1 = \sum_{n=-\infty}^{\infty} \frac{(eE\tau)^2}{(eE\tau)^2 + n^2\pi^2} = 2 \sum_{n=1}^{\infty} \frac{\tau^2}{\tau^2 + \tau_n^2}, \quad \tau_n \equiv \frac{n\pi}{eE}. \quad (14.445)$$

The relevant poles lie at $\tau = -i\tau_n$ and yield the result

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \sum_{n=1}^{\infty} \frac{1}{n^2} e^{-n\pi M^2/eE}. \quad (14.446)$$

A technical remark is necessary at this place concerning the integral (14.444). At first sight it may appear as if the second subtraction term in the integrand

$e^2 E^2 \tau^2 / 3$ can be omitted [29]. First, it is unnecessary to arrive at a finite integral in the imaginary part, and second, it seems to contribute only to the real part, since for all even powers $\alpha > 2$, the integral

$$\int_0^\infty \frac{d\tau}{\tau^3} \tau^\alpha e^{-i\tau(M^2 - i\eta)} = \frac{1}{(iM^2)^{\alpha-2}} \Gamma(\alpha - 2) \quad (14.447)$$

is real. The limit at hand $\alpha \rightarrow 2$, however, is an exception since for $\alpha \approx 2$, the integral possesses an imaginary part due to the divergence at small τ

$$\frac{1}{(iM^2)^{\alpha-2}} \Gamma(\alpha - 2) \approx -\gamma - \log M^2 - i \frac{\pi}{2} + \mathcal{O}(\alpha - 1). \quad (14.448)$$

The right-hand side of Eq. (14.446) is a polylogarithmic function (2.274), so that we may write

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \zeta_2(e^{-\pi M^2 / eE}). \quad (14.449)$$

For large fields, this has the so-called *Robinson expansion* [30]

$$\zeta_\nu(e^{-\alpha}) = \Gamma(1 - \nu) \alpha^{\nu-1} + \zeta(\nu) + \sum_{k=1}^{\infty} \frac{1}{k!} (-\alpha)^k \zeta(\nu - k). \quad (14.450)$$

This expansion plays an important role in the discussion of Bose-Einstein condensation [31]. For $\nu \rightarrow 2$, the Robinson expansion becomes

$$\zeta_2(e^{-\alpha}) = \frac{\pi^2}{6} + (-1 + \log \alpha) \alpha - \frac{\alpha^2}{4} + \frac{\alpha^3}{72} + \mathcal{O}(\alpha^5). \quad (14.451)$$

Hence we find the strong-field expansion

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \left\{ \frac{\pi^2}{6} + \left[-1 + \log \frac{\pi M^2}{eE} \right] \left(\frac{\pi M^2}{eE} \right) - \frac{1}{4} \left(\frac{\pi M^2}{eE} \right)^2 + \frac{1}{72} \left(\frac{\pi M^2}{eE} \right)^3 + \dots \right\}. \quad (14.452)$$

For bosons, we expand

$$\frac{e\varepsilon\tau}{\sinh e\varepsilon\tau} - 1 = 2 \sum_{n=1}^{\infty} (-1)^n \frac{(eE\tau)^2}{(eE\tau)^2 + n^2\pi^2} = 2 \sum_{n=1}^{\infty} (-1)^n \frac{\tau^2}{\tau^2 + \tau_n^2}, \quad \tau_n \equiv \frac{n\pi}{eE}. \quad (14.453)$$

Comparison with (14.445) shows that the bosonic result for the decay rate differs from the fermionic (14.446) by an alternating sign, accounting for the different statistics. There is also a factor $1/2$, since there is no spin. Thus we find the decay rate per volume

$$\frac{\Gamma_{\text{KG}}}{V} = \frac{e^2 E^2}{4\pi^3} \frac{1}{2} \sum_{n=1}^{\infty} (-1)^{n-1} \frac{1}{n^2} e^{-n\pi M^2 / eE}. \quad (14.454)$$

The sum can again be expressed in terms of the polylogarithmic function (14.450) as follows:

$$\tilde{\zeta}_\nu(z) \equiv \sum_{k=1}^{\infty} \frac{(-1)^{k-1} z^k}{k^\nu} = \sum_{k=1}^{\infty} \frac{z^k}{k^\nu} - 2 \sum_{k=1}^{\infty} \frac{z^{2k}}{(2k)^\nu} = \zeta_\nu(z) - 2^{1-\nu} \zeta_\nu(z^2). \quad (14.455)$$

For $z = e^{-\alpha} \approx 1$, the Robinson expansion (14.451) yields

$$\tilde{\zeta}_2(e^{-\alpha}) = \frac{\pi^2}{12} - \alpha \log 2 + \frac{\alpha^2}{4} - \frac{\alpha^3}{24} + \frac{\alpha^5}{960} + \mathcal{O}(\alpha^8). \quad (14.456)$$

The expansion $\tilde{\zeta}_2(e^{-\alpha})$ replaces the curly bracket in (14.452), if we set $\alpha = \pi M^2/eE$.

14.18.2 Constant Electric and Magnetic Background Fields

In the presence of both $\mathbf{E}$ and $\mathbf{B}$ fields, Eq. (6.253) reads

$$\exp\left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau\right) = \begin{pmatrix} e^{-ie\sigma\cdot(\mathbf{B}-i\mathbf{E})\tau} & 0 \\ 0 & e^{-ie\sigma\cdot(\mathbf{B}+i\mathbf{E})\tau} \end{pmatrix}. \quad (14.457)$$

The trace of this can be found by adding the traces of the 2×2 block matrices $e^{e\sigma\cdot(-i\mathbf{B}\mp\mathbf{E})\tau}$ separately. These are equal to $e^{-e\lambda_1\tau} + e^{-e\lambda_2\tau}$ and their complex conjugates, respectively, where λ_1, λ_2 are the eigenvalues of the matrix $\sigma\cdot(-i\mathbf{B}-\mathbf{E})$:

$$\lambda_{1,2} = \pm\sqrt{(\mathbf{E}+i\mathbf{B})^2} = \pm\sqrt{\mathbf{E}^2 - \mathbf{B}^2 + 2i\mathbf{E}\mathbf{B}}. \quad (14.458)$$

Thus we find

$$\text{tr} \exp\left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau\right) = 2(\cos e\lambda_1 + \cos e\lambda_1^*). \quad (14.459)$$

The eigenvalues are, of course, Lorentz-invariant quantities. They depend only on the two quadratic Lorentz invariants of the electromagnetic field: the scalar S and the pseudoscalar P defined by

$$S \equiv -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2), \quad P \equiv -\frac{1}{4}F_{\mu\nu}\tilde{F}^{\mu\nu} = \mathbf{E}\mathbf{B}. \quad (14.460)$$

In terms of these, Eq. (14.458) reads

$$\lambda_{1,2} = \pm\sqrt{2}\sqrt{S+iP}, \quad (14.461)$$

which can be rewritten as

$$\lambda_{1,2} = \pm\sqrt{2}(S^2 + P^2)^{1/4}(\cos \varphi/2 + i \sin \varphi/2), \quad (14.462)$$

where

$$\tan \varphi = \frac{P}{S}, \quad (14.463)$$

so that

$$\cos \varphi = \frac{S}{\sqrt{S^2 + P^2}}, \quad \sin \varphi = \frac{P}{\sqrt{S^2 + P^2}}, \quad (14.464)$$

implying that $\cos \varphi/2 = \sqrt{(1 + \cos \varphi)/2}$ and $\sin \varphi/2 = \sqrt{(1 - \cos \varphi)/2}$, or

$$\begin{cases} \cos \varphi/2 \\ \sin \varphi/2 \end{cases} = \frac{\sqrt{\sqrt{S^2 + P^2} \pm S}}{\sqrt{2}(S^2 + P^2)^{1/4}}. \quad (14.465)$$

We shall abbreviate the result (14.462) by

$$\lambda_{1,2} = \pm (\varepsilon + i\beta), \quad (14.466)$$

where

$$\begin{cases} \varepsilon \\ \beta \end{cases} \equiv \sqrt{\sqrt{S^2 + P^2} \pm S} = \frac{1}{\sqrt{2}} \sqrt{\sqrt{(\mathbf{E}^2 - \mathbf{B}^2)^2 + 4(\mathbf{E} \mathbf{B})^2} \pm (\mathbf{E}^2 - \mathbf{B}^2)}. \quad (14.467)$$

In terms of ε and β , the invariants S and P in (14.460) become

$$S \equiv -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2) = \frac{1}{2}(\varepsilon^2 - \beta^2), \quad P \equiv -\frac{1}{4}F_{\mu\nu}\tilde{F}^{\mu\nu} = \mathbf{E} \mathbf{B} = \varepsilon\beta, \quad (14.468)$$

and the trace (14.459) is simply

$$\text{tr exp} \left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau \right) = 2 \cosh(\varepsilon + i\beta) + 2 \cosh(\varepsilon - i\beta) = 4 \cosh \varepsilon \cos \beta. \quad (14.469)$$

Some special cases will simplify the upcoming formulas:

1. If $\mathbf{B} = 0$, then ε reduces to $|\mathbf{E}|$, whereas for $\mathbf{E} = 0$, β reduces to $|\mathbf{B}|$.
2. If $\mathbf{E} \neq 0$ and $\mathbf{B} \neq 0$ are orthogonal to each other, then we have either $\beta = 0$ for $E > B$, or $\varepsilon = 0$ for $B > E$. The formulas are then the same as for pure electric or magnetic fields.
3. If $\mathbf{E} \neq 0$ and $\mathbf{B} \neq 0$ are parallel to each other, then $\varepsilon = |\mathbf{E}| \neq 0$, $\beta = |\mathbf{B}| \neq 0$.

In all these cases, the calculation of the exponential (14.457) can be done very simply. Take the third case. Due to rotational symmetry, we can assume the fields to point in the z -direction, $\mathbf{B} = B\hat{\mathbf{z}}$, $\mathbf{E} = E\hat{\mathbf{z}}$, and the exponential (14.457) has the matrix form

$$\begin{aligned} \exp \left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau \right) &= \begin{pmatrix} e^{-ie\sigma_3(B-iE)\tau} & 0 \\ 0 & e^{-ie\sigma_3(B+iE)\tau} \end{pmatrix} \\ &= \begin{pmatrix} e^{-ie(B-iE)\tau} & 0 & 0 & 0 \\ 0 & e^{ie(B-iE)\tau} & 0 & 0 \\ 0 & 0 & e^{-ie(B+iE)\tau} & 0 \\ 0 & 0 & 0 & e^{ie(B+iE)\tau} \end{pmatrix}. \end{aligned} \quad (14.470)$$

This has the trace

$$\text{tr exp} \left(-i\frac{e}{2}\sigma^\mu{}_\nu F_\mu{}^\nu \tau \right) = 2 \cosh(E + iB)\tau + 2 \cosh(E - iB)\tau = 4 \cosh E\tau \cos B\tau, \quad (14.471)$$

in agreement with (14.469). In fact, given an arbitrary constant field configuration $\mathbf{B}$ and $\mathbf{E}$, it is always possible to perform a Lorentz transformation to a coordinate frame in which the transformed fields, call them $\mathbf{B}_{\text{CF}}$ and $\mathbf{E}_{\text{CF}}$, are parallel. This frame is called *center-of-fields* frame. The transformation has the form (4.285) and (4.286) with a velocity of the transformation determined by

$$\frac{\mathbf{v}/c}{1 + (|\mathbf{v}|/c)^2} = \frac{\mathbf{E} \times \mathbf{B}}{|\mathbf{E}|^2 + |\mathbf{B}|^2}. \quad (14.472)$$

By Lorentz invariance, we see that

$$\mathbf{E}^2 - \mathbf{B}^2 = \mathbf{E}_{\text{CF}}^2 - \mathbf{B}_{\text{CF}}^2, \quad \mathbf{E} \cdot \mathbf{B} = \mathbf{E}_{\text{CF}} \cdot \mathbf{B}_{\text{CF}}, \quad (14.473)$$

which shows that $|\mathbf{E}_{\text{CF}}|$ and $|\mathbf{B}_{\text{CF}}|$ in Eq. (14.471) coincide with ε and β in Eq. (14.468). This is the reason why Eq. (14.471) gives the general result for arbitrary constant fields, if E and B are replaced by $|\mathbf{E}_{\text{CF}}| = \varepsilon$ and $|\mathbf{B}_{\text{CF}}| = \beta$.

These considerations permit us to present a simple alternative calculation of a determinantal prefactor that occurred much earlier in Chapter 6, in particular in Eqs. (6.214) and (6.225). For a general constant field strength $F_\mu{}^\nu$, the basic matrix that had to be diagonalized was $e^{eF\tau}$ in Eq. (6.245). For an electric field pointing in the z -direction, this has the form $e^{-iM_3 eE\tau}$. In contrast to (6.253), this is a boost matrix with rapidity $\zeta = eE\tau$ in the defining 4×4 -representation [compare (4.63)]. The fact that the rapidity in the Dirac representation (6.252) was twice as large, has its origin in the value of the gyromagnetic ratio 2 of the Dirac particle in Eq. (6.119).

If the field points in any direction, the obvious generalization is $e^{-i\mathbf{M}\mathbf{E}e\tau}$. In the presence of a magnetic field, the generators of the rotation group (4.57) enter and (6.245) can be written as $e^{eF\tau} = e^{-ie(\mathbf{M}\mathbf{E} + \mathbf{L}\mathbf{B})\tau}$. This is the defining four-dimensional representation of the complex Lorentz transformation, whose chiral Dirac representation was written down in (14.457), apart from the factor 2 multiplying the rapidity and the rotation vectors.

As before in the Dirac representation, much labor is saved by working in the center-of-fields frame where electric and magnetic fields are parallel and point in the z -direction. Their lengths have the invariant values ε and β , respectively. The associated transformation $e^{eF\tau}$ has then the simple form

$$e^{eF\tau} = e^{-i(M_3\varepsilon + L_3\beta)e\tau} = \begin{pmatrix} \cosh \varepsilon e\tau & 0 & 0 & -\sinh \varepsilon e\tau \\ 0 & \cos \beta e\tau & -\sin \beta e\tau & 0 \\ 0 & \sin \beta e\tau & \cos \beta e\tau & 0 \\ -\sinh \varepsilon e\tau & 0 & 0 & \cosh \varepsilon e\tau \end{pmatrix}. \quad (14.474)$$

From this we find a matrix for $\sin eF\tau = [e^{-i(M_3\varepsilon + L_3\beta)e\tau} - e^{i(M_3\varepsilon + L_3\beta)e\tau}]/2$:

$$\sin eF\tau = \begin{pmatrix} 0 & 0 & 0 & -\sinh \varepsilon e\tau \\ 0 & 0 & -\sin \beta e\tau & 0 \\ 0 & \sin \beta e\tau & 0 & 0 \\ -\sinh \varepsilon e\tau & 0 & 0 & 1 \end{pmatrix}, \quad (14.475)$$

and from this

$$eF\tau = \begin{pmatrix} 0 & 0 & 0 & -\varepsilon e\tau \\ 0 & 0 & -\beta e\tau & 0 \\ 0 & \beta e\tau & 0 & 0 \\ -\varepsilon e\tau & 0 & 0 & 1 \end{pmatrix}. \quad (14.476)$$

This leads to the desired prefactor in the amplitude (6.225)

$$\det^{-1/2} \left(\frac{\sinh eF\tau}{eF\tau} \right) = e\varepsilon\beta\tau^2 \frac{e\varepsilon\beta\tau^2}{\sinh \varepsilon\tau \sin \beta e\tau}. \quad (14.477)$$

Thus we can obtain the imaginary part of the vacuum energy in a constant electromagnetic field if we simply replace the term $eE\tau \coth eE\tau$ in the integrand of the rate formula (14.439) as follows:

$$\frac{eE\tau}{\tanh eE\tau} \rightarrow \frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} \frac{e\beta\tau}{\tan e\beta\tau}. \quad (14.478)$$

14.18.3 Decay Rate in a Constant Electromagnetic Field

magnetic field the effective Lagrangian density (14.433) becomes, after the replacement (14.478)

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left[\frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} \frac{e\beta\tau}{\tan e\beta\tau} - 1 - \frac{e^2(\varepsilon^2 - \beta^2)}{3} \right] e^{-i\tau(M^2 - i\eta)}. \quad (14.479)$$

The subtracted small- τ divergence lies in the integral [recall the equality $\varepsilon^2 - \beta^2 = \mathbf{E}^2 - \mathbf{B}^2$ from Eq. (14.468)]

$$\Delta\mathcal{L}_{\text{div}}^{\text{eff}} = \frac{e^2}{2} (\mathbf{E}^2 - \mathbf{B}^2) \frac{1}{3(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2 - i\eta)}, \quad (14.480)$$

which is proportional to the full original Maxwell Lagrangian density in (4.237), and can therefore be absorbed into it by a renormalization of the charge as in (14.435) and of the fields

$$\mathbf{B}_R \equiv \frac{e}{e_R} \mathbf{B}, \quad \mathbf{E}_R \equiv \frac{e}{e_R} \mathbf{E}. \quad (14.481)$$

From twice the imaginary part of (14.489) we obtain the decay rate per unit volume extending Eq. (14.439) in an obvious manner. Inserting the expansion (14.445), extending the integral over the entire τ -axis and rotating the contour of integration as we did in evaluating (14.439), we find the generalization of Eq. (14.446) to constant electromagnetic fields

$$\frac{\Gamma_{\text{KG}}}{V} = \frac{e^2 E^2}{4\pi^3} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{n\pi\beta/\varepsilon}{\tanh n\pi\beta/\varepsilon} e^{-n\pi M^2/eE}. \quad (14.482)$$

For bosons obeying the Klein-Gordon equation, we obtain, by analogy, the extension of (14.454) to constant electromagnetic fields:

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \frac{1}{2} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^2} \frac{n\pi\beta/\varepsilon}{\sinh n\pi\beta/\varepsilon} e^{-n\pi M^2/e\varepsilon}. \quad (14.483)$$

14.18.4 Effective Action in a Purely Magnetic Field

If there is only a magnetic field, magnetic field the effective Lagrangian density (14.433) becomes, after the replacement (14.478)

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left[\frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} \frac{e\beta\tau}{\tan e\beta\tau} - 1 - \frac{e^2(\varepsilon^2 - \beta^2)}{3} \right] e^{-i\tau(M^2 - i\eta)}. \quad (14.484)$$

The subtracted small- τ divergence lies in the integral [recall the equality $\varepsilon^2 - \beta^2 = \mathbf{E}^2 - \mathbf{B}^2$ from Eq. (14.468)]

$$\Delta\mathcal{L}_{\text{div}}^{\text{eff}} = \frac{e^2}{2}(\mathbf{E}^2 - \mathbf{B}^2) \frac{1}{3(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2 - i\eta)}, \quad (14.485)$$

which is proportional to the full original Maxwell Lagrangian density in (4.237), and can therefore be absorbed into it by a renormalization of the charge as in (14.435) and of the fields

$$\mathbf{B}_R \equiv \frac{e}{e_R} \mathbf{B}, \quad \mathbf{E}_R \equiv \frac{e}{e_R} \mathbf{E}. \quad (14.486)$$

From twice the imaginary part of (14.489) we obtain the decay rate per unit volume extending Eq. (14.439) in an obvious manner. Inserting the expansion (14.445), extending the integral over the entire τ -axis and rotating the contour of integration as we did in evaluating (14.439), we find the generalization of Eq. (14.446) to constant electromagnetic fields

$$\frac{\Gamma_{\text{KG}}}{V} = \frac{e^2 E^2}{4\pi^3} \sum_{n=1}^\infty \frac{1}{n^2} \frac{n\pi\beta/\varepsilon}{\tanh n\pi\beta/\varepsilon} e^{-n\pi M^2/eE}. \quad (14.487)$$

For bosons obeying the Klein-Gordon equation, we obtain, by analogy, the extension of (14.454) to constant electromagnetic fields:

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \frac{1}{2} \sum_{n=1}^\infty \frac{(-1)^{n-1}}{n^2} \frac{n\pi\beta/\varepsilon}{\sinh n\pi\beta/\varepsilon} e^{-n\pi M^2/e\varepsilon}. \quad (14.488)$$

14.18.5 Effective Action in a Purely Magnetic Field

If there is only a magnetic field, For a constant electromagnetic field the effective Lagrangian density (14.433) becomes, after the replacement (14.478)

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left[\frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} \frac{e\beta\tau}{\tan e\beta\tau} - 1 - \frac{e^2(\varepsilon^2 - \beta^2)}{3} \right] e^{-i\tau(M^2 - i\eta)}. \quad (14.489)$$

The subtracted small- τ divergence lies in the integral [recall the equality $\varepsilon^2 - \beta^2 = \mathbf{E}^2 - \mathbf{B}^2$ from Eq. (14.468)]

$$\Delta\mathcal{L}_{\text{div}}^{\text{eff}} = \frac{e^2}{2}(\mathbf{E}^2 - \mathbf{B}^2) \frac{1}{3(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(M^2 - i\eta)}, \quad (14.490)$$

which is proportional to the full original Maxwell Lagrangian density in (4.237), and can therefore be absorbed into it by a renormalization of the charge as in (14.435) and of the fields

$$\mathbf{B}_R \equiv \frac{e}{e_R} \mathbf{B}, \quad \mathbf{E}_R \equiv \frac{e}{e_R} \mathbf{E}. \quad (14.491)$$

From twice the imaginary part of (14.489) we obtain the decay rate per unit volume extending Eq. (14.439) in an obvious manner. Inserting the expansion (14.445), extending the integral over the entire τ -axis and rotating the contour of integration as we did in evaluating (14.439), we find the generalization of Eq. (14.446) to constant electromagnetic fields

$$\frac{\Gamma_{\text{KG}}}{V} = \frac{e^2 E^2}{4\pi^3} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{n\pi\beta/\varepsilon}{\tanh n\pi\beta/\varepsilon} e^{-n\pi M^2/eE}. \quad (14.492)$$

For bosons obeying the Klein-Gordon equation, we obtain, by analogy, the extension of (14.454) to constant electromagnetic fields:

$$\frac{\Gamma}{V} = \frac{e^2 E^2}{4\pi^3} \frac{1}{2} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^2} \frac{n\pi\beta/\varepsilon}{\sinh n\pi\beta/\varepsilon} e^{-n\pi M^2/e\varepsilon}. \quad (14.493)$$

14.18.6 Effective Action in a Purely Magnetic Field

If there is only a magnetic field, the integral representation (14.489) reduces to [32, 33]

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left(\frac{eB\tau}{\tan eB\tau} - 1 + \frac{e^2 B^2 \tau^2}{3} \right) e^{-i\tau(M^2 - i\eta)}. \quad (14.494)$$

The integral still contains a divergence at small τ . The associated divergent integral is precisely a magnetic version of Eq. (14.434). It can be removed by the same type of subtraction as before, with E^2 replaced by B^2 . Going to renormalized quantities as in (14.435) and (14.491) and rotating the contour of integration clockwise to move it away from the poles, a trivial change of the integration variable leads to

$$\Delta\mathcal{L}_R^{\text{eff}} = -\frac{e^2 B^2}{2(2\pi)^2} \int_0^\infty \frac{ds}{s^2} \left(\coth s - \frac{1}{s} - \frac{s}{3} \right) e^{-sM^2/eB}. \quad (14.495)$$

This is a typical Borel transformation of the expression in parentheses. It implies that its power series expansion leads to coefficients of B^{2n} which grow like $(2n)!$. The expansion has therefore a vanishing radius of convergence. It is an asymptotic series, and we shall understand later the physical origin of this.

For Klein-Gordon particles, the result becomes

$$\Delta\mathcal{L}_{\text{RKG}} = \frac{e^2 B^2}{(2\pi)^2} \int_0^\infty \frac{ds}{s^2} \left(\frac{1}{\sin s} - \frac{1}{s} + \frac{s}{6} \right) e^{-sM^2/eB}. \quad (14.496)$$

14.18.7 Heisenberg-Euler Lagrangian

By expanding (14.478) in powers of e , we obtain

$$\begin{aligned} \frac{1}{\tau^3} \frac{e\beta\tau}{\tan e\beta\tau} \frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} &= \frac{1}{\tau^3} + \frac{e^2}{3\tau} (\varepsilon^2 - \beta^2) - e^4 \frac{\tau}{45} (\varepsilon^4 + 5\varepsilon^2\beta^2 + \beta^4) \\ &+ e^6 \frac{\tau^3}{945} (2\varepsilon^6 + 7\varepsilon^4\beta^2 - 7\varepsilon^2\beta^4 - 2\beta^6) + \dots \end{aligned} \quad (14.497)$$

Inserting this into (14.489) and performing the integral over τ leads to an expansion in powers of the fields, whose lowest terms are, with $e^2 = 4\pi\alpha$:

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{2\alpha^2}{45M^4} \{(\mathbf{E}^2 - \mathbf{B}^2)^2 + 7(\mathbf{E}\mathbf{B})^2\} + \frac{16\pi\alpha^3}{315M^8} \{2(\mathbf{E}^2 - \mathbf{B}^2)^3 + 13(\mathbf{E}^2 - \mathbf{B}^2)(\mathbf{E}\mathbf{B})^2\}. \quad (14.498)$$

In each term we can replace α by $\alpha_R = \alpha(1 + \mathcal{O}(\alpha))$, and the fields by the renormalized fields via (14.491). Then we obtain the same series as in (14.498) but for the physical renormalized quantities, plus higher-order corrections in α for each coefficient, which we ignore in this lowest-order calculation.

Each coefficient is exact to leading order in α . To illustrate the form of the higher-order corrections we include, without derivation, the leading correction into the first term, which becomes (see Appendix 14C for details)

$$\Delta\mathcal{L}_R^{\text{eff}} = \frac{2\alpha^2}{45m_e^4} \left\{ \left(1 + \frac{40\alpha}{9\pi}\right) (\mathbf{E}^2 - \mathbf{B}^2)^2 + 7 \left(1 + \frac{1315\alpha}{252\pi}\right) (\mathbf{E} \cdot \mathbf{B})^2 \right\} + \dots \quad (14.499)$$

Electrons in a Constant Magnetic Field

For Dirac particles in arbitrary constant fields we expand

$$e\varepsilon\tau \coth e\varepsilon\tau = \sum_{n=-\infty}^{\infty} \frac{(e\varepsilon\tau)^2}{(e\varepsilon\tau)^2 + n^2\pi^2} = \sum_{n=-\infty}^{\infty} \frac{\tau^2}{\tau^2 + \tau_{n,\varepsilon}^2}, \quad \tau_{n,\varepsilon} \equiv \frac{n\pi}{e\varepsilon}, \quad (14.500)$$

$$e\beta\tau \cot e\beta\tau = \sum_{m=-\infty}^{\infty} \frac{(e\beta\tau)^2}{(e\beta\tau)^2 - m^2\pi^2} = \sum_{m=-\infty}^{\infty} \frac{\tau^2}{\tau^2 - \tau_{m,\beta}^2}, \quad \tau_{m,\beta} \equiv \frac{m\pi}{e\beta}. \quad (14.501)$$

The $i\eta$ accompanying the mass term in the τ -integral (14.439) is equivalent to replacing $e^{-i\tau(M^2-i\eta)}$ by $e^{-i\tau(1-i\eta)M^2}$, implying that the integral over all τ has to be performed slightly below the real axis. Equivalently we may shift the $\tau_{m,\beta}$ slightly upwards in the complex plane to $\tau_{m,\beta} + i\epsilon$. This leads to an additional contribution to the action corresponding to a constant electromagnetic field $\Delta\mathcal{L}^{\text{eff}} = \Delta\mathcal{L}_{\text{div}}^{\text{eff}} + \Delta\mathcal{L}_R^{\text{eff}}$. It contains a logarithmically divergent part

$$\Delta\mathcal{L}_{\text{div}}^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau} e^{-i\tau(1-i\eta)M^2} 2 \left(\sum_{n=1}^{\infty} \frac{1}{\tau_{n,\varepsilon}^2} - \sum_{m=1}^{\infty} \frac{1}{\tau_{m,\beta}^2} \right), \quad (14.502)$$

and the finite part

$$\Delta \mathcal{L}_R^{\text{eff}} = \frac{1}{2(2\pi)^2} \int_0^\infty \frac{d\tau}{\tau^3} \left[\sum_{n,m=-\infty}^\infty \frac{\tau^2}{\tau^2 + \tau_{n,\varepsilon}^2} \frac{\tau^2}{\tau^2 - \tau_{m,\beta}^2} - 1 - 2\tau^2 \left(\sum_{n=0}^\infty \frac{1}{\tau_{n,\varepsilon}^2} - \sum_{m=1}^\infty \frac{1}{\tau_{m,\beta}^2} \right) \right] \times e^{-i\tau(1-i\eta)M^2}. \quad (14.503)$$

Performing the sums

$$\sum_{n=1}^\infty \frac{1}{\tau_{n,\varepsilon}^k} = \left(\frac{e\varepsilon}{\pi} \right)^k \zeta(k), \quad \sum_{m=1}^\infty \frac{1}{\tau_{m,\beta}^k} = \left(\frac{e\beta}{\pi} \right)^k \zeta(k), \quad (14.504)$$

we see that (14.502) coincides with (14.490), as it should. The remaining sum is finite:

$$\Delta \mathcal{L}_R^{\text{eff}} = \frac{1}{8\pi^2} \sum'_{n,m=-\infty}^\infty \frac{1}{\tau_{n,\varepsilon}^2 + \tau_{m,\beta}^2} \int_0^\infty d\tau \left[\frac{\tau e^{-\tau M^2}}{\tau^2 - \tau_{n,\varepsilon}^2 + i\eta} - \frac{\tau e^{-\tau M^2}}{\tau^2 + \tau_{m,\beta}^2 - i\eta} \right] - \dots, \quad (14.505)$$

where the dots indicate the subtractions. Now we decompose à la Sochocki [recall Footnote 9 in Chapter 1]:

$$\frac{\tau}{\tau^2 - \tau_{n,\varepsilon}^2 + i\eta} = i \frac{\pi}{2} \delta(\tau + \tau_{n,\varepsilon}) - i \frac{\pi}{2} \delta(\tau - \tau_{n,\varepsilon}) + \tau \frac{\mathcal{P}}{\tau^2 - \tau_{n,\varepsilon}^2}, \quad (14.506)$$

where $\mathcal{P}$ indicates the principal value under the integral. The integrals over the δ -functions contribute

$$\Delta_\delta \mathcal{L}^{\text{eff}} = \frac{i}{8\pi} \sum_{n>0, m \neq 0} \frac{1}{\tau_{n,\varepsilon}^2 + \tau_{m,\beta}^2} e^{-\tau_{n,\varepsilon} M^2} = i \frac{e^2 \varepsilon^2 \beta^2}{8\pi^3} \sum_{n>0, m \geq 0}^\infty \frac{1}{n^2 \beta^2 + m^2 \varepsilon^2} e^{-n\pi M^2 / e\varepsilon}. \quad (14.507)$$

This leads to a decay rate per volume which agrees with (14.493) if we expand in that expression [recall (14.445) and (14.425)]:

$$\frac{n\pi\beta/\varepsilon}{\tanh n\pi\beta/\varepsilon} = 1 + \sum_{m \neq 0} \frac{(n\pi\beta/\varepsilon)^2}{(n\pi\beta/\varepsilon)^2 + m^2 \pi^2} = 1 + \sum_{m \neq 0} \frac{n^2 \beta^2}{n^2 \beta^2 + m^2 \varepsilon^2}. \quad (14.508)$$

It remains to do the principal-value integrals. Here we use the formula⁹

$$J(z) \equiv \mathcal{P} \int_0^\infty d\tau \frac{\tau e^{-\tau}}{\tau^2 - z^2} = -\frac{1}{2} \left[e^{-z} \text{Ei}(z) + e^z \text{Ei}(-z) \right], \quad (14.509)$$

where

$$\text{Ei}(z) \equiv \int_{-\infty}^z dt \frac{\mathcal{P}}{t} e^t = \log(-z) + \sum_{k=1}^\infty \frac{z^k}{k \, k!} \quad (14.510)$$

⁹I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980, Formulas 3.354.4 and 8.211.

is the exponential integral, γ being the Euler-Mascheroni constant

$$\gamma = 0.577216 \dots \quad (14.511)$$

The function (14.509) has the small- z expansion

$$\begin{aligned} J(z) = & -\frac{1}{2} \left[e^z \log(z) + e^{-z} \log(-z) \right] - \gamma \cosh z \\ & - \sum_{l=1}^{\infty} \frac{z^{2l}}{(2l)(2l)!} \cosh z + \sum_{l=1}^{\infty} \frac{z^{2l+1}}{(2l+1)(2l+1)!} \sinh z, \end{aligned} \quad (14.512)$$

and behaves for large z like

$$J(z) = -\frac{1}{z^2} - \frac{6}{z^4} - \frac{120}{z^6} - \frac{5040}{z^8} + \dots \quad (14.513)$$

Using these formulas, we find from the principal-value integrals in (14.505) [34]:

$$\Delta_{\mathcal{P}} \mathcal{L}^{\text{eff}} = -\frac{e^2}{4\pi^4} \sum_{n=1}^{\infty} \frac{1}{n^2} (\beta^2 a_n + \varepsilon^2 b_n), \quad (14.514)$$

with

$$a_n = \frac{n\pi\varepsilon/\beta}{\tanh n\pi\varepsilon/\beta} \left[\text{Ci} \left(\frac{n\pi m^2}{e\beta} \right) \cos \frac{n\pi m^2}{e\beta} + \text{si} \left(\frac{n\pi m^2}{e\beta} \right) \sin \frac{n\pi m^2}{e\beta} \right], \quad (14.515)$$

$$b_n = -\frac{1}{2} \frac{n\pi\beta/\varepsilon}{\tanh n\pi\beta/\varepsilon} \left[\exp \left(\frac{n\pi m^2}{e\varepsilon} \right) \text{Ei} \left(-\frac{n\pi m^2}{e\varepsilon} \right) + \exp \left(-\frac{n\pi m^2}{e\varepsilon} \right) \text{Ei} \left(\frac{n\pi m^2}{e\varepsilon} \right) \right], \quad (14.516)$$

where $\text{Ci}(z) \equiv \frac{1}{2i} [\text{Ei}(iz) + \text{Ei}(-iz)]$ and $\text{si}(z) \equiv \frac{1}{2i} [\text{Ei}(iz) - \text{Ei}(-iz)] = \text{Si}(z) - \pi/2$ are the cosine and sine integrals with the integral representations [35]:

$$\text{Ci}(z) \equiv -\int_z^{\infty} \frac{dt}{t} \cos t = \gamma + \log z + \int_0^z \frac{dt}{t} (\cos t - 1), \quad \text{si}(z) \equiv -\int_z^{\infty} \frac{dt}{t} \sin t. \quad (14.517)$$

The prefactors in (14.515) and (14.516) come once more from sums of the type (14.508).

For large arguments of $J(z)$, the expansion (14.513) becomes

$$\Delta_{\mathcal{P}} \mathcal{L}^{\text{eff}} = \frac{1}{8\pi^2} \sum_{n,m=-\infty}^{\infty} \frac{1}{\tau_{n,\varepsilon}^2 + \tau_{m,\beta}^2} \left[\frac{1}{\tau_{n,\varepsilon}^2 M^4} + \frac{6}{\tau_{n,\varepsilon}^4 M^8} + \frac{120}{\tau_{n,\varepsilon}^6 M^{12}} + \dots \right]. \quad (14.518)$$

Applying the summation formulas (14.504), this is seen to agree with the small-field expansion (14.498).

For $\mathbf{E} = 0$, the sum (14.514) contains only the $n = 0$ -terms. If $\mathbf{B}$ is large, the n -sum is dominated by the first term in the expansion (14.512), and yields

$$\Delta_{\mathcal{P}} \mathcal{L}^{\text{eff}} = \frac{1}{8\pi^2} 2 \sum_{m=1}^{\infty} \frac{1}{\tau_{m,\beta}^2} \log(\tau_{m,\beta} M^2). \quad (14.519)$$

The leading part of this is

$$\Delta_{\mathcal{P}}\mathcal{L}^{\text{eff}} = \frac{1}{4\pi^2} \sum_{m=1}^{\infty} \frac{e^2 B^2}{\pi^2 m^2} \log \frac{M^2}{eB} + \dots = -\frac{1}{24\pi^2} e^2 B^2 \log \frac{eB}{M^2}, \quad (14.520)$$

as derived first by Weisskopf [36].

Note that this logarithmic behavior can be understood as the result of a lowest expansion in e^2 of an anomalous power behavior of the effective action

$$\Delta\mathcal{L}^{\text{eff}} = \frac{1}{2}(E^2 - B^2)^{1+e^2/12\pi^2}. \quad (14.521)$$

Due to the smallness of e^2 , this power can be observed only at very large field strengths. In self-focussing materials, however, it is visible in present-day laser beams [37].

14.18.8 Alternative Derivation for a Constant Magnetic Field

The case of a constant magnetic field can also be treated in a different way [38]. The eigenvalues of the euclidean Klein-Gordon operator of a free scalar field

$$\mathcal{O}_{\text{KG}} = -\hbar^2 \partial^2 + M^2 c^2 \quad (14.522)$$

are

$$\lambda_p = p^2 + M^2 c^2. \quad (14.523)$$

If a constant magnetic field is present that points in the z -direction, the kinetic energy $p_1^2 + p_2^2$ in the xy -plane changes to Landau energies:

$$p_1^2 + p_2^2 \rightarrow 2M \times \frac{p_1^2 + p_2^2}{2M} = 2M \times \hbar\omega_L \left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots, \quad (14.524)$$

where $\omega_L = eB/Mc$ is the Landau frequency. Thus the eigenvalues become

$$\lambda_{n,\mathbf{p}_{\perp}} = \mathbf{p}_{\perp}^2 + 2\frac{\hbar e}{c}B(n + 1/2) + M^2 c^2, \quad (14.525)$$

where $\mathbf{p}_{\perp}$ is the two-dimensional momentum in the $x_3 - x_4$ -plane.

For a Dirac electron satisfying the Pauli equation (6.110), this changes to

$$\lambda_{n,\mathbf{p}_{\perp}} = \mathbf{p}_{\perp}^2 + 2\frac{\hbar e}{c}B(n + 1/2 + s_3) + M^2 c^2, \quad s_3 = \pm 1/2. \quad (14.526)$$

In this expression, the famous g -factor which accounts for the anomalous magnetic moment is approximated by the Dirac value 2. Radiative corrections would insert a factor $g/2$ in front of σ_3 , with $g = 2 + \alpha/\pi + \dots$.

The contribution of electrons to the effective action in Eq. (14.427) can therefore be written as

$$i\Delta\mathcal{A}^{\text{eff}} = \frac{1}{2} \left(\sum_{n,\sigma} \int \frac{d^2 p_{\perp}}{(2\pi\hbar)^2} \log \lambda_{n,\mathbf{p}_{\perp}} - \int \frac{d^4 p}{(2\pi\hbar)^4} \log \lambda_p \right). \quad (14.527)$$

These are divergent expressions. In order to deal with them efficiently it is useful to introduce the Hurwitz ζ -function employed in number theory [39, 40]:

$$\zeta_H(s, z) = \sum_{n=0}^{\infty} \frac{1}{(n+z)^s}, \quad \text{Re}(s) > 1, \quad v \neq 0, -1, -2, \dots \quad (14.528)$$

This Hurwitz ζ -function can be analytically continued in the s -plane to define an analytic function with a single simple pole at $s = 1$. In quantum field theory, one may extend this definition to an arbitrary eigenvalue spectrum of an operator $\mathcal{O}$ as

$$\zeta_{\mathcal{O}}(s) = \sum \frac{1}{(\lambda/\mu^d)^s}, \quad (14.529)$$

where μ is some mass parameter to make the eigenvalues of mass dimension d dimensionless. For large enough s , this is always convergent. By analytic continuation in s , one can derive a finite value for the functional determinant of $\mathcal{O}$:

$$\text{Det } \mathcal{O} = e^{\text{Tr log } \mathcal{O}}, \quad \text{Tr log } \mathcal{O} = -\zeta'_{\mathcal{O}}(0). \quad (14.530)$$

For the Dirac spectrum (14.526), the ζ -function becomes, in natural units,

$$\zeta_D(s) = \frac{eB}{2\pi} \sum_{n=0}^{\infty} \sum_{\pm} \int \frac{d^2 k_{\perp}}{(2\pi)^2} \left[\frac{M^2 + k_{\perp}^2 + eB(2n+1 \pm 1)}{\mu^2} \right]^{-s}, \quad (14.531)$$

where the prefactor of $eB/2\pi$ is the degeneracy of the Landau levels which ensures that the sum $(eB/2\pi) \sum_n$ converges in the limit $B \rightarrow 0$ against the momentum integral $\int dk^1 dk^2 / (2\pi)^2 = \int dk^2 / 4\pi$. Performing the integral over the momenta $p_{\perp}$ yields

$$\zeta_D(s) = \frac{B}{8\pi^2} \mu^{2s} \frac{1}{s-1} \left\{ [M^2 + 2eBn]^{1-s} + [M^2 + 2eB(n+1)]^{1-s} \right\}. \quad (14.532)$$

This can be expressed in terms of the Hurwitz ζ -function (14.528) as

$$\zeta_D(s) = \frac{M^4}{4\pi^2} \left(\frac{eB}{M^2} \right)^2 \sum_{n=0}^{\infty} \left(\frac{\mu^2}{2eB} \right)^s \frac{1}{s-1} \left[2\zeta_H \left(s-1, \frac{M^2}{2eB} \right) - \left(\frac{M^2}{2eB} \right)^{1-s} \right]. \quad (14.533)$$

From this we obtain

$$\begin{aligned} \zeta'_D(0) &= \frac{(eB)^2}{4\pi^2} \left\{ -2\zeta'_H \left(-1, \frac{M^2}{2eB} \right) - \frac{M^2}{2eB} \log \left(\frac{M^2}{2eB} \right) \right. \\ &\quad \left. + \left[\frac{1}{6} + \left(\frac{M^2}{2eB} \right)^2 \right] \left[1 + \log \left(\frac{\mu^2}{2eB} \right) \right] \right\}. \end{aligned} \quad (14.534)$$

Choosing $\mu = M$ and subtracting the zero-field contribution, which is simply $-3M^4/32\pi^2$, we find

$$\Delta \mathcal{L}^{\text{eff}} = \frac{(eB)^2}{2\pi^2} \left\{ \zeta'_H \left(-1, \frac{M^2}{2eB} \right) + \zeta_H \left(-1, \frac{M^2}{2eB} \right) \log \left(\frac{M^2}{2eB} \right) - \frac{1}{12} + \frac{1}{4} \left(\frac{M^2}{2eB} \right)^2 \right\}, \quad (14.535)$$

where we have used the property [41, 39]

$$\zeta_H(-1, z) = -\frac{1}{12} + \frac{z}{2} - \frac{z^2}{2}. \quad (14.536)$$

Contact with the previous result in (14.495) is established with the help of the integral representation of the Hurwitz ζ -function [41]:

$$\zeta_H(s, z) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{e^{-zt} t^{s-1}}{1 - e^{-t}} dt \quad , \quad \text{Re}(s) > 1 \quad , \quad \text{Re}(z) > 0. \quad (14.537)$$

The integral can be rewritten as

$$\zeta_H(s, z) = \frac{z^{1-s}}{s-1} + \frac{z^{-s}}{2} + \frac{sz^{-1-s}}{12} + \frac{2^{s-1}}{\Gamma(s)} \int_0^\infty \frac{dt}{t^{1-s}} e^{-2zt} \left(\coth t - \frac{1}{t} - \frac{t}{3} \right), \quad (14.538)$$

this expression being valid for $\text{Re}(s) > -2$, where the integral converges [42]. From this we evaluate the s -derivative at $s = -1$ as follows:

$$\zeta'_H(-1, z) = \frac{1}{12} - \frac{z^2}{4} - \zeta_H(-1, z) \log z - \frac{1}{4} \int_0^\infty \frac{dt}{t^2} e^{-2zt} \left(\coth t - \frac{1}{t} - \frac{t}{3} \right). \quad (14.539)$$

Inserting this into (14.535) we recover exactly the previous Eq. (14.495).

Let us now derive the strong-field limit. For this we use the following relation between the Hurwitz ζ -function and the Γ -function [41, 39]:

$$\zeta'_H(-1, z) = \zeta'(-1) - \frac{z}{2} \log(2\pi) - \frac{z}{2}(1-z) + \int_0^z \log \Gamma(x) dx. \quad (14.540)$$

This identity follows from an integration of Binet's integral representation [43] of $\log \Gamma(z)$. Thus we can write

$$\begin{aligned} \Delta \mathcal{L}^{\text{eff}} = & \frac{(eB)^2}{2\pi^2} \left\{ -\frac{1}{12} + \zeta'(-1) - \frac{M^2}{4eB} + \frac{3}{4} \left(\frac{M^2}{2eB} \right)^2 - \frac{M^2}{4eB} \log(2\pi) \right. \\ & \left. + \left[-\frac{1}{12} + \frac{M^2}{4eB} - \frac{1}{2} \left(\frac{M^2}{2eB} \right)^2 \right] \log \left(\frac{M^2}{2eB} \right) + \int_0^{M^2/2eB} dx \log \Gamma(x) \right\}. \quad (14.541) \end{aligned}$$

In the strong-field limit, the range of integration in the last term vanishes, so we can use the Taylor expansion [41, 44] of $\log \Gamma(x)$:

$$\log \Gamma(x) = -\log x - \gamma x + \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \zeta(n) x^n, \quad (14.542)$$

where $\zeta(n)$ is the usual Riemann ζ -function. This leads to :

$$\begin{aligned} \Delta \mathcal{L}^{\text{eff}} = & \frac{(eB)^2}{2\pi^2} \left\{ -\frac{1}{12} + \zeta'(-1) - \frac{M^2}{4eB} + \frac{3}{4} \left(\frac{M^2}{2eB} \right)^2 - \frac{M^2}{4eB} \log(2\pi) \right. \\ & + \left[-\frac{1}{12} + \frac{M^2}{4eB} - \frac{1}{2} \left(\frac{M^2}{2eB} \right)^2 \right] \log \left(\frac{M^2}{2eB} \right) - \frac{\gamma}{2} \left(\frac{M^2}{2eB} \right)^2 \\ & \left. + \frac{M^2}{2eB} \left[1 - \log \left(\frac{M^2}{2eB} \right) \right] + \sum_{n=2}^{\infty} \frac{(-1)^n \zeta(n)}{n(n+1)} \left(\frac{M^2}{2eB} \right)^{n+1} \right\}. \quad (14.543) \end{aligned}$$

The leading behavior in the strong-field limit is

$$\Delta\mathcal{L}^{\text{eff}} = \frac{(eB)^2}{24\pi^2} \log \frac{2eB}{M^2} + \dots, \quad (14.544)$$

in agreement with Weisskopf's result (14.520).

Charged Scalar Field in a Constant Magnetic Field

For a charged scalar field obeying the Klein-Gordon equation there is no spin sum and the ζ -function (14.531) becomes

$$\begin{aligned} \zeta_{\text{KG}}(s) &= \frac{eB}{2\pi} \sum_{n=0}^{\infty} \int \frac{d^2k_{\perp}}{(2\pi)^2} \left[\frac{M^2 + k_{\perp}^2 + eB(2n+1)}{\mu^2} \right]^{-s} \\ &= \frac{(eB)^2}{4\pi^2} \left[\left(\frac{\mu^2}{2eB} \right)^s \frac{1}{(s-1)} \zeta_H \left(s-1, \frac{1}{2} + \frac{M^2}{2eB} \right) \right]. \end{aligned} \quad (14.545)$$

Setting again $\mu = m$, and subtracting the zero field contribution $3m^4/64\pi^2$, we obtain

$$\begin{aligned} \Delta\mathcal{L}_{\text{KG}}^{\text{eff}} &= -\frac{(eB)^2}{4\pi^2} \left\{ \zeta'_H \left(-1, \frac{1}{2} + \frac{M^2}{2eB} \right) + \frac{3}{4} \left(\frac{M^2}{2eB} \right)^2 \right. \\ &\quad \left. + \left[1 + \log \left(\frac{M^2}{2eB} \right) \right] \zeta_H \left(-1, \frac{1}{2} + \frac{M^2}{2eB} \right) \right\}. \end{aligned} \quad (14.546)$$

In the Bose case, the equivalence with the previous result is shown with the help of the integral representations of the Hurwitz ζ -function [compare (14.538)]

$$\begin{aligned} \zeta_H(s, 1/2 + z) &= \frac{1}{\Gamma(s)} \int_0^{\infty} e^{-zt} t^{s-1} \frac{e^{-t/2}}{1 - e^{-t}} dt, \quad \text{Re}(s) > 1, \text{Re}(z) > -\frac{1}{2} \\ &= \frac{z^{1-s}}{s-1} - \frac{sz^{-1-s}}{24} + \frac{2^{s-1}}{\Gamma(s)} \int_0^{\infty} \frac{dt}{t^{1-s}} e^{-2zt} \left(\frac{1}{\sinh t} - \frac{1}{t} + \frac{t}{6} \right). \end{aligned} \quad (14.547)$$

The second expression is valid for $\text{Re}(s) > -2$, where the subtracted integral converges. We can therefore use it to find the derivative at $s = -1$ required in Eq. (14.546):

$$\begin{aligned} \zeta'_H(-1, 1/2 + z) &= -\frac{1}{24}(1 + \log z) - \frac{z^2}{4} + \frac{z^2}{2} \log z \\ &\quad - \frac{1}{4} \int_0^{\infty} \frac{dt}{t^2} e^{-2zt} \left(\frac{1}{\sinh t} - \frac{1}{t} + \frac{t}{6} \right). \end{aligned} \quad (14.548)$$

Inserting this into (14.546), we recover exactly the previous result (14.496).

In order to find a strong-field expansion of $\Delta\mathcal{L}_{\text{KG}}^{\text{eff}}$ we use the following relation between the Hurwitz ζ -function and the log of the Γ -function [41, 43]:

$$\zeta'_H(-1, 1/2 + z) = -\frac{1}{2} \zeta'(-1) - \frac{z}{2} \log 2\pi - \frac{\log 2}{24} + \frac{z^2}{2} + \int_0^z dz \log \Gamma(x + \tfrac{1}{2}), \quad (14.549)$$

where we have used the formula [42, 45, 46]

$$\int_0^{\frac{1}{2}} \log \Gamma(x) dx = \frac{5}{24} \log 2 + \frac{1}{4} \log \pi + \frac{1}{8} - \frac{3}{2} \zeta'(-1) . \quad (14.550)$$

Then we expand

$$\log \Gamma(x + 1/2) = \frac{1}{2} \log \pi - (\gamma + 2 \log 2) x + \sum_{n=2}^{\infty} \frac{(-1)^{n-1}(1-2^n)}{n} \zeta(n) x^n, \quad (14.551)$$

and obtain the strong-field expansion

$$\begin{aligned} \Delta \mathcal{L}_{\text{KG}}^{\text{eff}} = & -\frac{(eB)^2}{4\pi^2} \left\{ \frac{5}{4} \left(\frac{M^2}{2eB} \right)^2 + \left[\frac{1}{24} - \frac{1}{2} \left(\frac{M^2}{2eB} \right)^2 \right] \left[1 + \log \left(\frac{M^2}{2eB} \right) \right] \right. \\ & - \frac{1}{2} \zeta'(-1) - \frac{\log 2}{24} - \frac{M^2}{4eB} \log 2 - \frac{1}{2} \left(\frac{M^2}{2eB} \right)^2 (\gamma + 2 \log 2) \\ & \left. + \sum_{n=2}^{\infty} \frac{(-1)^{n-1}(1-2^n)\zeta(n)}{n(n+1)} \left(\frac{M^2}{2eB} \right)^{n+1} \right\}, \quad (14.552) \end{aligned}$$

with the leading behavior

$$\Delta \mathcal{L}_{\text{KG}}^{\text{eff}} = \frac{(eB)^2}{96\pi^2} \log \frac{2eB}{M^2} + \dots \quad (14.553)$$

Appendix 14A Propagator of the Bilocal Pair Field

Consider the Bethe-Salpeter equation (14.300) with a potential λV instead of V

$$\Gamma = -i\lambda V G_0 G_0 \Gamma. \quad (14A.1)$$

Take this as an eigenvalue problem in λ at fixed energy-momentum $q = (q^0, \mathbf{q}) = (E, \mathbf{q})$ of the bound states. Let $\Gamma_n(P|q)$ be all solutions, with eigenvalues $\lambda_n(q)$. Then the convenient normalization of Γ_n is:

$$-i \int \frac{d^4 P}{(2\pi)^4} \Gamma_n^\dagger(P|q) G_0 \left(\frac{q}{2} + P \right) G_0 \left(\frac{q}{2} - P \right) \Gamma_{n'}(P|q) = \delta_{nn'}. \quad (14A.2)$$

If all solutions are known, there is a corresponding completeness relation (the sum may comprise an integral over a continuous part of the spectrum)

$$-i \sum_n G_0 \left(\frac{q}{2} + P \right) G_0 \left(\frac{q}{2} - P \right) \Gamma_n(P|q) \Gamma_n^\dagger(P'|q) = (2\pi)^4 \delta^{(4)}(P - P'). \quad (14A.3)$$

This completeness relation makes the object given in (14.315) the correct propagator of Δ . In order to see this, write the free Δ -action $\mathcal{A}_2[\Delta^\dagger \Delta]$ as

$$\mathcal{A}_2 = \frac{1}{2} \Delta^\dagger \left(\frac{1}{\lambda V} + i G_0 \times G_0 \right) \Delta \quad (14A.4)$$

where we have used λV instead of V . The propagator of Δ would have to satisfy

$$\left(\frac{1}{\lambda V} + iG_0 \times G_0\right) \bar{\Delta} \Delta^\dagger = i. \quad (14A.5)$$

Indeed, by performing a short calculation, we can verify that this equation is fulfilled by the spectral expansion (14.315). We merely have to use the fact that Γ_n and λ_n are eigenfunctions and eigenvalues of Eq. (14A.1), and find that that

$$\begin{aligned} & \left(\frac{1}{\lambda V} + iG_0 \times G_0\right) \times \left\{ -i\lambda \sum_n \frac{\Gamma_n \Gamma_n^\dagger}{\lambda - \lambda_n(q)} \right\} \\ &= -i\lambda \sum_n \frac{\frac{1}{\lambda V} \Gamma_n \Gamma_n^\dagger + iG_0 \times G_0 \Gamma_n \Gamma_n^\dagger}{\lambda - \lambda_n(q)} \\ &= i\lambda \sum_n \frac{-\frac{\lambda_n(q)}{\lambda} + 1}{\lambda - \lambda_n(q)} (-iG_0 \times G_0 \Gamma_n \Gamma_n^\dagger) \\ &= i \left(-i \sum_i G_0 \times G_0 \Gamma_i \Gamma_i^\dagger \right) = i. \end{aligned} \quad (14A.6)$$

Note that the expansion of the spectral representation of the propagator in powers of λ

$$\bar{\Delta} \Delta^\dagger = -i\lambda \sum_n \frac{\Gamma_n \Gamma_n^\dagger}{\lambda - \lambda_n(q)} = i \sum_k \left(\sum_n \left(\frac{\lambda}{\lambda_n(q)} \right)^k \Gamma_n \Gamma_n^\dagger \right) \quad (14A.7)$$

corresponds to the graphical sum over one, two, three, etc. exchanges of the potential λV . For $n = 1$ this is immediately obvious since (14A.1) implies that

$$i \sum_n \frac{\lambda}{\lambda_n(q)} \Gamma_n \Gamma_n^\dagger = \sum_n \frac{\lambda}{\lambda_n(q)} \lambda_n(q) V G_0 \times G_0 \Gamma_n \Gamma_n^\dagger = i\lambda V. \quad (14A.8)$$

For $n = 2$ one can rewrite, using the orthogonality relation,

$$i \sum_n \left(\frac{\lambda}{\lambda_n(q)} \right)^2 \Gamma_n \Gamma_n^\dagger = \sum_{nn'} \frac{\lambda}{\lambda_n(q)} \Gamma_n \Gamma_n^\dagger G_0 \times G_0 \Gamma_{n'} \Gamma_{n'}^\dagger \frac{\lambda}{\lambda_{n'}(q)} = \lambda V G_0 \times G_0 \lambda V. \quad (14A.9)$$

This displays the exchange of two λV terms with particles propagating in between. The same procedure applies at any order in λ . Thus the propagator has the expansion

$$\bar{\Delta} \Delta^\dagger = i\lambda V - i\lambda V G_0 \times G_0 i\lambda V + \dots \quad (14A.10)$$

If the potential is instantaneous, the intermediate $\int dP_0/2\pi$ can be performed replacing

$$G_0 \times G_0 \rightarrow i \frac{1}{E - E_0(\mathbf{P}|q)} \quad (14A.11)$$

where

$$E_0(\mathbf{P}|q) = \xi \left(\frac{\mathbf{q}}{2} + \mathbf{P} \right) + \xi \left(\frac{\mathbf{q}}{2} - \mathbf{P} \right)$$

is the free particle energy which may be considered as the eigenvalue of an operator H_0 . In this case the expansion (14A.10) reads

$$\bar{\Delta} \Delta^\dagger = i \left(\lambda V + \lambda V \frac{1}{E - H_0} \lambda V + \dots \right) = i\lambda V \frac{E - H_0}{E - H_0 - \lambda V}. \quad (14A.12)$$

We see it related to the resolvent of the complete Hamiltonian as

$$\overline{\Delta} \Delta^\dagger = i\lambda V(R\lambda V + 1) \quad (14A.13)$$

where

$$R \equiv \frac{1}{E - H_0 - \lambda V} = \sum_n \frac{\psi_n \psi_n^\dagger}{E - E_n} \quad (14A.14)$$

with ψ_n being the Schrödinger amplitudes in standard normalization. We can now easily determine the normalization factor N in the connection between Γ_n and the Schrödinger amplitude ψ_n . Eq. (29A.3) gives in the instantaneous case

$$\int \frac{d^3 P}{(2\pi)^3} \Gamma_n^\dagger(\mathbf{P}|q) \frac{1}{E - H_0} \Gamma_{n'}(\mathbf{P}|q) = \delta_{nn'}. \quad (14A.15)$$

Inserting ψ from (14.306) renders

$$\frac{1}{N^2} \int \frac{d^3 P}{(2\pi)^3} \psi_n^\dagger(\mathbf{P}|q) (E - H_0) \psi_{n'}(\mathbf{P}|q) = \delta_{nn'}. \quad (14A.16)$$

Using finally the Schrödinger equation

$$(E - H_0)\psi = \lambda V\psi, \quad (14A.17)$$

we find

$$\frac{1}{N^2} \int \frac{d^3 P}{(2\pi)^3} \psi_n^\dagger(\mathbf{P}|q) \lambda V \psi_{n'}(\mathbf{P}|q) = \delta_{nn'}. \quad (14A.18)$$

For the wave functions $\psi_n(\mathbf{P}|q)$ in standard normalization, the integral is equal to the energy differential

$$\lambda \frac{dE}{d\lambda}.$$

For a typical calculation of a resolvent, the reader is referred to Schwinger's treatment [47] of the Coulomb problem. His result may directly be used for a propagator of electron hole pairs bound to excitons.

Appendix 14B Fluctuations around the Composite Field

Here we show that the quantum mechanical fluctuations around the *classical* equations of motion (14.237) are quite simple to calculate. The exponent of (14.232) is extremized by the field

$$\varphi(x) = \int dy V(x, y) \psi^\dagger(y) \psi(y). \quad (14B.1)$$

Similarly, the extremum of the exponent of (14.278) yields

$$\Delta(x, y) = V(x - y) \psi(x) \psi(y). \quad (14B.2)$$

For this let us compare the Green functions of $\varphi(x)$ or $\Delta(x, y)$ with those of the composite operators on the right-hand side of Eqs. (14B.1) or (14B.2). The Green functions of $\varphi(x)$ or $\Delta(x, y)$ are generated by adding to the final actions (14.242) or (14.284) external currents $\int dx \varphi(x) I(x)$ or

$1/2 \int dx dy (\Delta(y, x) I^\dagger(x, y) + \text{h.c.})$, respectively, and by forming functional derivatives $\delta/\delta I$. The Green functions of the composite operators, on the other hand, are obtained by adding

$$\int dx \left(\int dy V(x, y) \psi^\dagger(y) \psi(y) \right) K(x) \quad (14B.3)$$

$$\frac{1}{2} \int dx \int dy V(x - y) \psi(x) \psi(y) K^\dagger(x, y) + \text{h.c.} \quad (14B.4)$$

to the original actions (14.235) or (14.278), respectively, and by forming functional derivatives $\delta/\delta K$. It is obvious that the sources $K(x)$ and $K(x, y)$ can be included in the final actions (14.242) and (14.284) by simply replacing

$$\varphi(x) \rightarrow \varphi'(x) = \varphi(x) - \int dx' K(x') V(x', x), \quad (14B.5)$$

or

$$\Delta(x, y) \rightarrow \Delta'(x, y) = \Delta(x, y) - K(x, y). \quad (14B.6)$$

If one now shifts the functional integrations to these new translated variables and drops the irrelevant superscript “prime”, the actions can be rewritten as

$$\begin{aligned} \mathcal{A}[\varphi] = & \pm i \text{Tr} \log(iG_\varphi^{-1}) + \frac{1}{2} \int dx dx' \varphi(x) V^{-1}(x, x') \varphi(x') + i \int dx dx' \eta^\dagger(x) G_\varphi(x, x') \eta(x) \\ & + \int dx \varphi(x) [I(x) + K(x)] + \frac{1}{2} \int dx dx' K(x) V(x, x') K(x'), \end{aligned} \quad (14B.7)$$

or

$$\begin{aligned} \mathcal{A}[\Delta] = & \pm \frac{i}{2} \text{Tr} \log(i\mathbf{G}_\Delta^{-1}) + \frac{1}{2} \int dx dx' |\Delta(x, x')|^2 \frac{1}{V(x, x')} \\ & + \frac{i}{2} \int dx dx' j^\dagger(x) \mathbf{G}_\Delta(x, x') \frac{1}{V(x, x')} \\ & + \frac{1}{2} \int dx dx' \{ \Delta(y, x) [I^\dagger(x, y) + K^\dagger(x, y)] + \text{h.c.} \} \\ & + \frac{1}{2} \int dx dx' |K(x, x')|^2 V(x, x'). \end{aligned} \quad (14B.8)$$

In this form the actions display clearly the fact that derivatives with respect to the sources K or I coincide exactly, except for all possible insertions of the direct interaction V . For example, the propagators of the plasmon field $\varphi(x)$ and of the composite operator $\int dy V(x, y) \psi^\dagger(y) \psi(y)$ are related by

$$\begin{aligned} \overline{\varphi(x) \varphi(x')} &= -\frac{\delta^{(2)} Z}{\delta I(x) \delta I(x')} = V^{-1}(x, x') - \frac{\delta^{(2)} Z}{\delta K(x) \delta K(x')} \\ &= V^{-1}(x, x') + \langle 0 | \left(\int dy V(x, y) \psi^\dagger(y) \psi(y) \right) \left(\int dy' V(x', y') \psi^\dagger(y') \psi(y') \right) | 0 \rangle, \end{aligned} \quad (14B.9)$$

in agreement with (14.238). Similarly, one finds for the pair fields:

$$\begin{aligned} \overline{\Delta(x, x') \Delta^\dagger(y, y')} &= \delta(x - y) \delta(x' - y') iV(x - x') \\ &+ \langle 0 | (V(x', x) \psi(x') \psi(x)) (V(y', y) \psi^\dagger(y) \psi^\dagger(y')) | 0 \rangle. \end{aligned} \quad (14B.10)$$

Note that the latter relation is manifestly displayed in the representation (14A.10) of the propagator Δ . Since

$$\overline{\Delta \Delta}^\dagger = iV G^{(4)} V, \quad (14B.11)$$

one has from (14B.10)

$$\langle 0|V(\psi\psi)(\psi^\dagger\psi^\dagger V)|0\rangle = V G^{(4)}V, \quad (14B.12)$$

which is correct remembering that $G^{(4)}$ is the full four-point Green function. In the equal-time situation relevant for an instantaneous potential, $G^{(4)}$ is replaced by the resolvent R .

Appendix 14C Two-Loop Heisenberg-Euler Effective Action

The next correction to the Heisenberg-Euler Lagrangian density (14.489) is [38, 48]

$$\begin{aligned} \Delta^{(2)}\mathcal{L}^{\text{eff}} = & -\frac{ie^2}{128\pi^4} \int_0^\infty d\tau \int_0^\infty d\tau' \frac{e^4\beta^2\varepsilon^2}{\sin e\beta\tau \sin e\beta\tau' \sinh e\varepsilon\tau \sinh e\varepsilon\tau'} e^{-i(M^2-i\eta)(\tau+\tau')} \\ & \times \left\{ 4M^2 [S(\tau)S(\tau') + P(\tau)P(\tau')] I_0 - iI \right\}, \end{aligned} \quad (14C.1)$$

where

$$S(\tau) \equiv \cos e\beta\tau \cosh e\varepsilon\tau, \quad P(\tau) \equiv \sin e\beta\tau \sinh e\varepsilon\tau,$$

and

$$\begin{aligned} I_0 &\equiv \frac{1}{b-a} \log \frac{b}{a}, & I &\equiv \frac{(q-p)}{(b-a)^2} \log \frac{b}{a} - \frac{aq-bp}{ba(b-a)}, \\ a &\equiv e\beta(\cot e\beta\tau + \cot e\beta\tau'), & b &\equiv e\varepsilon(\coth e\varepsilon\tau + \coth e\varepsilon\tau'), \\ p &\equiv \frac{2e^2\beta^2 \cosh e\varepsilon(\tau-\tau')}{\sin e\beta\tau \sin(e\beta\tau')}, & q &\equiv \frac{2e^2\varepsilon^2 \cos e\beta(\tau-\tau')}{\sinh e\varepsilon\tau \sinh e\varepsilon\tau'}. \end{aligned} \quad (14C.2)$$

This expression contains divergences which require renormalization. First, there is a subtraction of an infinity to make $\Delta^{(2)}\mathcal{L}^{\text{eff}}$ vanish for zero fields. Then there are both charge and wave function renormalizations, just as for the one-loop effective Lagrangian, which involves identifying a divergent term in $\Delta^{(2)}\mathcal{L}^{\text{eff}}$ of the form of the zero-loop Maxwell Lagrangian. This is done simply by expanding the integrand to quadratic order in the fields β and ε . This divergence can be absorbed by redefining the electric charge and the fields as

$$e_R = e Z_3^{1/2}, \quad \mathbf{B}_R = \mathbf{B} Z_3^{-1/2}, \quad \mathbf{E}_R = \mathbf{E} Z_3^{-1/2} \quad (14C.3)$$

where Z_3 is some divergent normalization constant, which was given by (14.435) in the previous result (14.491). The invariants β and ε are renormalized accordingly: $\beta_R = \beta Z_3^{-1/2}$, $\varepsilon_R = \varepsilon Z_3^{-1/2}$.

Then we re-express $\Delta^{(2)}\mathcal{L}^{\text{eff}}$ in terms of the renormalized charges and fields. Finally, we have to renormalize the mass:

$$\begin{aligned} m_R^2 &= m_0^2 + \delta M^2, \\ \Delta^{(1)}\mathcal{L}_R^{\text{eff}}(m_R^2) &= \mathcal{L}_R^{(1)}(m_0^2) + \delta M^2 \frac{\partial \mathcal{L}_R^{(1)}(m_0^2)}{\partial m_0^2}. \end{aligned} \quad (14C.4)$$

The second term in (14C.4) is of the order α^2 , since δM^2 and $\Delta^{(1)}\mathcal{L}_R^{\text{eff}}$ are both of order α . For details of removing the divergencies, see the original papers in Refs. [48]. The final answer for the renormalized two loop effective Lagrangian is

$$\begin{aligned} \Delta^{(2)}\mathcal{L}_R^{\text{eff}} = & -\frac{ie^2}{64\pi^4} \int_0^\infty d\tau \int_0^\tau d\tau' \left[K(\tau, \tau') - \frac{K_0(\tau)}{\tau'} \right] \\ & -\frac{ie^2}{64\pi^4} \int_0^\infty d\tau K_0(\tau) \left[\log(iM^2\tau) + \gamma - \frac{5}{6} \right] \end{aligned} \quad (14C.5)$$

where $\gamma \approx 0.577\dots$ is Euler's constant, and the functions $K(\tau, \tau')$ and $K_0(\tau)$ are

$$\begin{aligned} K(\tau, \tau') &= e^{-iM^2(\tau+\tau')} \left\{ \frac{(e\beta)^2(e\varepsilon)^2}{P(\tau)P(\tau')} [4M^2(S(\tau)S(\tau') + P(\tau)P(\tau'))I_0 - iI] \right. \\ &\quad \left. - \frac{1}{\tau\tau'(\tau+\tau')} \left[4M^2 - \frac{2i}{\tau+\tau'} + \frac{e^2(\beta^2 - \varepsilon^2)}{3} \left(2M^2(\tau\tau' - 2\tau^2 - 2\tau'^2) - \frac{5i\tau\tau'}{\tau+\tau'} \right) \right] \right\} \\ K_0(\tau) &= e^{-iM^2\tau} \left(4M^2 + i\frac{\partial}{\partial\tau} \right) \frac{1}{\tau^2} \left[\frac{e\beta\tau}{\tan e\beta\tau} \frac{e\varepsilon\tau}{\tanh e\varepsilon\tau} - 1 + \frac{e^2(\beta^2 - \varepsilon^2)\tau^2}{3} \right]. \end{aligned} \quad (14C.6)$$

The fields in this expression can be replaced by the renormalized fields, and everything is finite. The lowest contribution is of the fourth power in the fields and reads

$$\Delta^{(2)}\mathcal{L}^{\text{eff}} = \frac{e^6}{64\pi^4 m^4} \left[\frac{16}{81}(\beta^2 - \varepsilon^2)^2 + \frac{263}{162}(\beta\varepsilon)^2 \right] + \dots, \quad (14C.7)$$

which has been added to the one-loop result in Eq. (14.499). In the limit of strong magnetic fields it yields

$$\Delta^{(2)}\mathcal{L}^{\text{eff}} = \frac{e^4\beta^2}{128\pi^4} \left[\log \left(\frac{e\beta}{\pi M^2} \right) + \text{constant} \right] + \dots. \quad (14C.8)$$

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*It is best to do things systematically,
since we are only human, and disorder is our worst enemy.*
HESIOD (~800 BC)

15

Systematic Graphical Construction of Feynman Diagrams and Their Multiplicities

In Section 13.4 we have calculated the generating functional for the connected Green functions $W[j]$ by solving the functional differential equation (13.29) with respect to the source j of the scalar field. Alternatively, $W[j]$ may also be considered as a functional of the free propagator G_0 that was used to calculate the Feynman diagrams. As such it obeys a functional differential equation with respect to G_0 which can be turned into a recursion relation. This may also be solved order by order in the coupling constant to find all connected vacuum diagrams with their proper multiplicities. Let us apply this procedure here to $W[0]$ which contains all connected vacuum diagrams, first for a pure ϕ^4 -theory, subsequently for a theory with two scalar fields ϕ and A coupled to each other by a Yukawa-like interaction $\phi^2 A$. From this sum over all connected vacuum diagrams, all Feynman diagrams with external lines are obtained from functional derivatives with respect to the free correlation function G_0 .

The recursive graphical construction will be automatized by computer algebra with the help of a unique matrix notation for the Feynman diagrams. The methods developed in this chapter have been set up in the 1980s [1, 2], but for many years they have only been solved to low orders in the coupling strength. To all orders, the solution has been restricted to rather trivial zero-dimensional quantum field theories, in particular the anharmonic integral. Here we present a nontrivial extension of that work. It consists in an efficient graphical algorithm [3] for solving the functional differential equation for $W[0]$ as a functional of G_0 . We shall do this first for a multicomponent scalar ϕ^4 -theory, then also for a theory with two scalar fields ϕ and A with an interaction $\phi^2 A$.

In a second step, the connected vacuum diagrams are used to derive all connected diagrams with external lines. For that we make use of functional derivatives of the connected vacuum diagrams with respect to G_0 . This operation will be represented graphically by cutting lines. Finally, we automatize our construction method by computer algebra. For this we shall develop a unique matrix notation for Feynman diagrams.

15.1 Generalized Scalar ϕ^4 -Theory

The following treatment will involve somewhat lengthy equations such that it is useful to introduce a shorter notation for the symbols used. For the free propagator $G_0(x_1, x_2)$ we shall employ a functional matrix notation G_{12} . The fully interacting two-point function $G(x_1, x_2)$ will be denoted by $\mathbf{G}_{12}$. The D -dimensional integral $\int d^D x_1$ will simply be written as $\int_1$. We shall further work in euclidean spacetime to avoid factors of i . The scalar field ϕ is allowed to have N components, and the thermal fluctuations are controlled by a euclidean action which plays the role of an energy functional:

$$E[\phi] = \frac{1}{2} \int_{12} G_{12}^{-1} \phi_1 \phi_2 + \frac{g}{4!} \int_{1234} V_{1234} \phi_1 \phi_2 \phi_3 \phi_4, \quad (15.1)$$

with some coupling constant g . The functional matrix G_{12}^{-1} is the inverse of the free propagator G_{12} . Both contain, in addition, a Kronecker δ for the indices of N field components ϕ_a ($a = 1, \dots, N$), which we suppress. Throughout the manipulations to follow, the functional matrix G_{12} will be considered as a completely general symmetric nonsingular functional matrix, such that G_{12}^{-1} exists. Only at the end shall we specify G_{12} , identifying it with the free propagator, i.e., for the inverse

$$G_{12}^{-1} \rightarrow G_{a_1 a_2}^{-1}(x_1, x_2) = \delta_{a_1 a_2} \left(-\partial_{x_1}^2 + m^2 \right) \delta(x_1 - x_2). \quad (15.2)$$

In applications to critical phenomena to be discussed in Chapter 20, the mass m^2 will be proportional to the temperature distance $T - T_c$ from the critical point.

The interaction will likewise be considered as a completely general symmetric function of four arguments, $gV(x_1, x_2, x_3, x_4)$, where g parametrizes the coupling strength and serves as an expansion parameter. In the short-hand notation, it is a symmetric functional tensor of rank four, and will eventually be identified with the true interaction

$$\begin{aligned} V_{1234} &\rightarrow V_{a_1 a_2 a_3 a_4}(x_1, x_2, x_3, x_4) \\ &= \frac{1}{3} \{ \delta_{a_1 a_2} \delta_{a_3 a_4} + \delta_{a_1 a_3} \delta_{a_2 a_4} + \delta_{a_1 a_4} \delta_{a_2 a_3} \} \delta(x_1 - x_2) \delta(x_1 - x_3) \delta(x_1 - x_4). \end{aligned} \quad (15.3)$$

By using natural units, in which the Boltzmann constant k_B times the temperature T equals unity, the partition function is determined as a functional integral over the Boltzmann weight $e^{-E[\phi]}$

$$Z = \int \mathcal{D}\phi e^{-E[\phi]}. \quad (15.4)$$

It may be evaluated perturbatively as a power series in the coupling constant g . From this we obtain the negative free energy $W = \ln Z$ as an expansion

$$W = \sum_{p=0}^{\infty} \frac{1}{p!} \left(\frac{-g}{4!} \right)^p W^{(p)}. \quad (15.5)$$

The coefficients $W^{(p)}$ may be displayed as connected vacuum diagrams constructed from lines and vertices. Each line represents a free correlation function

$$1 \text{ --- } 2 \equiv G_{12}, \quad (15.6)$$

whose functional inverse G^{-1} appears in the energy functional (15.1), defined by

$$\int_2 G_{12} G_{23}^{-1} = \delta_{13}. \quad (15.7)$$

The vertices represent an integral over the interaction

$$\times \equiv \int_{1234} V_{1234}. \quad (15.8)$$

To construct in perturbation theory all connected vacuum diagrams contributing to $W^{(p)}$ one connects p vertices with $4p$ legs in all possible ways according to Feynman's rules. This yields an increasing number of Feynman diagrams, each with a certain multiplicity which follows from combinatorics. In total there are $4!^p p!$ ways of ordering the $4p$ legs of the p -vertices. This number is reduced by permutations of the legs and the vertices which leave a vacuum diagram invariant. Denoting the number of self-, double-, triple-, and fourfold connections with S, D, T, F , there are $2!^S, 2!^D, 3!^T, 4!^F$ leg permutations. An additional reduction arises from the number N of identical vertex permutations where the vertices remain attached to the lines emerging from them in the same way as before. The resulting multiplicity of a connected vacuum diagram in the ϕ^4 -theory is therefore given by the formula [4]

$$M_{\phi^4}^{E=0} = \frac{4!^p p!}{2!^{S+D} 3!^T 4!^F N}. \quad (15.9)$$

The superscript E records that the number of external legs of the connected vacuum diagrams is zero. The diagrammatic representation of the coefficients $W^{(p)}$ in the expansion (15.5) of the negative free energy W is displayed in Table 15.1 on page 1043 up to five loops [5].

In higher orders, the factorially increasing number of diagrams makes it more and more difficult to construct all topologically different diagrams and to count their multiplicities. In particular, it becomes quite hard to identify by inspection the number N of identical vertex permutations. This identification problem will be solved by introducing a unique matrix notation for the graphs, to be explained in detail below in Section 15.10.

In the following, we shall generate iteratively all connected vacuum diagrams. We start in Section 15.2 by identifying graphical operations associated with functional derivatives with respect to the inverse propagator G^{-1} , or the propagator G . In Section 15.3 we show that these operations can be applied to the one-loop contribution of the free partition function to generate all perturbative contributions to the partition function Z . In Sections 15.4 and 15.8 we derive a nonlinear functional differential equation for the negative free energy W , whose graphical solutions in Sections 15.5 and 15.9 yield all connected vacuum diagrams order by order in the coupling strength.

15.2 Basic Graphical Operations

Each Feynman diagram is composed of integrals over products of free correlation functions G and may thus be considered as a functional of the inverse propagator G^{-1} . The connected vacuum diagrams satisfy a certain functional differential equation, from which they will be constructed recursively. This will be done by a graphical procedure, for which we set up the necessary graphical rules in this subsection. First we observe that functional derivatives with respect to the inverse propagator G^{-1} or to the free propagator G correspond to the graphical prescriptions of cutting or of removing a single line of a diagram in all possible ways, respectively.

15.2.1 Cutting Lines

Since ϕ is a real scalar field, the inverse propagator G^{-1} is a symmetric functional matrix. This property has to be taken into account when performing functional derivatives with respect to the inverse propagator G^{-1} . The basic rule is

$$\frac{\delta G_{12}^{-1}}{\delta G_{34}^{-1}} = \frac{1}{2} \{ \delta_{13} \delta_{42} + \delta_{14} \delta_{32} \} . \quad (15.10)$$

From the identity (15.7) and the functional chain rule, we find the effect of this derivative on the free propagator

$$-2 \frac{\delta G_{12}}{\delta G_{34}^{-1}} = G_{13} G_{42} + G_{14} G_{32} . \quad (15.11)$$

This has the graphical representation

$$-2 \frac{\delta}{\delta G_{34}^{-1}} \text{ 1 — 2 } = \text{ 1 — 3 4 — 2 } + \text{ 1 — 4 3 — 2 } . \quad (15.12)$$

Thus differentiating a propagator with respect to the inverse propagator G^{-1} amounts to cutting the associated line into two pieces. The differentiation rule (15.10) ensures that the spatial indices of the inverse propagator are symmetrically attached to the newly created line ends in two possible ways. When differentiating a general Feynman integral with respect to G^{-1} , the product rule of functional differentiation leads to a sum of diagrams in which each line is cut once.

With this graphical operation, the product of two fields can be rewritten as a derivative of the energy functional with respect to the inverse propagator

$$\phi_1 \phi_2 = 2 \frac{\delta E[\phi]}{\delta G_{12}^{-1}} , \quad (15.13)$$

as follows directly from (15.1) and (15.10). Applying the substitution rule (15.13) to the functional integral for the fully interacting two-point function

$$\mathbf{G}_{12} = \frac{1}{Z} \int \mathcal{D}\phi \phi_1 \phi_2 e^{-E[\phi]} , \quad (15.14)$$

we obtain the fundamental identity

$$\mathbf{G}_{12} = -2 \frac{\delta W}{\delta G_{12}^{-1}}. \quad (15.15)$$

Thus, by cutting a line of the connected vacuum diagrams in all possible ways, we obtain all diagrams of the fully interacting two-point function. Analytically, this has a Taylor series expansion in powers of the coupling constant g similar to (15.5)

$$\mathbf{G}_{12} = \sum_{p=0}^{\infty} \frac{1}{p!} \left(\frac{-g}{4!} \right)^p \mathbf{G}_{12}^{(p)} \quad (15.16)$$

with coefficients

$$\mathbf{G}_{12}^{(p)} = -2 \frac{\delta W^{(p)}}{\delta G_{12}^{-1}}. \quad (15.17)$$

The cutting prescription (15.15) converts the vacuum diagrams of p th order in the coefficients $W^{(p)}$ in Table 15.1 on page 1043 to the corresponding ones in the coefficients $\mathbf{G}_{12}^{(p)}$ of the two-point function. The results are shown in Table 15.2 on page 1044 up to four loops. The numbering of diagrams used in Table 15.2 reveals from which connected vacuum diagrams they are obtained by cutting a line.

For instance, the diagrams labeled by #15.1-#15.5 in Table 15.2, together with their multiplicities, follow from the connected vacuum diagrams labeled by #15 in Table 15.1. We observe that the multiplicity of a diagram of a two-point function obeys a formula similar to (15.9):

$$M_{\phi^4}^{E=2} = \frac{4!^p p! 2!}{2!^{S+D} 3!^T N}. \quad (15.18)$$

In the numerator, the $4!^p p!$ permutations of the $4p$ legs of the p vertices are multiplied by a factor $2!$ for the permutations of the $E = 2$ end points of the two-point function. The number N in the denominator counts the identical permutations of both the p vertices and the two end points.

Performing a differentiation of the two-point function (15.14) with respect to the inverse propagator G^{-1} yields

$$-2 \frac{\delta \mathbf{G}_{12}}{\delta G_{34}^{-1}} = \mathbf{G}_{1234} - \mathbf{G}_{12} \mathbf{G}_{34}, \quad (15.19)$$

where $\mathbf{G}_{1234}$ denotes the fully interacting four-point function

$$\mathbf{G}_{1234} = \frac{1}{Z} \int \mathcal{D}\phi \phi_1 \phi_2 \phi_3 \phi_4 e^{-E[\phi]}. \quad (15.20)$$

The term $\mathbf{G}_{12} \mathbf{G}_{34}$ in (15.19) subtracts a certain set of disconnected diagrams from $\mathbf{G}_{1234}$. By subtracting *all* disconnected diagrams from $\mathbf{G}_{1234}$, we obtain the connected four-point function

$$\mathbf{G}_{1234}^c \equiv \mathbf{G}_{1234} - \mathbf{G}_{12} \mathbf{G}_{34} - \mathbf{G}_{13} \mathbf{G}_{24} - \mathbf{G}_{14} \mathbf{G}_{23} \quad (15.21)$$

in the form

$$\mathbf{G}_{1234}^c = -2 \frac{\delta \mathbf{G}_{12}}{\delta G_{34}^{-1}} - \mathbf{G}_{13} \mathbf{G}_{24} - \mathbf{G}_{14} \mathbf{G}_{23}. \quad (15.22)$$

The first term contains all diagrams obtained by cutting a line in the diagrams of the two-point-function $\mathbf{G}_{12}$. The second and third terms remove from these the disconnected diagrams. In this way we obtain the perturbative expansion

$$\mathbf{G}_{1234}^c = \sum_{p=1}^{\infty} \frac{1}{p!} \left(\frac{-g}{4!} \right)^p \mathbf{G}_{1234}^{c,(p)} \quad (15.23)$$

with coefficients

$$\mathbf{G}_{1234}^{c,(p)} = -2 \frac{\delta \mathbf{G}_{12}^{(p)}}{\delta G_{34}^{-1}} - \sum_{q=0}^p \binom{p}{q} \left(\mathbf{G}_{13}^{(p-q)} \mathbf{G}_{24}^{(q)} + \mathbf{G}_{14}^{(p-q)} \mathbf{G}_{23}^{(q)} \right). \quad (15.24)$$

They are listed diagrammatically in Table 15.3 on page 1045 up to three loops. As before in Table 15.2 on page 1044, the multiple numbering in Table 15.3 indicates the origin of each diagram of the connected four-point function. For instance, the diagrams #11.2.2, #11.4.3, #14.1.2, #14.3.3 in Table 15.3 on page 1045 (together with their multiplicities) stem from the diagrams #11.2, #11.4, #14.1, #14.3 in Table 15.2. on page 1044.

The multiplicity of each diagram of a connected four-point function obeys a formula similar to (15.18):

$$M_{\phi^4}^{E=4} = \frac{4!^p p! 4!}{2!^{S+D} 3!^T N}. \quad (15.25)$$

This multiplicity decomposes into equal parts if the spatial indices 1, 2, 3, 4 are assigned to the $E = 4$ end points of the connected four-point function, for instance:

$$62208 \quad \text{Diagram} \equiv 20736 \quad \text{Diagram}_1 + 20736 \quad \text{Diagram}_2 + 20736 \quad \text{Diagram}_3. \quad (15.26)$$

We now generalize the multiplicities (15.9), (15.18), and (15.25) of connected vacuum diagrams as well as of two- and four-point functions to those with an arbitrary even number E of end points. The multiplicities are [4]

$$M_{\phi^4}^E = \frac{4!^p p! E!}{2!^{S+D} 3!^T 4!^F N}, \quad (15.27)$$

where N counts the number of permutations of vertices and external lines which leave the diagram unchanged.

15.2.2 Removing Lines

Let us now study the graphical effect of functional derivatives with respect to the free propagator G . The basic differentiation rule (15.10) is

$$\frac{\delta G_{12}}{\delta G_{34}} = \frac{1}{2} \{ \delta_{13} \delta_{42} + \delta_{14} \delta_{32} \} . \quad (15.28)$$

We represent this operation graphically by extending the elements of Feynman diagrams by an open dot with two labeled line ends representing the delta function:

$$1 \text{ --- } 2 = \delta_{12} . \quad (15.29)$$

Thus we can write the differentiation (15.28) graphically as follows:

$$\frac{\delta}{\delta 3 \text{ --- } 4} \quad 1 \text{ --- } 2 = \frac{1}{2} \left\{ \begin{array}{c} 1 \text{ --- } 3 \quad 4 \text{ --- } 2 \\ + \quad 1 \text{ --- } 4 \quad 3 \text{ --- } 2 \end{array} \right\} . \quad (15.30)$$

Differentiating a line with respect to the free correlation function removes the line and leaves, in a symmetrized way, the spatial indices of the free correlation function on the vertices to which the line was connected.

The effect of this derivative is illustrated by displaying the diagrammatic effect of the operator

$$\hat{L} = \int_{12} G_{12} \frac{\delta}{\delta G_{12}} . \quad (15.31)$$

Applying $\hat{L}$ to a connected vacuum diagram in $W^{(p)}$, the functional derivative $\delta/\delta G_{12}$ removes successively each of its $2p$ lines. Subsequently, the removed lines are again reinserted, so that the connected vacuum diagrams $W^{(p)}$ are eigenfunctions of $\hat{L}$, whose eigenvalues $2p$ count the lines of the diagrams:

$$\hat{L} W^{(p)} = 2p W^{(p)} . \quad (15.32)$$

As an example, take the explicit first-order expression for the vacuum diagrams, i.e.

$$W^{(1)} = 3 \int_{1234} V_{1234} G_{12} G_{34} , \quad (15.33)$$

and apply the basic rule (15.28), leading to the desired eigenvalue 2.

15.3 Perturbation Theory for Vacuum Energy

For the calculation of the vacuum energy we use functional derivatives with respect to the inverse propagator G^{-1} in the energy functional (15.1) rather than with respect to the current j . This allows us to substitute the previous expression (14.53) for the partition function by

$$Z[0] \equiv e^{W[0]} = \exp \left\{ -\frac{g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right\} e^{W^{(0)}[0]} , \quad (15.34)$$

where the zeroth order of the negative free energy has the diagrammatic representation

$$W^{(0)}[0] = -\frac{1}{2} \text{Tr} \ln G^{-1} \equiv \frac{1}{2} \bigcirc . \quad (15.35)$$

Expanding again the exponential in a power series, we obtain

$$\begin{aligned} Z[0] = & \left\{ 1 + \frac{-g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right. \\ & \left. + \frac{1}{2} \left(\frac{-g}{6} \right)^2 \int_{12345678} V_{1234} V_{5678} \frac{\delta^4}{\delta G_{12}^{-1} \delta G_{34}^{-1} \delta G_{56}^{-1} \delta G_{78}^{-1}} + \dots \right\} e^{W^{(0)}[0]} . \end{aligned} \quad (15.36)$$

Thus we need only half as many functional derivatives as in the expansion derived with the help of the currents j . Taking into account (15.10), (15.11), and (14.23), we obtain

$$\frac{\delta W^{(0)}}{\delta G_{12}^{-1}} = -\frac{1}{2} G_{12} , \quad \frac{\delta^2 W^{(0)}}{\delta G_{12}^{-1} \delta G_{34}^{-1}} = \frac{1}{4} \{G_{13} G_{24} + G_{14} G_{23}\} , \quad (15.37)$$

such that the partition function Z becomes

$$\begin{aligned} Z[0] = & \left\{ 1 + \frac{-g}{4!} 3 \int_{1234} V_{1234} G_{12} G_{34} + \frac{1}{2} \left(\frac{-g}{4!} \right)^2 \int_{12345678} V_{1234} V_{5678} \right. \\ & \left. \times \left[9 G_{12} G_{34} G_{56} G_{78} + 24 G_{15} G_{26} G_{37} G_{48} + 72 G_{12} G_{35} G_{46} G_{78} \right] + \dots \right\} e^{W^{(0)}[0]} . \end{aligned} \quad (15.38)$$

This has the diagrammatic representation

$$\begin{aligned} Z[0] = & \left\{ 1 + \frac{-g}{4!} 3 \bigcirc \bigcirc \right. \\ & \left. + \frac{1}{2} \left(\frac{-g}{4!} \right)^2 \left[9 \bigcirc \bigcirc \bigcirc \bigcirc + 24 \bigcirc \bigcirc \bigcirc \bigcirc + 72 \bigcirc \bigcirc \bigcirc \bigcirc \right] + \dots \right\} e^{W^{(0)}[0]} . \end{aligned} \quad (15.39)$$

All diagrams in this expansion follow directly by successively cutting lines of the basic one-loop vacuum diagram (15.35) according to (15.36). By going to the logarithm of the partition function $Z[0]$, we find a diagrammatic expansion for the negative free energy $W[0]$

$$W[0] = \frac{1}{2} \bigcirc + \frac{-g}{4!} 3 \bigcirc \bigcirc + \frac{1}{2} \left(\frac{-g}{4!} \right)^2 \left\{ 24 \bigcirc \bigcirc \bigcirc \bigcirc + 72 \bigcirc \bigcirc \bigcirc \bigcirc \right\} + \dots , \quad (15.40)$$

which turns out to contain precisely all connected diagrams in (15.39) with the same multiplicities. In the next section we show that this diagrammatic expansion for the negative free energy can be derived more efficiently by solving a differential equation.

15.4 Functional Differential Equation for Free Energy in Scalar Theory

Regarding the partition function $Z[0]$ as a functional of the inverse propagator G^{-1} , we derive a functional differential equation for $Z[0]$. We start out with the trivial identity

$$\int \mathcal{D}\phi \frac{\delta}{\delta\phi_1} \left\{ \phi_2 e^{-E[\phi]} \right\} = 0, \quad (15.41)$$

which follows via functional integration by parts from the vanishing of the exponential at infinite fields. Taking into account the explicit form of the energy functional (15.1), we perform the functional derivative with respect to the field and obtain

$$\int \mathcal{D}\phi \left\{ \delta_{12} - \int_3 G_{13}^{-1} \phi_2 \phi_3 - \frac{g}{6} \int_{345} V_{1345} \phi_2 \phi_3 \phi_4 \phi_5 \right\} e^{-E[\phi]} = 0. \quad (15.42)$$

Applying the substitution rule (15.13), this equation can be expressed in terms of the partition function (15.4) and its derivatives with respect to the inverse propagator G^{-1} :

$$\delta_{12} Z + 2 \int_3 G_{13}^{-1} \frac{\delta Z}{\delta G_{23}^{-1}} = \frac{2}{3} g \int_{345} V_{1345} \frac{\delta^2 Z}{\delta G_{23}^{-1} \delta G_{45}^{-1}}. \quad (15.43)$$

Note that this linear functional differential equation for the partition function Z is, indeed, solved by (15.34) due to the commutation relation

$$\begin{aligned} & \exp \left\{ -\frac{g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right\} G_{56}^{-1} - G_{56}^{-1} \exp \left\{ -\frac{g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right\} \\ &= -\frac{g}{3} \int_{78} V_{5678} \frac{\delta}{\delta G_{78}^{-1}} \exp \left\{ -\frac{g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right\}. \end{aligned} \quad (15.44)$$

This follows directly from the canonical rule

$$\frac{\delta}{\delta G_{12}^{-1}} G_{34}^{-1} - G_{34}^{-1} \frac{\delta}{\delta G_{12}^{-1}} = \frac{1}{2} \{ \delta_{13} \delta_{24} + \delta_{14} \delta_{23} \}. \quad (15.45)$$

Going over from $Z = Z[0]$ to $W = \ln Z$, the linear functional differential equation (15.43) turns into a nonlinear equation:

$$\delta_{12} + 2 \int_3 G_{13}^{-1} \frac{\delta W}{\delta G_{23}^{-1}} = \frac{2}{3} g \int_{345} V_{1345} \left\{ \frac{\delta^2 W}{\delta G_{23}^{-1} \delta G_{45}^{-1}} + \frac{\delta W}{\delta G_{23}^{-1}} \frac{\delta W}{\delta G_{45}^{-1}} \right\}. \quad (15.46)$$

If the coupling constant g vanishes, this is immediately solved by (15.35). For a non-vanishing coupling constant g , the right-hand side in (15.46) produces corrections to (15.35) which we shall denote with $W^{(\text{int})}$. Thus the negative free energy W decomposes according to (all at zero external current j)

$$W = W^{(0)} + W^{(\text{int})}. \quad (15.47)$$

Inserting this into (15.46) and taking into account (15.37), we obtain the following functional differential equation for the interaction negative free energy $W^{(\text{int})}$:

$$\begin{aligned} \int_{12} G_{12}^{-1} \frac{\delta W^{(\text{int})}}{\delta G_{12}^{-1}} &= \frac{g}{4} \int_{1234} V_{1234} G_{12} G_{34} - \frac{g}{3} \int_{1234} V_{1234} G_{12} \frac{\delta W^{(\text{int})}}{\delta G_{34}^{-1}} \\ &+ \frac{g}{3} \int_{1234} V_{1234} \left\{ \frac{\delta^2 W^{(\text{int})}}{\delta G_{12}^{-1} \delta G_{34}^{-1}} + \frac{\delta W^{(\text{int})}}{\delta G_{12}^{-1}} \frac{\delta W^{(\text{int})}}{\delta G_{34}^{-1}} \right\}. \end{aligned} \quad (15.48)$$

With the help of the functional chain rule, the first and second derivatives with respect to the inverse propagator G^{-1} , are rewritten as

$$\frac{\delta}{\delta G_{12}^{-1}} = - \int_{34} G_{13} G_{24} \frac{\delta}{\delta G_{34}} \quad (15.49)$$

and

$$\begin{aligned} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} &= \int_{5678} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2}{\delta G_{56} \delta G_{78}} \\ &+ \frac{1}{2} \int_{56} \{ G_{13} G_{25} G_{46} + G_{14} G_{25} G_{36} + G_{23} G_{15} G_{46} + G_{24} G_{15} G_{36} \} \frac{\delta}{\delta G_{56}}, \end{aligned} \quad (15.50)$$

respectively, so that the functional differential equation (15.48) for $W^{(\text{int})}$ takes the form [6]:

$$\begin{aligned} \int_{12} G_{12} \frac{\delta W^{(\text{int})}}{\delta G_{12}} &= -\frac{g}{4} \int_{1234} V_{1234} G_{12} G_{34} - g \int_{123456} V_{1234} G_{12} G_{35} G_{46} \frac{\delta W^{(\text{int})}}{\delta G_{56}} \\ &- \frac{g}{3} \int_{12345678} V_{1234} G_{15} G_{26} G_{37} G_{48} \left\{ \frac{\delta^2 W^{(\text{int})}}{\delta G_{56} \delta G_{78}} + \frac{\delta W^{(\text{int})}}{\delta G_{56}} \frac{\delta W^{(\text{int})}}{\delta G_{78}} \right\}. \end{aligned} \quad (15.51)$$

15.5 Recursion Relation and Graphical Solution in Scalar Theory

We now convert the functional differential equation (15.51) into a recursion relation by expanding $W^{(\text{int})}$ into a power series in G :

$$W^{(\text{int})} = \sum_{p=1}^{\infty} \frac{1}{p!} \left(\frac{-g}{4!} \right)^p W^{(p)}. \quad (15.52)$$

Using the property pointed out in Eq. (15.32) that the coefficient $W^{(p)}$ is an eigenfunction of the line number operator (15.31), we obtain the recursion relation

$$\begin{aligned} W^{(p+1)} &= 12 \int_{123456} V_{1234} G_{12} G_{35} G_{46} \frac{\delta W^{(p)}}{\delta G_{56}} + 4 \int_{12345678} V_{1234} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2 W^{(p)}}{\delta G_{56} \delta G_{78}} \\ &+ 4 \sum_{q=1}^{p-1} \binom{p}{q} \int_{12345678} V_{1234} G_{15} G_{26} G_{37} G_{48} \frac{\delta W^{(p-q)}}{\delta G_{56}} \frac{\delta W^{(q)}}{\delta G_{78}}, \quad p \geq 1. \end{aligned} \quad (15.53)$$

This must be solved with the initial condition (15.33). Employing the graphical rules of Subsection 15.2, the recursion relation (15.53) can be written diagrammatically as follows:

$$\begin{aligned}
 W^{(p+1)} = & 4 \frac{\delta^2 W^{(p)}}{\delta_1 \text{---} 2 \delta_3 \text{---} 4} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \diagup \\ \diagdown \\ \diagup \\ \diagdown \end{array} + 12 \frac{\delta W^{(p)}}{\delta_1 \text{---} 2} \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \diagup \\ \diagdown \end{array} \\
 & + 4 \sum_{q=1}^{p-1} \binom{p}{q} \frac{\delta W^{(p-q)}}{\delta_1 \text{---} 2} \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \diagup \\ \diagdown \end{array} \begin{array}{c} 3 \\ 4 \end{array} \frac{\delta W^{(q)}}{\delta_3 \text{---} 4}, \quad p \geq 1. \quad (15.54)
 \end{aligned}$$

This is iterated starting from

$$W^{(1)} = 3 \begin{array}{c} \bigcirc \quad \bigcirc \end{array}. \quad (15.55)$$

The right-hand side of (15.54) contains three different graphical operations. The first two are linear and involve one or two line amputations of the previous perturbative order. The third operation is nonlinear and mixes two different one-line amputations of lower orders.

An alternative way of formulating the above recursion relation may be based on the graphical rules:

$$W^{(p)} = \begin{array}{c} \bigcirc \\ p \end{array}, \quad \frac{\delta W^{(p)}}{\delta G_{12}} = \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \bigcirc \\ p \end{array}, \quad \frac{\delta^2 W^{(p)}}{\delta G_{12} \delta G_{34}} = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \bigcirc \\ p \end{array}. \quad (15.56)$$

With these, the recursion relation (15.54) takes the form

$$(p+1) = 4 \begin{array}{c} \bigcirc \\ p \end{array} + 12 \begin{array}{c} \bigcirc \quad \bigcirc \\ p \end{array} + 4 \sum_{q=1}^{p-1} \binom{p}{q} \begin{array}{c} \bigcirc \quad \bigcirc \\ p-q \quad q \end{array}. \quad (15.57)$$

To demonstrate the application of (15.54), we calculate the connected vacuum diagrams up to five loops. Applying the linear operations to (15.53), we obtain immediately

$$\frac{\delta W^{(1)}}{\delta_1 \text{---} 2} = 6 \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \bigcirc \end{array}, \quad \frac{\delta^2 W^{(1)}}{\delta_1 \text{---} 2 \delta_3 \text{---} 4} = 6 \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \diagup \\ \diagdown \end{array} \begin{array}{c} 3 \\ 4 \end{array}. \quad (15.58)$$

Inserted into (15.54), these lead to the three-loop vacuum diagrams

$$W^{(2)} = 24 \begin{array}{c} \bigcirc \quad \bigcirc \quad \bigcirc \\ 2 \quad 3 \\ 4 \end{array} + 72 \begin{array}{c} \bigcirc \quad \bigcirc \quad \bigcirc \end{array}. \quad (15.59)$$

Proceeding to the next order, we have to perform one- and two-line amputations on the vacuum graphs in (15.59), leading to

$$\frac{\delta W^{(2)}}{\delta_1 \text{---} 2} = 96 \text{ } 1 \text{---} \bigcirc \text{---} 2 + 144 \text{ } 1 \text{---} \bigcirc \text{---} 2 + 144 \text{ } 1 \text{---} \bigcirc \text{---} 2, \quad (15.60)$$

and subsequently to

$$\begin{aligned} \frac{\delta^2 W^{(2)}}{\delta_1 \text{---} 2 \delta_3 \text{---} 4} = & 288 \text{ } 1 \text{---} \bigcirc \text{---} 2 + 144 \text{ } 1 \text{---} \bigcirc \text{---} 3 + 288 \text{ } 2 \text{---} \bigcirc \text{---} 4 \\ & + 144 \text{ } 3 \text{---} \bigcirc \text{---} 2 + 144 \text{ } 1 \text{---} \bigcirc \text{---} 4 + 144 \text{ } 1 \text{---} \bigcirc \text{---} 3. \end{aligned} \quad (15.61)$$

Inserting (15.60) and (15.61) into (15.54), and taking into account (15.58), we find the connected vacuum diagrams of order $p = 3$ with their multiplicities as shown in Table 15.1 on page 1043. We observe that the nonlinear operation in (15.54) does not lead to topologically new diagrams. It only corrects the multiplicities of the diagrams generated from the first two operations. This is true also in higher orders. The connected vacuum diagrams of the subsequent order $p = 4$ and their multiplicities are listed in Table 15.1.

As a cross-check we can also determine the total multiplicities $M^{(p)}$ of all connected vacuum diagrams contributing to $W^{(p)}$. To this end we recall that each of the $M^{(p)}$ diagrams in $W^{(p)}$ consists of $2p$ lines. The amputation of one or two lines therefore leads to $2pM^{(p)}$ and $2p(2p-1)M^{(p)}$ diagrams with $2p-1$ and $2p-2$ lines, respectively. Considering only the total multiplicities, the graphical recursion relations (15.54) reduce to the form derived before [7]:

$$M^{(p+1)} = 16p(p+1)M^{(p)} + 16 \sum_{q=1}^{p-1} \frac{p!}{(p-q-1)!(q-1)!} M^{(q)} M^{(p-q)}; \quad p \geq 1. \quad (15.62)$$

These are solved starting with the initial value

$$M^{(1)} = 3, \quad (15.63)$$

leading to the total multiplicities

$$M^{(2)} = 96, \quad M^{(3)} = 9504, \quad M^{(4)} = 1880064, \quad (15.64)$$

which agree with the results listed in Table 15.1 on page 1043. In addition we note that the next orders would contain

$$M^{(5)} = 616108032, \quad M^{(6)} = 301093355520, \quad M^{(7)} = 205062331760640 \quad (15.65)$$

connected vacuum diagrams.

15.6 Scalar Yukawa-like Theory

For the sake of generality, let us also study the situation where the quartic interaction of the ϕ^4 -theory is generated by a scalar field A from a Yukawa-like $\phi^2 A$ -interaction. The associated energy functional

$$E[\phi, A] = E^{(0)}[\phi, A] + E^{(\text{int})}[\phi, A] \quad (15.66)$$

decomposes into the free part

$$E^{(0)}[\phi, A] = \frac{1}{2} \int_{12} G_{12}^{-1} \phi_1 \phi_2 + \frac{1}{2} \int_{12} H_{12}^{-1} A_1 A_2 \quad (15.67)$$

and the interaction

$$E^{(\text{int})}[\phi, A] = \frac{\sqrt{g}}{2} \int_{123} V_{123} \phi_1 \phi_2 A_3. \quad (15.68)$$

Indeed, as the field A appears only quadratically in (15.66), the functional integral for the partition function

$$Z = \int \mathcal{D}\phi \mathcal{D}A e^{-E[\phi, A]} \quad (15.69)$$

can be exactly evaluated with respect to the field A , yielding

$$Z = \int \mathcal{D}\phi e^{-E^{(\text{eff})}[\phi]} \quad (15.70)$$

with the effective energy functional

$$E^{(\text{eff})}[\phi] = -\frac{1}{2} \text{Tr} \ln H^{-1} + \frac{1}{2} \int_{12} G_{12}^{-1} \phi_1 \phi_2 - \frac{g}{8} \int_{123456} V_{125} V_{346} H_{56} \phi_1 \phi_2 \phi_3 \phi_4. \quad (15.71)$$

Apart from a trivial shift due to the negative free energy of the field A , the effective energy functional (15.71) coincides with the earlier one of a ϕ^4 -theory in (15.1), except that the quartic δ -function interaction is replaced by the finite-range Yukawa interaction

$$V_{1234} = -3 \int_{56} V_{125} V_{346} H_{56}. \quad (15.72)$$

We must only supplement the previous Feynman rules (15.6) and (15.8) by the free correlation function of the field A

$$1 \text{ --- } 2 \quad \equiv \quad H_{12} \quad (15.73)$$

and the cubic interaction

$$\text{---} \text{---} \text{---} \text{---} \text{---} \quad \equiv \quad \int_{123} V_{123}. \quad (15.74)$$

The intimate relation (15.72) between the ϕ^4 -theory and the $\phi^2 A$ -theory can be graphically illustrated by

$$\begin{array}{c} \diagup \quad \diagdown \\ \times \end{array} = - \begin{array}{c} \diagup \quad \diagdown \\ \text{---} \text{---} \text{---} \end{array} - \begin{array}{c} \diagup \quad \diagdown \\ \text{---} \text{---} \text{---} \\ \diagdown \quad \diagup \end{array} - \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \\ \text{---} \text{---} \end{array} . \quad (15.75)$$

This corresponds to a photon exchange in the so-called s -, t - and u -channels of Mandelstam's theory of the scattering matrix. Their infinite repetitions yield the relevant forces in the Hartree-Fock-Bogoliubov approximations of many-body physics.

In the sequel we analyze the $\phi^2 A$ -theory along similar lines as done before with the ϕ^4 -theory.

15.7 Perturbation Theory for the Yukawa-like Theory

Expanding the exponential in the partition function (15.69) in powers of the coupling constant g , the resulting perturbation series reads

$$Z = \sum_{p=0}^{\infty} \frac{1}{(2p)!} \left(\frac{g}{4} \right)^p \int \mathcal{D}\phi \mathcal{D}A \left(\int_{123456} V_{123} V_{456} \phi_1 \phi_2 \phi_4 \phi_5 A_3 A_6 \right)^p e^{-E^{(0)}[\phi, A]} . \quad (15.76)$$

Substituting the product of two fields ϕ or A by a functional derivative with respect to the inverse propagators G^{-1} or H^{-1} , we conclude from (15.76)

$$Z = \sum_{p=0}^{\infty} \frac{(-2g)^p}{(2p)!} \left(\int_{123456} V_{123} V_{456} \frac{\delta^3}{\delta G_{12}^{-1} \delta G_{45}^{-1} \delta H_{36}^{-1}} \right)^p e^{W^{(0)}} , \quad (15.77)$$

where the zeroth order of the negative free energy reads

$$W^{(0)} = -\frac{1}{2} \text{Tr} \ln G^{-1} - \frac{1}{2} \text{Tr} \ln H^{-1} \equiv \frac{1}{2} \bigcirc + \frac{1}{2} \text{---} \text{---} \text{---} . \quad (15.78)$$

Inserting (15.78) into (15.77), the first-order contribution to the negative free energy yields

$$W^{(1)} = 2 \int_{123456} V_{123} V_{456} H_{36} G_{14} G_{25} + \int_{123456} V_{123} V_{456} H_{36} G_{12} G_{45} , \quad (15.79)$$

which corresponds to the Feynman diagrams

$$W^{(1)} = 2 \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \end{array} . \quad (15.80)$$

15.8 Functional Differential Equation for the Free Energy in the Yukawa-like Theory

The derivation of a functional differential equation for the negative free energy W requires the combination of two independent steps. Consider first the identity

$$\int \mathcal{D}\phi \mathcal{D}A \frac{\delta}{\delta \phi_1} \left\{ \phi_2 e^{-E[\phi, A]} \right\} = 0 , \quad (15.81)$$

If applied to the energy functional (15.66), it yields

$$\delta_{12}Z + 2 \int_3 G_{13}^{-1} \frac{\delta Z}{\delta G_{23}^{-1}} + 2\sqrt{g} \int_{34} V_{134} \frac{\delta \{\langle A \rangle Z\}}{\delta G_{23}^{-1}} = 0, \quad (15.82)$$

where $\langle A \rangle$ denotes the expectation value of the field A . In order to close the functional differential equation, we consider a similar second identity

$$\int \mathcal{D}\phi \mathcal{D}A \frac{\delta}{\delta A_1} e^{-E[\phi, A]} = 0, \quad (15.83)$$

which leads to

$$\langle A_1 \rangle Z = \sqrt{g} \int_{234} V_{234} H_{14} \frac{\delta Z}{\delta G_{23}^{-1}}. \quad (15.84)$$

Inserting (15.84) into (15.82), we arrive at the desired functional differential equation for the negative free energy $W = \ln Z$:

$$\delta_{12} + 2 \int_2 G_{13}^{-1} \frac{\delta W}{\delta G_{23}^{-1}} = -2g \int_{34567} V_{134} V_{567} H_{47} \left\{ \frac{\delta^2 W}{\delta G_{23}^{-1} \delta G_{56}^{-1}} + \frac{\delta W}{\delta G_{23}^{-1}} \frac{\delta W}{\delta G_{56}^{-1}} \right\}. \quad (15.85)$$

A subsequent separation (15.47) of the zeroth order (15.78) leads to a functional differential equation for the interaction part of the free energy $W^{(\text{int})}$:

$$\begin{aligned} \int_{12} G_{12}^{-1} \frac{\delta W^{(\text{int})}}{\delta G_{12}^{-1}} &= -\frac{g}{4} \int_{123456} V_{123} V_{456} H_{36} \{G_{12} G_{45} + 2G_{14} G_{25}\} \\ &+ g \int_{123456} V_{123} V_{456} G_{12} H_{36} \frac{\delta W^{(\text{int})}}{\delta G_{45}^{-1}} \\ &- g \int_{123456} V_{123} V_{456} H_{36} \left\{ \frac{\delta^2 W^{(\text{int})}}{\delta G_{12}^{-1} \delta G_{45}^{-1}} + \frac{\delta W^{(\text{int})}}{\delta G_{12}^{-1}} \frac{\delta W^{(\text{int})}}{\delta G_{45}^{-1}} \right\}. \end{aligned} \quad (15.86)$$

Taking into account the functional chain rules (15.49) and (15.50), the functional derivatives with respect to G^{-1} in (15.86) can be rewritten in terms of G :

$$\begin{aligned} \int_{12} G_{12} \frac{\delta W^{(\text{int})}}{\delta G_{12}} &= \frac{g}{4} \int_{123456} V_{123} V_{456} H_{36} \{G_{12} G_{45} + 2G_{14} G_{25}\} \\ &+ g \int_{123456} V_{123} V_{456} H_{36} \{G_{12} G_{47} G_{58} + 2G_{14} G_{27} G_{58}\} \frac{\delta W^{(\text{int})}}{\delta G_{78}} \\ &+ g \int_{123456789\bar{1}} V_{123} V_{456} H_{36} G_{17} G_{28} G_{39} G_{4\bar{1}} \left\{ \frac{\delta^2 W^{(\text{int})}}{\delta G_{78} \delta G_{9\bar{1}}} + \frac{\delta W^{(\text{int})}}{\delta G_{78}} \frac{\delta W^{(\text{int})}}{\delta G_{9\bar{1}}} \right\}. \end{aligned} \quad (15.87)$$

15.9 Recursion Relation and Graphical Solution in the Yukawa-like Theory

The functional differential equation (15.87) is now solved by the power series

$$W^{(\text{int})} = \sum_{p=1}^{\infty} \frac{1}{(2p)!} \left(\frac{g}{4}\right)^p W^{(p)}. \quad (15.88)$$

results which we shall not derive here in detail. Observe that the multiplicity of a connected vacuum diagram D in the $\phi^2 A$ -theory is given by a formula similar to (15.9) in the ϕ^4 -theory:

$$M_{\phi^2 A}^D = \frac{(2p)!4^p}{2^{S+D}N}. \quad (15.93)$$

Here S and D denote the number of self- and double connections, whereas N represents the number of identical vertex permutations.

The connected vacuum diagrams of the $\phi^2 A$ -theory are shown in Table 15.4 on page 1047. They can, of course, be converted to corresponding ones of the ϕ^4 -theory in Table 15.1 on page 1043, by shrinking wiggly lines to a point and dividing the resulting multiplicity by 3 in accordance with (15.75). This relation between connected vacuum diagrams in ϕ^4 - and $\phi^2 A$ -theory is emphasized by the numbering used in Table 15.4. For instance, the shrinking converts the five diagrams #4.1-#4.5 in Table 15.4 to the diagram #4 in Table 15.1. Taking into account the different combinatorial factors in the expansions (15.5) and (15.88) as well as the factor 3 when shrinking the wiggly line as in (15.75), the multiplicity $M_{\phi^4}^{E=0}$ of a ϕ^4 -diagram results from the corresponding one $M_{\phi^2 A}^{E=0}$ of the $\phi^2 A$ -partner diagrams via the rule

$$M_{\phi^4}^{E=0} = \frac{1}{(2p-1)!!} M_{\phi^2 A}^{E=0}. \quad (15.94)$$

Continuing the solution of the graphical recursion relations (15.54) and (15.90) to higher loops becomes an arduous task. We therefore automatize the procedure by computer algebra. Here we restrict ourselves to the ϕ^4 -theory because of its relevance for critical phenomena.

15.10 Matrix Representation of Diagrams

To implement the procedure on a computer we must represent Feynman diagrams in the ϕ^4 -theory by algebraic symbols. For this purpose, matrices were defined in Ref. [8]. Let p be the number of vertices of a given diagram and label them with indices from 1 to p . Set up a matrix $\mathbf{M}$ whose elements M_{ij} ($0 \leq i, j \leq p$) specify the number of lines joining the vertices i and j . The diagonal elements M_{ii} ($i > 0$) count the number of self-connections of the i th vertex. External lines of a diagram are labeled as if they were connected to a single additional dummy vertex with index 0. A matrix element M_{00} is set to zero, as a convention. The off-diagonal elements lie in the interval $0 \leq M_{ij} \leq 4$, while the diagonal elements for $i > 0$ are restricted by $0 \leq M_{ii} \leq 2$. We observe that the sum of the matrix elements M_{ij} in each row or column equals 4, where the diagonal elements count twice,

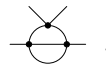
$$\sum_{j=0}^p M_{ij} + M_{ii} = \sum_{i=0}^p M_{ij} + M_{jj} = 4. \quad (15.95)$$

The matrix $\mathbf{M}$ is symmetric and is thus specified by $(p+1)(p+2)/2-1$ elements. Each matrix characterizes a unique diagram and determines its multiplicity via formula (15.27). From the matrix $\mathbf{M}$ we directly read off the number of self-, double-, triple-, and fourfold connections S, D, T, F and the number of external legs $E = \sum_{i=1}^p M_{0i}$. It also permits us to calculate the number N of identical vertex permutations. For this we observe that the matrix $\mathbf{M}$ is not unique, since so far the vertex numbering is arbitrary. In fact, N is the number of permutations of vertices and external lines which leave the matrix $\mathbf{M}$ unchanged [compare to the statement after (15.27)]. If n_M denotes the number of different matrices representing the same diagram, the number N is given by

$$N = \frac{p!}{n_M} \prod_{i=1}^p M_{0i}!. \quad (15.96)$$

The matrix elements M_{0i} count the number of external legs connected to the i th vertex. Inserting Eq. (15.96) into the formula (15.27) for $E = 0$, we obtain the multiplicity of the diagram represented by $\mathbf{M}$. This may be used to cross-check the multiplicities obtained before when solving the recursion relation (15.54).

As an example, consider the following diagram of the four-point function with $p = 3$ vertices:



$$. \quad (15.97)$$

This diagram can be represented by altogether $n_M = 3$ different matrices, depending on the labeling of the top vertex with two external legs by 1, 2, or 3:

0	0	2	1	1	0	0	1	2	1	0	0	1	1	2
1	2	0	1	1	1	1	0	1	2	1	1	0	2	1
2	1	1	0	2	2	2	1	0	1	2	1	2	0	1
3	1	1	2	0	3	1	2	1	0	3	2	1	1	0

$$. \quad (15.98)$$

From the zeroth row or column of these matrices or by inspecting the diagram (15.97), we read off that there exist two one-connections and one two-connection between external legs and vertices. Thus Eq. (15.96) states that the number of identical vertex permutations of the diagram (15.97) is $N = 4$.

The matrix $\mathbf{M}$ contains of course all information on the topological properties of a diagram. For this we define the submatrix $\tilde{\mathbf{M}}$ by removing the zeroth row and column from $\mathbf{M}$. This allows us to recognize the connectedness of a diagram: A diagram is disconnected if there is a vertex numbering for which $\tilde{\mathbf{M}}$ is a block matrix. Furthermore, it is a cutvertex, e.g., it is vertex which links two otherwise disconnected parts of its diagram, if the matrix $\tilde{\mathbf{M}}$ has an almost block-form. In

such a form the blocks overlap only on some diagonal element $\tilde{M}_{ii}$, i.e., the matrix $\tilde{\mathbf{M}}$ will acquire a block form if the i th row and column are removed. Similarly, the matrix $\tilde{\mathbf{M}}$ allows us to recognize a one-particle-reducible diagram, which falls into two pieces by cutting a certain line. Removing a line amounts to reducing the associated matrix elements in the submatrix $\tilde{\mathbf{M}}$ by one unit. If the resulting matrix $\tilde{\mathbf{M}}$ has a block form, the diagram is one-particle-reducible.

So far, the vertex numbering has been arbitrary, making the matrix representation of a diagram non-unique. To achieve uniqueness, we proceed as follows. With each matrix, we associate a number whose digits are composed of the matrix elements M_{ij} ($0 \leq j \leq i \leq p$), i.e. we form the number with the $(p+1)(p+2)/2 - 1$ elements

$$M_{10}M_{11}M_{20}M_{21}M_{22}M_{30}M_{31}M_{32}M_{33} \dots M_{pp}. \quad (15.99)$$

The smallest of these numbers is chosen to represent the diagram in a unique way. For instance, the three matrices (15.98) carry the numbers

$$201101120, \quad 102101210, \quad 101202110, \quad (15.100)$$

the smallest one being the last. Thus we uniquely represent the diagram (15.97) by this number.

15.11 Practical Generation

We are now prepared for the computer generation of Feynman diagrams. First the vacuum diagrams are generated from the recursion relation (15.54). From these the diagrams of the connected two- and four-point functions are obtained by cutting or removing lines. A MATHEMATICA program performs this task. The resulting unique matrix representations of the diagrams up to the order $p = 4$ are listed in Tables 15.6 and 15.7 on the pages 1049 and 1050. Higher-order results up to $p = 6$, containing all diagrams which are relevant for the five-loop renormalization of the ϕ^4 -theory in $d = 4 - \epsilon$ dimensions, are published in Ref. [3], with the associated computer programs on the www [35].

15.11.1 Connected Vacuum Diagrams

The computer solution of the recursion relation (15.54) necessitates to keep an exact record of the labeling of external legs of intermediate diagrams which arise from differentiating a vacuum diagram with respect to a line once or twice. To this end we have to extend our previous matrix representation of diagrams where the external legs are labeled as if they were connected to a simple additional vertex with number 0. For each matrix representing a diagram we define an associated vector which contains the labels of the external legs connected to each vertex. This vector has the length of the dimension of the matrix and will be prepended to the matrix. By doing so, it is understood that the rows and columns of the matrix are labeled from

0 to the number of vertices as explained in Section 15.10, so that we may omit these labels from now on. Consider, as an example, once more the diagram (15.97) of the four-point function with $p = 3$ vertices, where the spatial indices 1, 2, 3, 4 are assigned in a particular order:

$$\begin{array}{c} 1 \quad 2 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ 3 \quad 4 \end{array} . \quad (15.101)$$

In our extended matrix notation, such a diagram can be represented in total by six matrices:

$$\begin{aligned} & \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 0 & 1 & 1 \\ \{3\} & 1 & 1 & 0 & 2 \\ \{4\} & 1 & 1 & 2 & 0 \end{array} \right), & \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 2 & 1 \\ \{3\} & 1 & 0 & 1 & 2 \\ \{1,2\} & 2 & 1 & 0 & 1 \\ \{4\} & 1 & 2 & 1 & 0 \end{array} \right), & \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 2 \\ \{3\} & 1 & 0 & 2 & 1 \\ \{4\} & 1 & 2 & 0 & 1 \\ \{1,2\} & 2 & 1 & 1 & 0 \end{array} \right), \\ & \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 0 & 1 & 1 \\ \{4\} & 1 & 1 & 0 & 2 \\ \{3\} & 1 & 1 & 2 & 0 \end{array} \right), & \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 2 & 1 \\ \{4\} & 1 & 0 & 1 & 2 \\ \{1,2\} & 2 & 1 & 0 & 1 \\ \{3\} & 1 & 2 & 1 & 0 \end{array} \right), & \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 2 \\ \{4\} & 1 & 0 & 2 & 1 \\ \{3\} & 1 & 2 & 0 & 1 \\ \{1,2\} & 2 & 1 & 1 & 0 \end{array} \right). \end{aligned} \quad (15.102)$$

In the calculation of the vacuum diagrams from the recursion relation (15.54) that starts out with the two-loop diagram (15.55), we have to represent three different elementary operations in our extended matrix notation:

1. We must perform one or two derivatives on a vacuum diagram with respect to a line. For example, we apply this operation to the vacuum diagram #2 in Table 15.1

$$\begin{aligned} \frac{\delta^2}{\delta G_{12} \delta G_{34}} \text{ (vacuum diagram #2) } &= 2 \frac{\delta}{\delta G_{12}} \left[3 \text{ (line 1-2)} + 4 \text{ (line 3-4)} \right] \\ &= 3 \left[\begin{array}{c} 1 \quad 2 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ 3 \quad 4 \end{array} + \begin{array}{c} 2 \quad 1 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ 3 \quad 4 \end{array} + \begin{array}{c} 1 \quad 2 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ 4 \quad 3 \end{array} + \begin{array}{c} 2 \quad 1 \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \\ \diagup \quad \diagdown \\ 4 \quad 3 \end{array} \right]. \end{aligned} \quad (15.103)$$

This operation has the matrix representation

$$\begin{aligned} \frac{\delta^2}{\delta G_{12} \delta G_{34}} \left(\begin{array}{c|cccc} \{\} & 0 & 0 & 0 & 0 \\ \{\} & 0 & 0 & 4 & 0 \\ \{\} & 0 & 4 & 0 & 0 \end{array} \right) &= 2 \frac{\delta}{\delta G_{12}} \left[\left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 1 \\ \{3\} & 1 & 0 & 3 & 0 \\ \{4\} & 1 & 3 & 0 & 0 \end{array} \right) + \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 1 \\ \{4\} & 1 & 0 & 3 & 0 \\ \{3\} & 1 & 3 & 0 & 0 \end{array} \right) \right] \\ &= 3 \left[\left(\begin{array}{c|cccc} \{\} & 0 & 2 & 2 & 2 \\ \{1,3\} & 2 & 0 & 2 & 2 \\ \{2,4\} & 2 & 2 & 0 & 2 \end{array} \right) + \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 2 & 2 \\ \{2,3\} & 2 & 0 & 2 & 2 \\ \{1,4\} & 2 & 2 & 0 & 2 \end{array} \right) \right. \\ &\quad \left. + \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 2 & 2 \\ \{1,4\} & 2 & 0 & 2 & 2 \\ \{2,3\} & 2 & 2 & 0 & 2 \end{array} \right) + \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 2 & 2 \\ \{2,4\} & 2 & 0 & 2 & 2 \\ \{1,3\} & 2 & 2 & 0 & 2 \end{array} \right) \right]. \end{aligned} \quad (15.104)$$

The first and fourth matrix as well as the second and third matrix represent the same diagram in (15.104), as can be seen by permutating rows and columns of either matrix.

2. We must combine two or three diagrams to one. This is done by creating a block matrix of internal lines from the submatrices that represent the internal lines of the original diagrams. Then the zeroth row or column is added to represent the respective original external spatial arguments. Let us illustrate the combination of two diagrams by the example

$$\begin{aligned}
 1 \text{---} \bigcirc \text{---} 2 \quad 1 \text{---} \bigcirc \text{---} 2 &\equiv \left(\begin{array}{c|ccc} \{\} & 0 & 1 & 1 \\ \{1\} & 1 & 0 & 3 \\ \{2\} & 1 & 3 & 0 \end{array} \right) , \quad \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{1,2\} & 2 & 1 \end{array} \right) \\
 &\rightarrow \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 1 & 0 & 0 \\ \{1\} & 1 & 0 & 0 & 3 \\ \{2\} & 1 & 0 & 3 & 0 \end{array} \right) , \quad (15.105)
 \end{aligned}$$

and the combination of three diagrams by

$$\begin{aligned}
 \bigcirc \text{---} 1 \text{---} 2 , \quad 1 \text{---} \bigcirc \text{---} 3 \text{---} 4 , \quad 3 \text{---} \bigcirc \text{---} 4 &\equiv \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{1,2\} & 2 & 1 \end{array} \right) , \left(\begin{array}{c|cc} \{\} & 0 & 4 \\ \{1,2,3,4\} & 4 & 0 \end{array} \right) , \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{3,4\} & 2 & 1 \end{array} \right) \\
 &\rightarrow \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 4 & 2 \\ \{1,2\} & 2 & 1 & 0 & 0 \\ \{1,2,3,4\} & 4 & 0 & 0 & 0 \\ \{3,4\} & 2 & 0 & 0 & 1 \end{array} \right) . \quad (15.106)
 \end{aligned}$$

Observe that the ordering of the submatrices in the block matrix is arbitrary at this point. We merely must make sure to distribute correctly the spatial labels of the external legs.

3. When connecting external legs with the same label we must create an internal line. This is achieved in our extended matrix notation by eliminating the spatial labels of external legs which appear twice, and by performing an appropriate entry in the matrix for the additional line. Thus we obtain from (15.105)

$$\bigcirc \text{---} \bigcirc \text{---} \bigcirc \equiv \left(\begin{array}{c|cccc} \{\} & 0 & 0 & 0 & 0 \\ \{\} & 0 & 1 & 1 & 1 \\ \{\} & 0 & 1 & 0 & 3 \\ \{\} & 0 & 1 & 3 & 0 \end{array} \right) \quad (15.107)$$

and similarly, from (15.106),

$$\begin{array}{c} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \end{array} \equiv \left(\begin{array}{c|cccc} \{\} & 0 & 0 & 0 & 0 \\ \{\} & 0 & 1 & 2 & 0 \\ \{\} & 0 & 2 & 0 & 2 \\ \{\} & 0 & 0 & 2 & 1 \end{array} \right). \quad (15.108)$$

As we reobtain at this stage connected vacuum diagrams with no external legs to be labeled, we may omit the prepended vector.

The selection of a unique matrix representation for the resulting vacuum diagrams obtained at each stage of the recursion relation proceeds as explained in detail in Section 15.10. By comparing these with each other we find out which of the vacuum diagrams are topologically identical. From this we determine their individual multiplicities.

In a similar way, the recursion relation (15.54) is solved by a MATHEMATICA program up to the order $p = 6$. The results are shown in Table 15.5 on page 1048, available on the internet under the address [35]. To each order p , the numbers $n_p^{(0)}$ of topologically different connected vacuum diagrams are

p	1	2	3	4	5	6
$n_p^{(0)}$	1	2	4	10	28	97

(15.109)

15.11.2 Two- and Four-Point Functions G_{12} and G_{1234}^c from Cutting Lines

Having found all connected vacuum diagrams, we derive from these the diagrams of the connected two- and four-point functions by using the relations (15.17) and (15.24). In our matrix representation, cutting a line is essentially identical to removing a line, except that we now interpret the labels which represent the external spatial labels as sitting on the end of lines. Since we are not going to distinguish between trivially “crossed” graphs which are related by exchanging external labels in our computer implementation, we no longer need to carry around external spatial labels. Thus we omit the additional vector prepended to the matrix which represents a subdiagram in the generation of vacuum diagrams. As an example, consider cutting a line in diagram #3 in Table 15.1

$$-\frac{\delta}{\delta G^{-1}} \begin{array}{c} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \end{array} = 2 \begin{array}{c} \bigcirc \text{---} \bigcirc \end{array} + \begin{array}{c} \diagup \bigcirc \text{---} \bigcirc \diagdown \end{array} + \begin{array}{c} \bigcirc \text{---} \diagdown \bigcirc \diagup \end{array}. \quad (15.110)$$

This equation has the matrix representation

$$-\frac{\delta}{\delta G^{-1}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \end{pmatrix} = 2 \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 2 \\ 0 & 2 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 2 \\ 0 & 1 & 2 \\ 2 & 2 & 0 \end{pmatrix}. \quad (15.111)$$

Here the plus signs and multiplication by 2 have a set-theoretical meaning and are

not to be understood as matrix algebra operations. The last two matrices represent, incidentally, the same graph in (15.110) as can be seen by exchanging the last two rows and columns of either matrix.

To create the connected four-point function, we also have to consider second derivatives of vacuum diagrams with respect to G^{-1} . If an external line is cut, an additional external line will be created which is not connected to any vertex. It can be interpreted as a self-connection of the zeroth vertex which collects the external lines. This may be accommodated in the matrix notation by letting the matrix element M_{00} count the number of lines not connected to any vertex. For example, taking the derivative of the first diagram in Eq. (15.110) gives

$$-\frac{\delta}{\delta G^{-1}} \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + 2 \text{Diagram 5}, \quad (15.112)$$

with the matrix notation

$$-\frac{\delta}{\delta G^{-1}} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 3 & 1 \\ 3 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 3 \\ 1 & 1 & 1 \\ 3 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 2 & 2 \\ 2 & 1 & 0 \\ 2 & 0 & 1 \end{pmatrix} + 2 \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \quad (15.113)$$

The first two matrices represent the same diagram as can be seen from Eq. (15.112). The last two matrices in Eq. (15.113) correspond to disconnected diagrams: the first because of the absence of a connection between the two vertices, the second because of the disconnected line represented by the entry $M_{00} = 1$. In the full expression for the two loop contribution $G_{1234}^{c,(2)}$ to the four-point function in Eq. (15.24) all disconnected diagrams arising from cutting a line in $G_{12}^{(2)}$ are canceled by diagrams resulting from the sum. Therefore we may omit the sum, take only the first term and discard all disconnected graphs it creates. This is particularly useful for treating low orders by hand. If we include the sum, we use the prescription of combining two diagrams into one as described above in Subsection 15.11.1 (paragraph 2), except that we now omit the extra vector with the labels of spatial arguments.

15.11.3 Two- and Four-Point Function $\mathbf{G}_{12}$ and $\mathbf{G}_{1234}^c$ from Removing Lines

Instead of cutting lines of connected vacuum graphs once or twice, the perturbative coefficients of $\mathbf{G}_{12}$ and $\mathbf{G}_{1234}^c$ can also be obtained graphically by removing lines. Indeed, from (15.15), (15.37), (15.47) and (15.49) we get, for the two-point function:

$$\mathbf{G}_{12} = G_{12} + 2 \int_{34} G_{13} G_{24} \frac{\delta W^{(\text{int})}}{\delta G_{34}}, \quad (15.114)$$

so that we have, for $p > 0$:

$$\mathbf{G}_{12}^{(p)} = 2 \int_{34} G_{13} G_{24} \frac{\delta W^{(p)}}{\delta G_{34}}. \quad (15.115)$$

This can be used to compute the coefficients $\mathbf{G}_{12}^{(p)}$ via the removal of one line in the connected vacuum diagrams $W^{(p)}$, in all possible ways. The corresponding matrix operations are identical to those employed for cutting a line, so that in this respect there is no difference between both procedures to obtain $\mathbf{G}_{12}$.

Combining (15.114) with (15.11), (15.22), and (15.49), we obtain for the connected four-point function the equation:

$$\begin{aligned} \mathbf{G}_{1234}^c &= 4 \int_{5678} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2 W^{(\text{int})}}{\delta G_{56} \delta G_{78}} \\ &\quad - 4 \int_{5678} G_{15} G_{27} (G_{36} G_{48} + G_{46} G_{38}) \frac{\delta W^{(\text{int})}}{\delta G_{56}} \frac{\delta W^{(\text{int})}}{\delta G_{78}}. \end{aligned} \quad (15.116)$$

With the help of the recursion relation (15.57), this can be replaced by the sum

$$\begin{aligned} \mathbf{G}_{1234}^{c,(p)} &= 4 \int_{5678} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2 W^{(p)}}{\delta G_{56} \delta G_{78}} \\ &\quad - 4 \sum_{q=1}^{p-1} \binom{p}{q} \int_{5678} G_{15} G_{27} (G_{36} G_{48} + G_{46} G_{38}) \frac{\delta W^{(q)}}{\delta G_{56}} \frac{\delta W^{(p-q)}}{\delta G_{78}}. \end{aligned} \quad (15.117)$$

Again, the sum serves only to subtract disconnected diagrams which are created by the first term, so we may choose to discard both in the first term.

Now the problem of generating diagrams is reduced to the generation of vacuum diagrams and subsequently taking functional derivatives with respect to G_{12} . An advantage of this approach is that external lines do not appear at intermediate steps. So when one uses the cancellation of disconnected terms as a cross check, there are less operations to be performed than with cutting. At the end one just interprets external labels as sitting on external lines. Since all necessary operations on matrices have already been introduced, we omit examples here and just note that we can again omit external labels if we are not distinguishing between trivially “crossed” graphs.

The generation of diagrams of the connected two- and four-point functions has been implemented in both possible ways. Cutting or removing one or two lines in the connected vacuum diagrams up to the order $p = 6$ leads to the following numbers $n_p^{(2)}$ and $n_p^{(4)}$ of topologically different diagrams of $\mathbf{G}_{12}^{(p)}$ and $\mathbf{G}_{1234}^{c,(p)}$:

p	1	2	3	4	5	6
$n_p^{(2)}$	1	3	8	30	118	548
$n_p^{(4)}$	1	2	8	37	181	1010

(15.118)

TABLE 15.2 Two-point functions. Connected diagrams with their multiplicities in the ϕ^4 -theory up to four loops. The labels underneath each diagram contain the numbers $(S, D, T; N)$ specified in the previous figure.

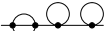
p	$\mathbf{G}_{12}^{(p)}$
1	#1.1 12 (1,0,0;2) 
2	#2.1 192 (0,0,1;2)  #3.1 288 (1,1,0;2)  #3.2 288 (2,0,0;2) 
3	#4.1 20736 (0,2,0;2)  #5.1 6912 (0,0,1;4)  #5.2 20736 (1,1,0;2)  #5.3 13824 (1,0,1;1) 
	#6.1 10368 (2,0,0;4)  #6.2 10368 (3,0,0;2)  #7.1 10368 (1,2,0;2)  #7.2 20736 (2,1,0;1) 
4	#8.1 995328 (0,3,0;2)  #9.1 1990656 (0,1,0;4)  #9.2 1990656 (0,2,0;2)  #10.1 221184 (0,0,2;2)  #10.2 663552 (0,1,1;2)  #11.1 995328 (0,2,0;4)  #11.2 1990656 (1,2,0;1)  #11.3 995328 (1,2,0;2)  #11.4 3981312 (1,1,0;1)  #12.1 995328 (2,1,0;2)  #12.2 331776 (2,0,1;2)  #12.3 663552 (2,0,1;1)  #12.4 663552 (1,0,1;2)  #13.1 995328 (2,0,0;4)  #13.2 995328 (1,1,0;4)  #13.3 1990656 (2,1,0;1)  #14.1 995328 (1,2,0;2)  #14.2 663552 (1,1,1;1)  #14.3 663552 (1,0,1;2)  #14.4 331776 (0,1,1;4)  #15.1 995328 (3,1,0;1)  #15.2 497664 (3,1,0;2)  #15.3 497664 (2,1,0;4)  #15.4 995328 (2,1,0;2)  #15.5 995328 (3,0,0;2)  #16.1 497664 (3,0,0;4)  #16.2 497664 (4,0,0;2)  #17.1 497664 (1,3,0;2)  #17.2 995328 (2,2,0;1)  #17.3 497664 (2,2,0;2) 

TABLE 15.3 Four-point functions. Connected diagrams with their multiplicities in the ϕ^4 -theory up to three loops. Each diagram is labelled by a vector $(S, D, T; N)$ analogous to the last figures.

p	$\mathbf{G}_{1234}^{c,(p)}$
1	$\begin{array}{c} \#1.1.1 \\ 24 \\ (0,0,0;24) \end{array} \quad \times$
2	$\begin{array}{cc} \#2.1.1, \#3.1.1 & \#3.1.2, \#3.2.1 \\ 1152, 576 & 1152, 1152 \\ 1728 & 2304 \\ (0,1,0;8) & (1,0,0;6) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \end{array}$
3	$\begin{array}{ccc} \#4.1.1, \#7.1.1 & \#4.1.2, \#5.1.1, \#5.2.1 & \#5.1.2, \#5.3.2 \\ 41472, 20736 & 165888, 41472, 41472 & 27648, 27648 \\ 62208 & 248832 & 55296 \\ (0,2,0;8) & (0,1,0;4) & (0,0,1;6) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#5.2.2, \#6.1.1 & \#5.2.3, \#5.3.1, \#7.1.2, \#7.2.1 & \#6.1.2, \#6.2.2, \#7.2.2 \\ 82944, 41472 & 82944, 82944, 41472, 41472 & 20736, 20736, 82944 \\ 124416 & 248832 & 124416 \\ (1,0,0;8) & (1,1,0;2) & (2,0,0;4) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#6.1.3, \#6.2.1 & \#7.1.3, \#7.2.3 \\ 41472, 41472 & 41472, 41472 \\ 82944 & 82944 \\ (2,0,0;6) & (1,1,0;6) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \end{array}$
4	$\begin{array}{ccc} \#8.1.1, \#17.1.1 & \#8.1.2, \#9.2.1, \#10.2.1 & \#8.1.3, \#11.1.2, \#11.3.1 \\ 1990656, 995328 & 3981312, 3981312, 3981312 & 7962624, 1990656, 1990656 \\ 2985984 & 11943936 & 11943936 \\ (0,3,0;8) & (0,2,0;4) & (0,2,0;4) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#9.1.1, \#13.2.1 & \#9.1.2 & \#9.1.3, \#9.2.3, \#11.1.1, \#11.4.1 \\ 3981312, 1990656 & 7962624 & 15925248, 15925248, 7962624, 7962624 \\ 5971968 & (0,0,0;24) & 47775744 \\ (0,1,0;16) & & (0,1,0;2) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#9.2.2, \#14.1.1, \#14.4.3 & \#10.1.1, \#10.2.3, \#14.2.1, \#14.4.2 & \#10.2.2, \#12.4.1 \\ 7962624, 1990656, 1990656 & 2654208, 2654208, 1327104, 1327104 & 2654208, 1327104 \\ 11943936 & 7962624 & 3981312 \\ (0,2,0;4) & (0,1,1;2) & (0,0,1;8) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#11.1.3, \#11.2.1 & \#11.2.2, \#11.4.3, \#14.1.2, \#14.3.3 & \#11.2.3, \#11.4.2, \#13.2.2, \#13.3.1 \\ 3981312, 3981312 & 7962624, 7962624, 3981312, 3981312 & 7962624, 7962624, 3981312, 3981312 \\ 7962624 & 23887872 & 23887872 \\ (0,2,0;6) & (1,1,0;2) & (1,1,0;2) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#11.2.4, \#11.3.2, \#17.1.2, \#17.2.1 & \#11.3.3, \#11.4.4, \#12.1.1, \#12.4.5 & \#11.4.5, \#15.3.1, \#15.4.1 \\ 3981312, 3981312, 1990656, 1990656 & 7962624, 7962624, 3981312, 3981312 & 7962624, 1990656, 1990656 \\ 11943936 & 23887872 & 11943936 \\ (1,2,0;2) & (1,1,0;2) & (1,1,0;4) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$ $\begin{array}{ccc} \#11.4.6, \#13.1.1, \#13.2.3 & \#12.1.2, \#12.2.2, \#13.3.3, \#17.2.2 & \#12.1.3, \#16.1.2 \\ 15925248, 3981312, 3981312 & 1990656, 1990656, 3981312, 3981312 & 3981312, 1990656 \\ 23887872 & 11943936 & 5971968 \\ (1,0,0;4) & (2,1,0;2) & (2,0,0;8) \end{array} \quad \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} \\ \text{diagram 3} \end{array}$

#12.1.4, #12.3.3, #15.1.1, #15.3.2 3981312, 3981312, 1990656, 1990656 11943936 (2,1,0;2)	#12.2.1, #12.4.2 1327104, 1327104 2654208 (1,0,1;6)	#12.3.2, #12.4.3, #14.2.2, #14.3.2 1327104, 1327104, 2654208, 2654208 7962624 (1,0,1;2)
#12.3.1, #12.4.4 1327104, 1327104 2654208 (1,0,1;6)	#13.1.2, #13.3.4, #15.4.2, #15.5.1 7962624, 7962624, 3981312, 3981312 23887872 (2,0,0;2)	#13.1.3, #16.1.1 1990656, 995328 2985984 (2,0,0;16)
#13.2.4, #13.3.5 3981312, 3981312 7962624 (1,1,0;6)	#13.3.2, #15.2.1, #15.3.3 3981312, 995328, 995328 5971968 (2,1,0;4)	#14.1.3, #14.2.3, #17.1.3, #17.3.1 3981312, 3981312, 1990656, 1990656 11943936 (1,2,0;2)
#14.1.4, #15.4.4 3981312, 1990656 5971968 (1,1,0;8)	#14.3.1, #14.4.1 1327104, 1327104 2654208 (0,0,1;12)	#15.1.2, #15.5.3, #16.1.3, #16.2.2 3981312, 3981312, 1990656, 1990656 11943936 (3,0,0;2)
#15.1.3, #15.4.3, #17.2.3, #17.3.2 1990656, 1990656, 3981312, 3981312 11943936 (2,1,0;2)	#15.1.4, #15.4.5 1990656, 1990656 3981312 (2,1,0;6)	#15.2.2, #15.5.2 1990656, 1990656 3981312 (3,0,0;6)
#15.2.3, #15.4.6 1990656, 1990656 3981312 (2,1,0;6)	#15.3.4, #15.5.4 1990656, 1990656 3981312 (2,0,0;12)	#16.1.4, #16.2.1 1990656, 1990656 3981312 (3,0,0;6)
#17.1.4, #17.2.4 1990656, 1990656 3981312 (1,2,0;6)		

TABLE 15.4 Vacuum diagrams. Connected graphs with their multiplicities in the Yukawa-like $\phi^2 A$ -theory up to four loops. Each diagram is labelled by the numbers $(S, D; N)$ specified in the previous figures.

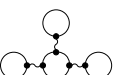
p	$W^{(p)}$
1	$\#1.1$ 2 (0,1;2)  $\#1.2$ 1 (2,0;2) 
2	$\#2.1$ 48 (0,0;8)  $\#2.2$ 24 (0,2;4)  $\#3.1$ 96 (0,0;4)  $\#3.2$ 96 (1,0;2)  $\#3.3$ 24 (2,1;2) 
3	$\#4.1$ 3840 (0,0;12)  $\#4.2$ 11520 (0,0;4)  $\#4.3$ 3840 (0,0;12)  $\#4.4$ 960 (0,3;6)  $\#4.5$ 5760 (0,1;4)  $\#5.1$ 11520 (0,1;2)  $\#5.2$ 23040 (0,0;2)  $\#5.3$ 11520 (1,0;2)  $\#5.4$ 5760 (1,1;2)  $\#6.1$ 7680 (0,0;6)  $\#6.2$ 11520 (1,0;2)  $\#6.3$ 5760 (2,0;2)  $\#6.4$ 960 (3,0;6)  $\#7.1$ 11520 (0,0;4)  $\#7.2$ 5760 (0,0;8)  $\#7.3$ 11520 (1,0;2)  $\#7.4$ 5760 (1,1;2)  $\#7.5$ 1440 (2,2;2)  $\#7.6$ 2880 (2,0;4) 

TABLE 15.5 Unique matrix representation of all connected *vacuum* diagrams of ϕ^4 -theory up to the order $p = 4$. The numbers in the first column correspond to their graphical representations in Table 15.1 on page 1043. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j , omitting $M_{i0} = 0$, for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T, F; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$W^{(1)}$: 1 diagram				
i	1			
j	1			
#	M_{ij}	$(S,D,T,F;N)$	M	W^{-1}
1	2	(2,1,0,0;1)	3	8

W ⁽²⁾ : 2 diagrams					
i	1	22			
j	1	12			
#	M _{ij}		(S,D,T,F;N)	M	W ⁻¹
2	0	40	(0,0,0,1;2)	24	48
3	1	21	(2,1,0,0;2)	72	16

$W^{(3)}$: 4 diagrams						
i	1	22	333			
j	1	12	123			
#	M_{ij}			$(S,D,T,F;N)$	M	W^{-1}
5	0	11	310	(1,0,1,0;2)	3456	24
4	0	20	220	(0,3,0,0;6)	1728	48
7	0	21	201	(2,2,0,0;2)	2592	32
6	1	11	111	(3,0,0,0;6)	1728	48

$W^{(4)}$: 10 diagrams							
i	1	22	333	4444			
j	1	12	123	1234			
#	M_{ij}	$(S,D,T,F;N)$	M	W^{-1}			
10	0	00	130	3100	(0,0,2,0;4)	55296	144
8	0	00	220	2200	(0,4,0,0;8)	62208	128
12	0	01	111	3100	(2,0,1,0;2)	165888	48
14	0	01	120	3010	(1,1,1,0;2)	165888	48
17	0	01	201	2200	(2,3,0,0;2)	124416	64
11	0	01	210	2110	(1,2,0,0;2)	497664	16
9	0	10	120	2110	(0,2,0,0;8)	248832	32
13	0	11	101	2110	(2,1,0,0;4)	248832	32
15	0	11	111	2001	(3,1,0,0;2)	248832	32
16	1	01	111	1101	(4,0,0,0;8)	62208	128

TABLE 15.6 Unique matrix representation of all connected *two-point* functions of ϕ^4 -theory up to the order $p = 4$. The numbers in the first column correspond to their graphical representation in Table 15.2. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j , omitting $M_{i0} = 0$ for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$\mathbf{G}_{12}^{(1)}$: 1 diagram				
i	11			
j	01			
#	M_{ij}	$(S, D, T; N)$	M	W^{-1}
1.1	21	(1,0,0;2)	12	4

$\mathbf{G}_{12}^{(3)}$: 8 diagrams						
i	11	222	3333			
j	01	012	0123			
#	M_{ij}			$(S, D, T; N)$	M	W^{-1}
7.1	00	021	2200	(1,2,0;2)	10368	16
5.1	00	030	2110	(0,0,1;4)	6912	24
5.3	00	111	1300	(1,0,1;1)	13824	12
4.1	00	120	1210	(0,2,0;2)	20736	8
6.1	01	011	2110	(2,0,0;4)	10368	16
7.2	01	101	1210	(2,1,0;1)	20736	8
5.2	01	110	1120	(1,1,0;2)	20736	8
6.2	01	111	1101	(3,0,0;2)	10368	16

$\mathbf{G}_{12}^{(2)}$: 3 diagrams					
i	11	222			
j	01	012			
#	M_{ij}		$(S, D, T; N)$	M	W^{-1}
3.1	01	220	(1,1,0;2)	288	8
2.1	10	130	(0,0,1;2)	192	12
3.2	11	111	(2,0,0;2)	288	8

$\mathbf{G}_{12}^{(4)}$: 30 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S, D, T; N)$	M	W^{-1}
17.1	00	001	0220	22000	(1,3,0;2)	497664	32
12.4	00	001	0310	21100	(1,0,1;2)	663552	24
14.2	00	001	1120	13000	(1,1,1;1)	663552	24
11.3	00	001	1210	12100	(1,2,0;2)	995328	16
14.4	00	010	0130	22000	(0,1,1;4)	331776	48
11.1	00	010	0220	21100	(0,2,0;4)	995328	16
10.1	00	010	1030	13000	(0,0,2;2)	221184	72
9.2	00	010	1120	12100	(0,2,0;2)	1990656	8
15.3	00	011	0111	22000	(2,1,0;4)	497664	32
15.4	00	011	0201	21100	(2,1,0;2)	995328	16
13.2	00	011	0210	21010	(1,1,0;4)	995328	16
12.3	00	011	1011	13000	(2,0,1;1)	663552	24
13.3	00	011	1101	12100	(2,1,0;1)	1990656	8
11.4	00	011	1110	12010	(1,1,0;1)	3981312	4
11.2	00	020	1011	12100	(1,2,0;1)	1990656	8
8.1	00	020	1020	12010	(0,3,0;2)	995328	16
9.1	00	020	1110	11110	(0,1,0;4)	1990656	8
17.2	00	021	1001	12010	(2,2,0;1)	995328	16
14.1	00	021	1100	11020	(1,2,0;2)	995328	16
15.2	00	021	1101	11001	(3,1,0;2)	497664	32
14.3	00	030	1001	11110	(1,0,1;2)	663552	24
10.2	00	030	1010	11020	(0,1,1;2)	663552	24
12.2	00	030	1011	11001	(2,0,1;2)	331776	48
16.1	01	001	0111	21100	(3,0,0;4)	497664	32
15.1	01	001	1011	12100	(3,1,0;1)	995328	16
17.3	01	001	1020	12010	(2,2,0;2)	497664	32
13.1	01	001	1110	11110	(2,0,0;4)	995328	16
15.5	01	011	1001	11110	(3,0,0;2)	995328	16
12.1	01	011	1010	11020	(2,1,0;2)	995328	16
16.2	01	011	1011	11001	(4,0,0;2)	497664	32

TABLE 15.7 Unique matrix representation of all connected *four-point* functions of ϕ^4 -theory up to the order $p = 4$. The numbers in the first column correspond to their graphical representation in Table 15.3. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j , omitting $M_{i0} = 0$ for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$\mathbf{G}_{1234}^{c,(1)}$: 1 diagram				
i	11			
j	01			
#	M_{ij}	$(S, D, T; N)$	M	W^{-1}
1.1.1	40	(0,0,0;24)	24	24

$\mathbf{G}_{1234}^{c,(2)}$: 2 diagrams					
i	11	222			
j	01	012			
#	M_{ij}	$(S, D, T; N)$	M	W^{-1}	
3.1.2, 3.2.1	11	310	(1,0,0;6)	2304	12
2.1.1, 3.1.1	20	220	(0,1,0;8)	1728	16

$\mathbf{G}_{1234}^{c,(3)}$: 8 diagrams						
i	11	222	3333			
j	01	012	0123			
#	M_{ij}			$(S, D, T; N)$	M	W^{-1}
5.1.2, 5.3.2	00	130	3100	(0,0,1;6)	55296	36
4.1.1, 7.1.1	00	220	2200	(0,2,0;8)	62208	32
6.1.3, 6.2.1	01	111	3100	(2,0,0;6)	82944	24
7.1.3, 7.2.3	01	120	3010	(1,1,0;6)	82944	24
5.2.2, 6.1.1	01	210	2110	(1,0,0;8)	124416	16
5.2.3, 5.3.1, 7.1.2, 7.2.1	10	111	2200	(1,1,0;2)	248832	8
4.1.2, 5.1.1, 5.2.1	10	120	2110	(0,1,0;4)	248832	8
6.1.2, 6.2.2, 7.2.2	11	101	2110	(2,0,0;4)	124416	16

$\mathbf{G}_{1234}^{c,(4)}$: 37 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S, D, T; N)$	M	W^{-1}
13.2.4, 13.3.5	00	011	1210	31000	(1,1,0;6)	7962624	24
12.3.1, 12.4.4	00	011	1300	30100	(1,0,1;6)	2654208	72
11.4.5, 15.3.1, 15.4.1	00	011	2110	22000	(1,1,0;4)	11943936	16
11.1.3, 11.2.1	00	020	1120	31000	(0,2,0;6)	7962624	24
8.1.1, 17.1.1	00	020	2020	22000	(0,3,0;8)	2985984	64
9.1.1, 13.2.1	00	020	2110	21100	(0,1,0;16)	5971968	32
15.2.3, 15.4.6	00	021	1101	31000	(2,1,0;6)	3981312	48
17.1.4, 17.2.4	00	021	1200	30010	(1,2,0;6)	3981312	48
14.1.4, 15.4.4	00	021	2100	21010	(1,1,0;8)	5971968	32
12.2.1, 12.4.2	00	030	1011	31000	(1,0,1;6)	2654208	72
14.3.1, 14.4.1	00	030	1110	30010	(0,0,1;12)	2654208	72
10.2.2, 12.4.1	00	030	2010	21010	(0,0,1;8)	3981312	48
11.2.4, 11.3.2, 17.1.2, 17.2.1	00	101	1210	22000	(1,2,0;2)	11943936	16

$\mathbf{G}_{1234}^{c,(4)}$: 37 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S,D,T;N)$	M	W^{-1}
12.3.2, 12.4.3, 14.2.2, 14.3.2	00	101	1300	21100	(1,0,1;2)	7962624	24
9.2.2, 14.1.1, 14.4.3	00	110	1120	22000	(0,2,0;4)	11943936	16
9.1.3, 9.2.3, 11.1.1, 11.4.1	00	110	1210	21100	(0,1,0;2)	47775744	4
10.1.1, 10.2.3, 14.2.1, 14.4.2	00	110	1300	20200	(0,1,1;2)	7962624	24
13.3.2, 15.2.1, 15.3.3	00	111	1101	22000	(2,1,0;4)	5971968	32
11.2.3, 11.4.2, 13.2.2, 13.3.1	00	111	1200	21010	(1,1,0;2)	23887872	8
8.1.3, 11.1.2, 11.3.1	00	120	1200	20110	(0,2,0;4)	11943936	16
15.1.4, 15.4.5	01	001	1120	31000	(2,1,0;6)	3981312	48
13.1.3, 16.1.1	01	001	2110	21100	(2,0,0;16)	2985984	64
16.1.4, 16.2.1	01	011	1011	31000	(3,0,0;6)	3981312	48
15.3.4, 15.5.4	01	011	1110	30010	(2,0,0;12)	3981312	48
12.1.3, 16.1.2	01	011	2010	21010	(2,0,0;8)	5971968	32
11.3.3, 11.4.4, 12.1.1, 12.4.5	01	100	1120	21100	(1,1,0;2)	23887872	8
14.1.3, 14.2.3, 17.1.3, 17.3.1	01	100	1210	20200	(1,2,0;2)	11943936	16
15.1.2, 15.5.3, 16.1.3, 16.2.2	01	101	1101	21100	(3,0,0;2)	11943936	16
13.1.2, 13.3.4, 15.4.2, 15.5.1	01	101	1110	21010	(2,0,0;2)	23887872	8
15.1.3, 15.4.3, 17.2.3, 17.3.2	01	101	1200	20110	(2,1,0;2)	11943936	16
12.1.4, 12.3.3, 15.1.1, 15.3.2	01	110	1101	20200	(2,1,0;2)	11943936	16
11.4.6, 13.1.1, 13.2.3	01	110	1110	20110	(1,0,0;4)	23887872	8
8.1.2, 9.2.1, 10.2.1	10	100	1120	12100	(0,2,0;4)	11943936	16
12.1.2, 12.2.2, 13.3.3, 17.2.2	10	101	1101	12100	(2,1,0;2)	11943936	16
11.2.2, 11.4.3, 14.1.2, 14.3.3	10	101	1110	12010	(1,1,0;2)	23887872	8
9.1.2	10	110	1110	11110	(0,0,0;24)	7962624	24
15.2.2, 15.5.2	10	111	1101	11001	(3,0,0;6)	3981312	48

Notes and References

The development in this chapter is taken from the textbook
H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4 -Theories*, World Scientific, Singapore 2001 (<http://klnrt.de/b8>).

The particular citations in this chapter refer to:

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- [2] H. Kleinert, Fortschr. Phys. **30**, 351 (1982) (<http://klnrt.de/84>).
- [3] H. Kleinert, A. Pelster, B. Kastening, and M. Bachmann, Phys. Rev. E **62**, 1537 (2000) ([hep-th/9907168](http://arxiv.org/abs/hep-th/9907168)). The associated algebraic computer programs and their outputs can be downloaded from the internet address [35].
- [4] See Eq. (2.28) in Ref. [3].
- [5] B. Kastening, Phys. Rev. D **54**, 3965 (1996); Phys. Rev. D **57**, 3567 (1998);
S.A. Larin, M. Mönnigmann, M. Strösser, V. Dohm, Phys. Rev. B **58**, 3394 (1998).
- [6] Compare Eq. (51) in Ref. [2].
- [7] See Ref. [2].
- [8] See Section 14.1 in the above textbook, and Ref. [3].
- [9] See the www address <http://klnrt.de/294/programs>.

16

Spontaneous Symmetry Breakdown

In the perturbation expansion developed in Chapter 10, the classical ground state carries no field. The associated vacuum state is called *normal*, since it is invariant under all symmetry transformations of the action. There are many physical systems where this is not true. As an example, we shall discuss here the ϕ^4 -theory with N components $\phi_1, \dots, \phi_N$ coupled in an $O(N)$ -symmetric way.

16.1 Scalar $O(N)$ -Symmetric ϕ^4 -Theory

The relevant Lagrangian reads

$$\mathcal{L} = \frac{1}{2} (\partial\phi_a)^2 - \frac{m^2}{2} \phi_a^2 - \frac{g}{4} (\phi_a^2)^2. \quad (16.1)$$

It is invariant under all N -dimensional rotations of its components

$$\phi_a \rightarrow R_{ab} \phi_b, \quad (16.2)$$

which conserve the length of the field vector $\Phi \equiv (\phi_a)$,

$$|\Phi| = \sqrt{\phi_a^2}. \quad (16.3)$$

The perturbation expansion of the ϕ^4 -theory discussed in Chapters 10 and 11 was based on a Taylor expansion of the total generating functional

$$Z[j] = e^{-i(g/4) \int_{-\infty}^{\infty} dt [-i\delta/\delta j(x)]^4} Z_0[j] \quad (16.4)$$

in powers of the interaction g , where $Z_0[j]$ is the generating functional of the free-field theory with a Lagrangian

$$\mathcal{L}_0 = \frac{1}{2} (\partial\phi_a)^2 - \frac{m^2}{2} \phi_a^2. \quad (16.5)$$

This expansion makes sense only for a positive square mass m^2 . Assuming a positive coupling constant g , the classical field potential

$$v(\phi_a) = \frac{m^2}{2} \phi_a^2 + \frac{g}{4} (\phi_a^2)^2 \quad (16.6)$$

has a minimum at the $O(N)$ -symmetric field configuration $\phi_a = \phi_a^0 = 0$. Only in this case can the perturbation expansion of the second-quantized field theory proceed around the free-field theory described by $\mathcal{L}_0$.

A non-trivial and physically very important situation is, however, described by the case $m^2 < 0$ (at $g > 0$). Then the classical field configuration minimizing $\mathcal{L}$ is given by a nonzero field

$$\phi_a^0 \neq 0. \quad (16.7)$$

This happens in various many-body systems, where field theories of the type (16.1) are used to describe orientational properties of materials, for instance the direction of magnetization. In that case $n = 3$, and the vector (ϕ_1, ϕ_2, ϕ_3) is identified with the local size and orientation of the local magnetization. The generating functional

$$Z[j] = \int \mathcal{D}\phi e^{i \int dx [\mathcal{L}(\phi, \partial\phi) + j_a \phi_a]} \quad (16.8)$$

can serve to understand the fluctuation phenomena in such systems. When comparing theory and experiment it turns out that there is usually a certain temperature T_c , above which the system can be described via the perturbation expansion given in the last chapter. As the temperature is lowered toward T_c , fluctuations increase drastically. This can be accounted for in field theory based on (16.1) by letting the mass parameter be temperature dependent such that m^2 vanishes for some temperature $T = T_c^{\text{MF}}$, say

$$m^2 = \mu^2 \left(\frac{T}{T_c^{\text{MF}}} - 1 \right) \equiv \mu^2 \tau, \quad (16.9)$$

where μ is some mass scale. The temperature $T = T_c^{\text{MF}}$ carries a superscript MF to indicate that this is the place where the *bare mass* changes sign, and the mean-field approximation has its phase transition. The fluctuations will shift this temperature downwards, making the true critical temperature T_c smaller than T_c^{MF} . In the low-temperature phase, the direction of the spin vectors ϕ_a is no more random, but the system settles at a specific non-zero expectation value of the field which we denoted before as

$$\Phi_a \equiv \langle 0 | \phi_a | 0 \rangle. \quad (16.10)$$

Take, for example, a magnetic system which can acquire a certain spontaneous magnetization. The existence of a nonzero expectation value (16.10) introduces a new qualitative feature into the theory. The ground state no longer has the symmetry which was contained in the action. A rotation $O(N)$ changes the direction of the ground state just as a magnet can be rotated in space. One speaks of a *spontaneous breakdown* of the original symmetry of the action.

The perturbative calculation order by order cannot account for this feature since, as we have seen, the evenness of the ϕ^4 -interaction prevents the existence of any odd-point function. The effect must therefore be due to a non-perturbative mechanism.

It is gratifying to note that this does not prevent us from giving a theoretical explanation of this phenomenon using perturbation-theoretic techniques. In fact, the effective action that was calculated in the proceeding chapters with perturbative techniques is the ideal tool for this purpose. Note that whatever symmetry is carried by the action $\mathcal{A}[\phi_a]$, this will also wind up in the effective action $\Gamma[\Phi_a]$. Indeed, if $\mathcal{A}[\phi_a]$ does not change under the transformation (16.2), then $W[j_a]$ is invariant under $j_a \rightarrow R_{ab}j_b$. Thus the field expectation value $\Phi_a \equiv \delta W / \delta j_a$ transforms according to the same law as the field ϕ_a itself, and $\Gamma[\Phi_a] = W[j_a] - j_a \Phi_a$ will also be invariant.

This statement is obvious at the lowest-order approximation to the effective action which is equal to the classical action $\mathcal{A}[\phi_a]$ taken at Φ_a :

$$\Gamma[\Phi_a] \approx \mathcal{A}[\Phi_a]. \quad (16.11)$$

At a constant field expectation Φ_a , this determines the effective potential

$$\Gamma[\Phi_a] = -Vv(\Phi_a), \quad (16.12)$$

where $V = d^Dx$ is the spacetime volume. For the Lagrange density (16.1), the effective potential is

$$v(\Phi_a) = \frac{1}{2}m^2\Phi_a^2 + \frac{g}{4}(\Phi_a^2)^2. \quad (16.13)$$

Already at this lowest approximation, the effective action is capable of describing a spontaneous symmetry breakdown. As long as $m^2 > 0$, this has an $O(N)$ -symmetric minimum at a single field point, the origin $\Phi_a = 0$. But if m^2 is lowered and becomes smaller than zero, the origin becomes unstable and the potential looks as shown in Fig. 16.1. The $O(N)$ -symmetry of the potential gives rise to an infinitely degenerate minimum characterized by a fixed length of the field vector Φ_a :

$$|\Phi^0| \equiv \sqrt{\Phi_a^2} = \sqrt{\frac{-m^2}{g}}. \quad (16.14)$$

The direction of this minimum in field space can be changed arbitrarily by an $O(N)$ -rotation without changing the energy.

The length scale over which the fluctuations take place is given by the mass term as

$$\xi = m^{-1} = \mu^{-1}\tau^{-1/2}. \quad (16.15)$$

Experimentally one finds the slightly different result

$$\xi = \mu^{-1}\tau^{-\nu}, \quad (16.16)$$

and the power ν is the *critical exponent* or *critical index* of the temperature dependence of the coherence length. In mean-field approximation to (16.10), where β is equal to $1/2$. The system is unstable at the origin. Small fluctuations which are

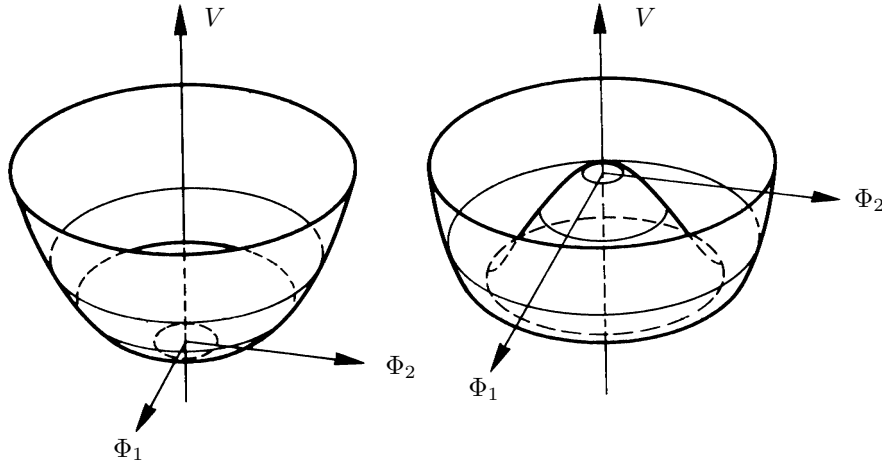


FIGURE 16.1 Effective potential of the ϕ^4 -theory for $N = 2$ in mean-field approximation. It is plotted for $m^2 > 0$ and $m^2 < 0$, corresponding to temperatures above and below the critical temperature, respectively.

neglected within the present classical approximation will drive the field down to a new minimum at Φ_0 . The non-perturbative aspect of the solution manifests itself in the power $1/\sqrt{g}$ appearing even at the level of no fluctuations.

Note how the symmetry is spontaneously broken: The system has now many directions to choose from, since there exists an entire surface of an $O(N)$ -sphere, the so-called $O(N)$ -shell, of minimal energy. It is pictured as a circle in Fig. 16.1. One says that for $m^2 < 0$, the vacuum is infinitely degenerate. As soon as Φ_a has made its directional choice, the ground state has lost its symmetry, which is said to be *spontaneously broken*.

From (16.14) we can calculate how the strength of the magnetization varies with temperature using (16.9):

$$|\Phi^0| = \frac{\mu}{\sqrt{g}} \sqrt{-\tau} = \frac{\mu}{\sqrt{g}} \sqrt{1 - \frac{T}{T_c^{\text{MF}}}}. \quad (16.17)$$

Experimentally, one finds a power law slightly different from this:

$$|\Phi^0| \propto (-\tau)^\beta, \quad (16.18)$$

where the power β is the *critical exponent* or *critical index* of the temperature behavior of the magnetic field. The data lie quite close to the mean-field approximation (16.17), where β has a value $\beta \approx 1/2$ with the plot shown in Fig. 16.2.

The deviation of ν and β from $1/2$ is due to fluctuations. In Section 20.8 we shall derive the deviation from $1/2$. It will emerge from an expansion of a general scaling relation to be discussed in the section leading to Eq. (20.174). Anticipating

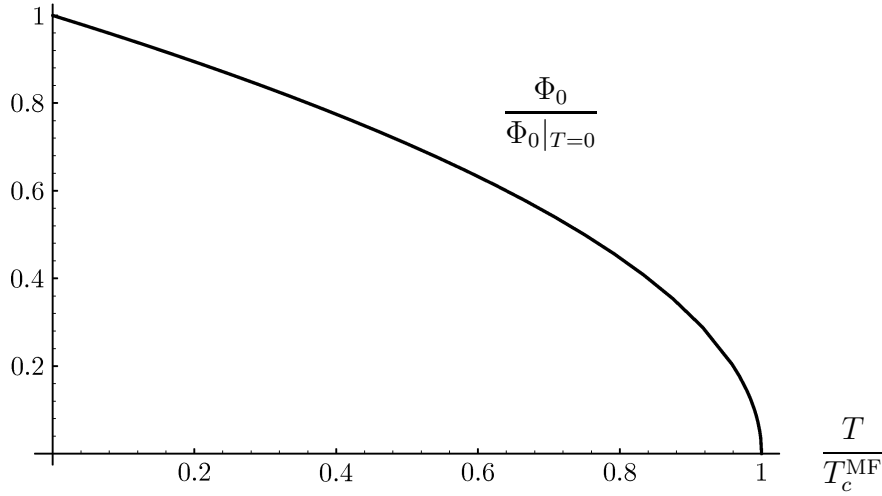


FIGURE 16.2 Magnetization Φ_0 in mean-field approximation as a function of the temperature ratio T/T_c^{MF} .

the result for the effective potential $v(\Phi_a)$, we shall find that it depends on $\Phi \equiv \sqrt{\Phi_a^2}$ like

$$v(\Phi_a) = \frac{g^*}{4} \Phi^\delta \left(1 + \text{const} \times \xi^{-\omega} \Phi^{-2\omega/(D-2+\eta)} + \dots \right), \quad (16.19)$$

where for $N = 2$, the critical exponents are $\delta = (D + 2 - \eta)/(D - 2 + \eta) \approx 4.7$, $\eta \approx 0.033$, $\nu \approx 2/3$, $\omega \approx 0.8$.

The expansion (16.19) is derived for positive m^2 . What can we say about $m^2 < 0$? Looking at the original one-loop formula we see that the whole effective action can be continued analytically to negative m^2 as long as Φ^2 is kept nonzero, so that

$$m^2 + \frac{g}{2} \Phi^2 > 0. \quad (16.20)$$

But this is too close to the new minimum which, with the normalization of the coupling used there implying $g_{\text{old}} = 3!g_{\text{new}}$, was at

$$\Phi^{02} = -\frac{m^2}{g} 3! \quad (16.21)$$

such that $m^2 + g\Phi^2/2 = -2m^2 > 0$. Moreover, the full loop expansion formula to all orders can be calculated for Φ close to this minimum since all propagators $\mathcal{D} = i/(-\partial^2 - m^2 - g\Phi^2/2)$ correspond to particles with a proper positive mass term.

Note that the renormalization procedure is well-defined order by order in the coupling constant g . The same counter terms which made the results finite above

T_c^{MF} , keep the results finite below T_c^{MF} . The only point to watch out is that the Φ never drops below a certain critical value

$$\Phi^2 < \frac{1}{3}\Phi^{02} = -2\frac{m^2}{g}, \quad (16.22)$$

at which place logarithms pick up negative arguments and give rise to imaginary parts. Thus, as long as we avoid the critical value (16.22) we may use (16.19) also for $m^2 < 0$, $T < T_c^{\text{MF}}$. Actually, that result was only derived for a one-component Φ -field. But it can easily be shown that the same form remains valid also for the $O(N)$ -field Φ_a , except with slightly different critical exponents β and γ .

We may now use the expansion (16.19) for the same discussion as before, and find a vacuum expectation below T_c^{MF} :

$$|\Phi^0| = \left(-\frac{m^2}{g}\right)^\beta = (-\tau)^\beta. \quad (16.23)$$

By comparing this one-loop corrected theoretical result with experiment, one does find an improvement in the right direction.

The theory of critical indices has been the subject of many investigations in the past years. Therefore they deserve a more detailed discussion which will be given in a separate chapter. Let us end this section by pointing out that the appearance of an imaginary part for $\Phi^2 < \Phi_c^2$ has a good physical reason: Imaginary parts in an energy are always related to an instability of the system. The origin of the instability for $\Phi^2 < \Phi_c^2$ can easily be found: Let us turn on an external field j which drives Φ into the region of instability. The effective potential becomes

$$v(\Phi) = \frac{m^2}{2}\Phi^2 + \frac{g}{4!}\Phi^4 - j\Phi \quad (16.24)$$

and looks as plotted in Fig. 16.1.

The value of Φ at the minimum increases with j . The other minimum at the diametrically opposite place, however, begins to move closer to the axis. We can display the two minima as a function of j by plotting, in Fig. 16.3, the result Φ_j of the equation $\partial v(\Phi)/\partial \Phi = 0$: // [2em]

$$j = m^2\Phi + \frac{g}{3!}\Phi^3. \quad (16.25)$$

For very large j or $-j$, there is only a single minimum on the right- or left-hand side, respectively. In a region $|j| \leq j_c$ there are three solutions, two minima and one maximum. The value j_c is determined from the maximum of the curve (16.25)

$$j_c = -\sqrt{\frac{2m^2}{g}}\frac{2}{3}m^2 \quad (16.26)$$

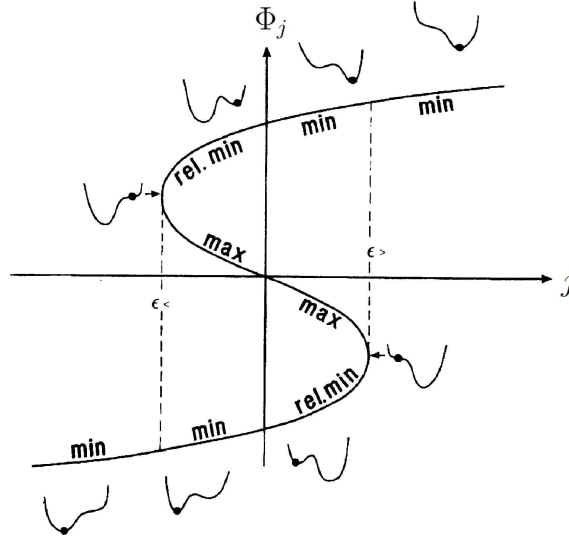


FIGURE 16.3 Magnetization Φ_j as a function of the external source j in mean-field approximation.

which lies at

$$\Phi_c^2 = -2m^2/g. \quad (16.27)$$

There the minimum fuses with the maximum and disappears. But this is precisely the place at which the effective potential develops an imaginary part. Thus the instability indicated by the appearance of an imaginary part in the effective potential is simply a signal for the fact that the local minimum at the elevated place can no longer be a solution of the field equation. The point becomes locally unstable. Note that the same instability point appears to all orders in the loop expansion, i.e., to all orders in the fluctuation expansion.

From our knowledge of simple quantum mechanical systems we may conclude that this result cannot contain the whole truth about phase stability. While the system certainly can be in the higher minimum, it always has a possibility of escaping through the potential barrier via tunneling. Thus there must be an imaginary part in the true effective potential as soon as $\Phi < \Phi^0$. Obviously, the loop expansion cannot account for this. Even the hope is futile that a full summation of all terms might produce a corresponding singularity at $\Phi = \Phi^0$. From quantum mechanics it is known that tunneling amplitudes carry an exponentially small suppression factor $e^{-a/g\hbar}$. Such a factor can never be derived from a loop expansion that is always a power series in g (the power series expansion of $e^{-a/g\hbar}$ would be $1 + 0 + 0 + \dots$). Note however, that approximate methods have been developed to describe physical effects of this type. They are based on variational perturbation theory (VPT) that will be described in Section 22.5.

16.2 Nambu-Goldstone Particles

16.2.1 The Mechanism

There is an important physical consequence of spontaneous symmetry breakdown. The system has an infinite choice between different directions of ϕ . Consider a field configuration which is not constant in space but changes smoothly from space-time point to space-time point along the degenerate $O(N)$ shell. Obviously, the energy of such a configuration can be made arbitrarily small. But this means that there is a large region in field space over which fluctuations hardly change the action. Thus the suppression of fluctuation cannot be very effective and the angular fluctuations of the field are large. Let us see this explicitly for the case $N = 2$ for which ϕ may be written as a single complex field $\phi = \phi_1 + i\phi_2$. Going to a radial decomposition

$$\phi = \rho e^{i\gamma}, \quad (16.28)$$

we may write the action as

$$\mathcal{A}[\phi] = \frac{1}{2} (\partial\rho)^2 - \frac{m^2}{2} \rho^2 + \frac{1}{2} \rho^2 (\partial\gamma)^2 - \frac{g}{4} \rho^4. \quad (16.29)$$

For $m^2 < 0$, consider variations of ρ around $\rho_0 = \sqrt{-m^2/g}$. If $\gamma(\mathbf{x})$ is kept constant we may expand $\rho = \rho_0 + \delta\rho$ and write

$$\delta^2 \mathcal{A}[\phi] = \frac{1}{2} (\partial\delta\rho)^2 + \frac{2m^2}{2} (\delta\rho)^2. \quad (16.30)$$

Note that the size fluctuations $\delta\rho$ take place with a mass twice the opposite of the $T > T_c^{\text{MF}}$ situation. An $O(2)$ -symmetric field theory with ϕ^4 -interaction can be used to describe the phase transition from normal to superfluid in liquid helium near 2.7 degrees Kelvin. The $O(2)$ -degeneracy of the ground state manifests itself by the independence of the action on γ . If γ has small space-time variations, we may write $\gamma = \gamma_0 + \delta\gamma$, and we get from the gradient term in (16.29) an additional piece in the action

$$\delta^2 \mathcal{A}[\phi] = \frac{1}{2} \rho_0^2 (\partial\delta\gamma)^2. \quad (16.31)$$

Consider now the eigenmodes of quadratic fluctuations. There is one mode associated with the size ρ of the field. From (16.30) we read off the propagator

$$G_{\delta\rho\delta\rho} = \frac{i}{-\partial^2 + 2m^2}. \quad (16.32)$$

The other fluctuation in the phase γ is seen from (16.31) to have a propagator

$$G_{\delta\gamma\delta\gamma} = \frac{1}{\rho_0^2} \frac{i}{-\partial^2}. \quad (16.33)$$

This is a massless mode, the famous *Nambu-Goldstone boson*. Its presence in the case of spontaneously broken symmetry was first discovered by Nambu, followed by a more rigorous treatment by Goldstone. If the action depends on an N -component vector field ϕ_a in an $O(N)$ -symmetric way, there are $N - 1$ Nambu-Goldstone bosons carried by the directional fluctuations $\delta\phi^0$ transverse to the direction Φ^0 of the ground state.

Remember that the physical origin is the arbitrarily small change of action for smooth continuous variations of the ground state directions.

At long distances, the only experimental correlations come from the massless modes. There exist many physical phenomena which are dominated by these. They can be studied approximately by ignoring completely the variations of the size of the field ρ , freezing it at the equilibrium value ρ_0 . This is called the *hydrodynamic limit* of the field theory. It describes only the Nambu-Goldstone boson. In the $O(N)$ -symmetric theory, the freezing of the size of the field leaves the directional vector $n_a = \phi_a/|\phi|$ free to fluctuate. Then the field theory model goes over into the classical Heisenberg model.

This limit will be discussed further in Section 19.2.

16.2.2 General Considerations

The necessity of a Nambu-Goldstone particle as a consequence of spontaneous symmetry breakdown can easily be proved for any continuous symmetry and to all orders in perturbation theory by using the full effective action. Let us look only at the case of $O(N)$ -symmetry. The infinitesimal symmetry transformations on the currents are

$$j_a \rightarrow j_a - i\epsilon_{cd} (L_{cd})_{ab} j_b \quad (16.34)$$

where L_{cd} are the $N(N - 1)/2$ generators of $O(N)$ -rotations. Under this, the generating functional is invariant

$$\delta W[j] = \int dx \frac{\delta W[j]}{\delta j_a(x)} i (L_{cd})_{ab} j_b \epsilon_{cd} = 0. \quad (16.35)$$

Let us insert the Legendre transformation laws for Φ and j . Then (16.35) amounts to

$$0 = \int dx \Phi_a(x) i (L_{cd})_{ab} \frac{\delta \Gamma[\Phi]}{\delta \Phi_b(x)} \epsilon_{cd}, \quad (16.36)$$

which expresses the infinitesimal invariance of the effective action under

$$\Phi_a \rightarrow \Phi_a - i\epsilon_{cd} (L_{cd})_{ab} \Phi_b.$$

The invariance law (16.36) is often called the *Ward-Takahashi identity* for the functional $\Gamma[\Phi]$. It can be used to find an infinite set of identities with this name for all vertex functions by forming higher functional derivatives and setting $\Phi = \Phi^0$ at the

end. For example, the first derivative of (16.36) gives (dropping the infinitesimal parameter ϵ_{cd})

$$0 = (L_{cd})_{ab} \frac{\delta\Gamma[\Phi]}{\delta\Phi_b(x)} + \int dx' \Phi_{a'}(x') (L_{cd})_{a'b} \frac{\delta^2\Gamma[\Phi]}{\delta\Phi_b(x')\delta\Phi_a(x)}. \quad (16.37)$$

Setting $\Phi = \Phi^0$, where $j_a = \delta\Gamma[\Phi]/\delta\Phi_b(x) = 0$, gives

$$\int dx' \Phi_{a'}^0(x') (L_{cd})_{a'b} \frac{\delta^2\Gamma[\Phi^0]}{\delta\Phi_b^0(x')\delta\Phi_a^0(x)}.$$

At $\Phi = \Phi^0$, the second derivative of $\Gamma[\Phi^0]$ is simply the vertex function $\Gamma^{(2)}$ at zero momentum which equals the inverse of the connected two-point function in momentum space $G_c(p)$, due to Eq. (13.45). Hence we obtain

$$\Phi_{a'}^0 (L_{cd})_{a'b} [G_c^{-1}]_{ba}(q=0) = 0. \quad (16.38)$$

This statement implies that certain fully interacting propagators have to contain a singularity at $q = 0$. In most cases this is caused by a pole in the momentum square variable q^2 . Then (16.38) implies the existence of a massless particle state in Hilbert space, the Nambu-Goldstone boson. We shall see later which exceptions are possible.

We have argued before that the directions of massless fluctuations must be associated with the valley of degenerate states in the effective potential. The above equation (16.38) is a mathematical expression of this conclusion.

As an example consider the case $N = 2$. Then $(L_{cd}\epsilon_{cd})_{ab}$ is simply the 2×2 -matrix

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \epsilon_{12}.$$

Let the vacuum expectation of the two-component field $\phi_a(x)$ be

$$\Phi^0 = (\Phi^0, 0).$$

Then (16.38) states that

$$[G_c^{-1}]_{22}(q=0) = 0, \quad (16.39)$$

calling for a massless mode along the second field direction. Translating this into the complex field language studied previously, we rewrite $\Phi_a = (\rho \cos \gamma, \rho \sin \gamma)$ as

$$\Phi = \rho e^{i\gamma}.$$

For ρ close to ρ_0 and small γ , this is precisely the massless mode in the azimuthal variable.

For $N = 3$, the rotations may be written as

$$(L_{cd}\epsilon_{cd})_{ab} = -\epsilon_{dab}\alpha_d,$$

where α is a small angle of rotation and $\epsilon_{123} = 1$. Then (16.38) becomes

$$\epsilon_{abd}\Phi_a^0[G_c^{-1}]_{bc}(q=0) = 0. \quad (16.40)$$

If Φ_a^0 points into the direction of the third axis of the $O(3)$ -sphere, the transverse modes $[G_c]_{11}^{(2)}$ and $[G_c]_{22}^{(2)}$ are massless.

Note that only statements on diagonal elements are non-trivial, since $[G_c^{(2)}]_{ij}$ vanishes unless $i = j$, as is obvious at the one-loop level and can be shown to hold for any invariant power $(\Phi_a^2)^n$ appearing in the effective action.

The Nambu-Goldstone theorem has an important exception if the field theory possesses a massless gauge boson from the outset. This is the case in a superconductor, where the electrons are coupled to an electromagnetic field. When a material is cooled below the transition temperature at which its resistance drops to zero, it also expels the magnetic field. This is called the Meissner-Ochsenfeld effect, discovered in 1933.¹ This effect constitutes the basis of present theories of weak interactions. It therefore deserves being discussed in detail in Chapters 17 and 27.

16.2.3 Experimental Consequences

The Nambu-Goldstone phenomenon has important observational consequences. The most simple experiment which can be done on a system is to study the change of energy as a function of an external field j . The functional derivative

$$\frac{\delta W[j]}{\delta j} = \langle 0|\phi(x)|0\rangle_{j=\text{const}} = \Phi \quad (16.41)$$

is observable directly as an order parameter of the system (say as a magnetization). The change of this order parameter with respect to changes in j is measured as the susceptibility $\chi(x, y)$:

$$\frac{\delta\Phi(x)}{\delta j(y)} = \frac{\delta^2 W[j]}{\delta j(x)\delta j(y)} = \langle 0|T\phi(x)\phi(y)|0\rangle \equiv \chi(x, y). \quad (16.42)$$

Its Fourier transform

$$(2\pi)^4\delta^{(4)}(q+q')\chi(q) = \int d^4x \int d^4x' e^{i(qx+q'x')}\chi(x, x') \quad (16.43)$$

at $q_0 = 0$ is called the static susceptibility. Using the identity (13.42), we may write equivalently

$$(2\pi)^4\delta^{(4)}(q+q')\chi^{-1}(q) = -\frac{\delta^2\Gamma[\Phi]}{\delta\Phi_a(q)\delta\Phi_b(q')}, \quad (16.44)$$

¹W. Meissner and R. Ochsenfeld, *Naturwissenschaften* 21, 787 (1933).

or

$$\chi^{-1}(0) = \frac{\partial^2 v}{\partial \Phi_a \partial \Phi_b}. \quad (16.45)$$

Let us calculate these quantities at the mean-field level. For $\tau > 0$ we find

$$\begin{aligned} \chi_{ab}^{-1}(q) &= (m^2 + \mathbf{q}^2 - q_0^2) \delta_{ab} = (\mu^2 \tau + \mathbf{q}^2 - q_0^2) \delta_{ab}, \\ \chi_{ab}^{-1}(0) &= m^2 \delta_{ab} = \mu^2 \tau \delta_{ab}. \end{aligned} \quad (16.46)$$

Thus χ^{-1} increases linearly with τ . It is a favorite quantity for experimental plots. Very close to a critical point, the measurements show deviations from this law due to fluctuations. Near $T = T_c^{\text{MF}}$, one measures a power law parametrized by

$$\chi_{ab}^{-1} = \mu^2 \tau^\gamma \delta_{ab}.$$

The value of γ is called the *critical index* of susceptibility above T_c^{MF} . The derivation of this power behavior will be given in Subsec. 20.9 [see Eq. (20.152)].

As the temperature passes below T_c^{MF} , the spontaneous breakdown of $O(N)$ symmetry leads to a drastic change: The susceptibility $\chi_{ab}(q)$ loses its isotropy in field space. The component $\chi_{\parallel}^{-1}(q)$ longitudinally to the direction Φ_a^0 is produced by the longitudinal projection matrix $(P_{\parallel})_{ab} \equiv \Phi_a^0 \Phi_b^0 / (\Phi^0)^2$ and behaves like

$$\begin{aligned} \chi_{\parallel}^{-1}(q) &= -2m^2 + q^2 - q_0^2 = -2\mu^2 \tau + q^2 - q_0^2, & \tau < 0, \\ \chi_{\parallel}^{-1}(0) &= -2m^2 = -2\mu^2 \tau, & \tau < 0. \end{aligned} \quad (16.47)$$

Then N transverse components of χ_{ab}^{-1} , on the other hand, are obtained from the transverse projection matrix $(P_{\perp})_{ab} \equiv \delta_{ab} - (P_{\parallel})_{ab}$. They vanish at $q = 0$:

$$\chi_{\perp}^{-1}(q) = G^{-1}(q) = q^2 - q_0^2. \quad (16.48)$$

Thus $\chi_{\perp}$ diverges for $q \rightarrow 0$, and this leads to a dramatic experimental effect: If the external source describes incoming waves with weak space-time dependence, the system scatters these very strongly. For example, if j corresponds to an electromagnetic field in the optical range (as is the case in nematic liquid crystals), the system becomes completely opaque (it looks milky). When cooling through T_c^{MF} , this phenomenon is called *critical opalescence*.

Note that a spontaneously broken *continuous* symmetry is necessary for the opalescence below T_c^{MF} . In the case of a single real ϕ field (Ising-like system) there are no Goldstone modes and there is no $\chi_{\perp}^{-1}$ which stays identically equal to zero for $T < T_c^{\text{MF}}$, $q = 0$. There, one sees critical opalescence just in the immediate vicinity of T_c^{MF} , and the system becomes again clear below T_c^{MF} .

16.3 Domain Walls in the $O(1)$ -Symmetric Theory

The field equations following from the Lagrangian (16.1) are

$$\left[\partial^2 + m^2 + g\phi_b^2(x) \right] \phi_a(x) = 0. \quad (16.49)$$

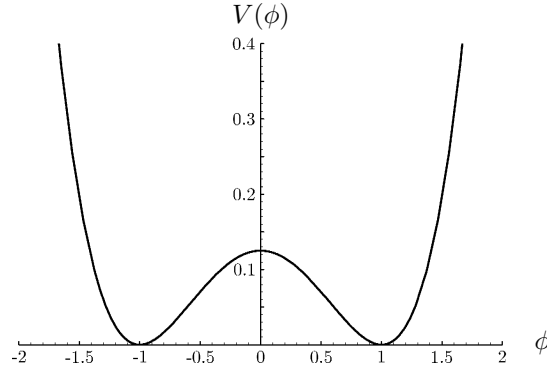


FIGURE 16.4 Plot of the symmetric double-well potential $V(x) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$. We have added a trivial constant $1/4$ to place the minima on the ϕ -axis.

For $m^2 < 0$, where the potential looks like the bottom of a champagne bottle in Fig. 16.1, these equations possess nontrivial static solutions solving the spatial part of the differential equation (16.49):

$$\left[-\nabla^2 + m^2 + g\phi_b^2(\mathbf{x})\right] \phi_a(\mathbf{x}) = 0. \quad (16.50)$$

The simplest nontrivial solution varies only along one axis, say the x -axis, and only in one field component. It will turn out to be a stable solution only if the other components are absent altogether. There the Lagrangian (16.1) possesses merely a reflection symmetry $\phi \rightarrow -\phi$, which in the general context is called an $O(1)$ -symmetry.

Thus we shall study the simplified field equation

$$\left[-\frac{d^2}{dx^2} + m^2 + g\phi^2(x)\right] \phi(x) = 0. \quad (16.51)$$

For a single field component, the potential has the form of a double-well pictured in Fig. 16.4. The equation (16.51) has two trivial constant solutions

$$\phi(x) \equiv \pm\phi_0 \equiv \sqrt{\frac{-m^2}{g}} \quad (16.52)$$

which lie at the two minima of the potential

$$V(\phi) = \frac{m^2}{2}V(x) = \frac{m^2}{2}\phi^2 + \frac{g}{4}\phi^4. \quad (16.53)$$

At the minimum, the potential has the value

$$V_c = -\frac{m^4}{g}, \quad (16.54)$$

which is called the *condensation energy* of the field system. It will be convenient to subtract this from $V(\phi)$ and write the subtracted potential

$$V(\phi) = \frac{m^2}{8\phi_0^2}(\phi - \phi_0)^2(\phi + \phi_0)^2, \quad (16.55)$$

exhibiting more directly the symmetric minima at $\phi = \pm\phi_0$ (see Fig. 16.4). The coupling strength is

$$g = m^2/2\phi_0^2. \quad (16.56)$$

Near the minima, the potential looks approximately like a harmonic oscillator potential $V_{\pm}(\phi_0) = m^2(x \mp \phi_0)^2/2$:

$$V(\phi) = \frac{m^2}{2}(\phi \mp \phi_0)^2 \left(1 \pm \frac{\phi \mp \phi_0}{\phi_0} + \dots \right) \equiv V_{\pm}(\phi) + \Delta V_{\pm}(\phi) + \dots \quad (16.57)$$

The height of the potential barrier at the center is

$$V_{\max} = \frac{(m\phi_0)^2}{8}. \quad (16.58)$$

In the limit $\phi_0 \rightarrow \infty$ at a fixed frequency m , the barrier height becomes infinite and the system decomposes into a sum of two independent harmonic-oscillator potentials widely separated from each other.

The nontrivial solution of the field equation connects the two trivial solutions (16.52) across the barrier. As we shall derive immediately, this reads

$$\phi(x) = \phi_{\text{cl}}^{\pm}(x) \equiv \pm\phi_0 \tanh[m(x - x_0)/2], \quad (16.59)$$

with an arbitrary parameter x_0 specifying the point on the x -axis where the crossing takes place. The crossing takes place over a distance of the order of $2/m$. For large positive and negative x , the solution approaches $\pm\phi_0$ exponentially (see Fig. 16.5).

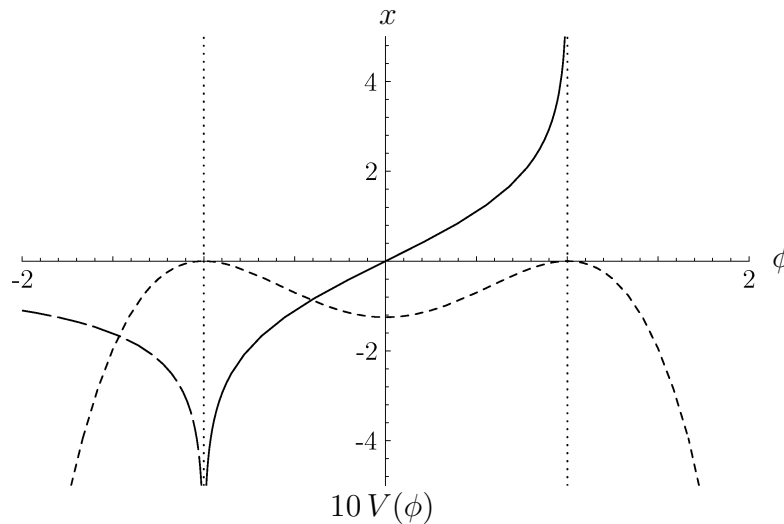


FIGURE 16.5 Classical kink solution (solid curve) in double-well potential (short-dashed curve with units marked on the lower half of the vertical axis). The solution connects the two degenerate maxima in the reversed potential. The long-dashed curve starts out at a maximum and slides down into the adjacent abyss.

The subscript cl on ϕ_{cl} emphasized that these solutions solve the classical field equations. Alluding to their shape, the solutions $\phi_{\text{cl}}^{\pm}(x)$ are called *kink* and *antikink* solutions, respectively.²

To derive these solutions, consider the equation of motion (16.51) in the pseudotime $t = ix$,

$$\ddot{\phi}(t) = -V'(\phi(t)), \quad (16.60)$$

where $V'(\phi) \equiv dV(\phi)/d\phi$. Since the differential equation is of second order, there is merely a sign change in front of the potential with respect to the spatial differential equation (16.51). The equation of motion (16.60) therefore corresponds to a usual equation of motion of a point particle as a function of the pseudotime t , whose potential is turned upside down with respect to Fig. 16.4. This is illustrated in Fig. 16.6. The reversed potential allows obviously a classical solution which starts

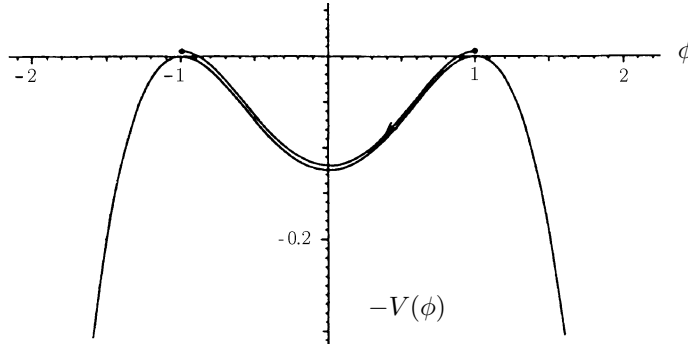


FIGURE 16.6 Reversed double-well potential governing the motion of the position ϕ as a function of the imaginary time x .

out at $\phi = -\phi_0$ for $x \rightarrow -\infty$ and arrives at $\phi = \phi_0$ for $x \rightarrow +\infty$. The particle needs an infinite time to leave the initial potential mountain and to climb up to the top of the final one. The movement through the central valley proceeds within the finite time $\approx 2/m$. If the particle does not start its movement exactly at the top but slightly displaced towards the valley, say at $\phi = -a + \epsilon$, it will reach $\phi = a - \epsilon$ after a finite time, then return to $\phi = -a + \epsilon$, and oscillate back and forth forever. In the limit $\epsilon \rightarrow 0$, the period of oscillation goes to infinity and only a single crossing of the valley remains.

To calculate this movement, the differential equation (16.49) is integrated once after multiplying it by $\phi' = dx/dx$ and rewriting it as

$$\frac{1}{2} \frac{d}{dx} x'^2 = \frac{d}{dx} V(\phi(x)). \quad (16.61)$$

²In much of the the field-theoretic literature, such solutions are also referred to as *instanton* or *anti-instanton* solutions, the name emphasizing the fact that the valley is crossed within a short time interval. See the references quoted at the end of the chapter.

The integration gives

$$\frac{x'^2}{2} + [-V(\phi(x))] = \text{const}. \quad (16.62)$$

If x is reinterpreted as the physical time, this is the law of *energy conservation* for motion in the reversed potential $-V(\phi)$. Thus we identify the integration constant in (16.62) as the total energy E in the reversed potential:

$$\text{const} \equiv E. \quad (16.63)$$

Integrating (16.62) further gives

$$x - x_0 = \pm \frac{1}{\sqrt{2}} \int_{\phi(x_0)}^{\phi(x)} \frac{d\phi}{\sqrt{E + V(\phi)}}. \quad (16.64)$$

A look at the potential in Fig. 16.6 shows that an orbit that starts out with the particle at rest for $x \rightarrow -\infty$ must have $E = 0$. Inserting the explicit potential (16.55) into (16.64), we obtain for $|\phi| < \phi_0$

$$\begin{aligned} x - x_0 &= \pm \frac{2\phi i_0}{m} \int_0^\phi \frac{d\phi'}{(\phi_0 - \phi')(\phi' + \phi_0)} = \pm \frac{1}{m} \log \frac{\phi_0 + \phi}{\phi_0 - \phi} \\ &= \pm \frac{2}{m} \text{artanh} \frac{\phi}{\phi_0}. \end{aligned} \quad (16.65)$$

Thus we find the kink and antikink solution (16.59) crossing the barrier.

The euclidean action of such a solution can be calculated as follows [using (16.62) and (16.63)]:

$$\begin{aligned} \mathcal{A}_{\text{cl}} &= \int_{-\infty}^{\infty} dx \left[\frac{\phi'_{\text{cl}}{}^2}{2} + V(\phi_{\text{cl}}(x)) \right] = \int_{-\infty}^{\infty} dx (\phi'_{\text{cl}}{}^2 - E) \\ &= -EL + \int_{-a}^a dx \sqrt{2[E + V(\phi)]}. \end{aligned} \quad (16.66)$$

The kink has $E = 0$, so that

$$\sqrt{2(E + V(\phi))} = \frac{m}{2\phi_0}(\phi_0^2 - \phi^2), \quad (16.67)$$

and the classical action becomes

$$\mathcal{A}_{\text{cl}} = \frac{m}{2\phi_0} \int_{-\phi_0}^{\phi_0} d\phi (\phi_0^2 - \phi^2) = \frac{2}{3} \phi_0^2 m = \frac{m^3}{3g}. \quad (16.68)$$

Note that for $E = 0$, the classical action is also given by the integral

$$\mathcal{A}_{\text{cl}} = \int_{-\infty}^{\infty} dx \frac{\phi'_{\text{cl}}{}^2}{2}. \quad (16.69)$$

There are also solutions starting out at the top of either mountain and sliding down into the adjacent exterior abyss, for instance (see again Fig. 16.6)

$$\begin{aligned} x - x_0 &= \mp \frac{2\phi_0}{m} \int_{\phi}^{\infty} \frac{d\phi'}{(\phi' - \phi_0)(\phi' + \phi_0)} = \pm \frac{1}{m} \log \frac{\phi + \phi_0}{\phi - \phi_0} \\ &= \pm \frac{2}{m} \operatorname{arccoth} \frac{\phi}{\phi_0}. \end{aligned} \quad (16.70)$$

However, these solutions cannot connect the bottoms of the double well with each other and will not be considered further.

The real ϕ^4 -theory can be used as a model for a spin system, in which the spins can point only in two directions. In statistical mechanics, such a system is usually described by the *Ising model* on a lattice. In fact, it can be shown that the Ising model can be transformed into a real ϕ^4 -field theory whose potential can be approximated, near the phase transition, by a ϕ^4 -potential. The two spin directions are represented in the ϕ^4 -theory by the two minima of the potential. The classical solution to the field equation may be interpreted as a domain wall between up and down directions. Domain walls can occur in many possible shapes which are too hard to calculate analytically. They possess a high configurational entropy, and the demagnetization transition can be understood as a transition in the ensemble of fluctuating domain walls of any shape. Their configurational entropy overcomes the energy consumed in the process of creating the domain walls.

Let us finally realize that domain walls in O(N)-symmetric theories cannot be stable: It is always possible to rotate the spin direction of one domain into another direction thereby lowering continuously the energy. This is impossible for a single-component real ϕ -field.

16.4 Vortex Lines in the O(2)-Symmetric Theory

The most important domain of application of the O(2)-symmetric theory is the study of the superfluid phase transition in liquid helium at $T_c \approx 2.3$ K. The two-component ϕ^4 theory is then referred to as *Landau-Pitaevskii theory*. Its euclidean action is written in terms of a complex field $\varphi = (\phi_1 + i\phi_2)/\sqrt{2}$ in $D = 3$ space dimensions as an energy density

$$\mathcal{H} = \varphi^*(\mathbf{x}) \left(-\frac{\hbar^2}{2M} \nabla^2 - \mu \right) \varphi(\mathbf{x}) + g|\varphi(\mathbf{x})|^4, \quad (16.71)$$

where μ is the chemical potential which passes through zero at some critical mean-field temperature T_c^{MF} :

$$\mu = \mu_0 \left(\frac{T}{T_c^{\text{MF}}} - 1 \right). \quad (16.72)$$

The quartic term approximates the repulsion between the helium atoms by a δ -function potential [recall the second-quantized Hamiltonian (2.139)].

The field equation which minimizes this energy density is

$$\left(-\frac{\hbar^2}{2M}\nabla^2 - \mu + g|\varphi|^2\right)\varphi = 0. \quad (16.73)$$

It possesses cylindrical solutions which are observable in the laboratory in the form of straight vortex lines. To find these, we decompose φ into its polar components as $\varphi = \rho e^{i\gamma}$, and find from the real and imaginary parts of Eq. (16.73) the two equations

$$\left\{-\frac{\hbar^2}{2M}[\nabla^2 - (\nabla\gamma)^2] - \mu + g\rho^2\right\}\rho = 0, \quad (16.74)$$

and

$$\nabla(\rho^2\nabla\gamma) = 0. \quad (16.75)$$

The latter equation is simply the radial-azimuthal form of the conservation law for the particle current $\mathbf{j}$:

$$\nabla\mathbf{j} = \nabla\left(\frac{1}{2i}\varphi^*\overleftrightarrow{\nabla}\varphi\right) = 0. \quad (16.76)$$

Equation (16.75) can be solved by a purely circular flow of particles, in which ρ depends on the spatial distance r from the cylindrical axis, and the phase γ of the complex field is an integer multiple of the azimuthal angle in space, $\theta \equiv \tan^{-1}(x_2/x_1)$, i.e.,

$$\gamma = n\theta. \quad (16.77)$$

Then, (16.74) reduces to the radial differential equation

$$-\frac{\hbar^2}{2M}\left(\partial_r^2 + \frac{1}{r} - \frac{n^2}{2}\right)\rho + g(\rho^2 - \rho_0^2)\rho = 0, \quad (16.78)$$

where $\rho_0 = |\varphi_0| = \sqrt{-\mu/g} = \sqrt{-\mu_0(T/T_c^{\text{MF}} - 1)/g}$ [compare (16.73)].

In order to solve Eq. (16.78), it is convenient to go to the reduced quantities

$$\bar{x} \equiv x/\xi, \quad \bar{r} \equiv r/\xi, \quad (16.79)$$

which measure the distances in units of the coherence length

$$\xi = \sqrt{2}\xi_{\text{size}} = \sqrt{\frac{\hbar^2}{2Mg\varphi_0^2}} = \sqrt{\frac{\hbar^2}{2M(-\mu_0)}}\sqrt{\frac{T}{T_c^{\text{MF}}} - 1}^{-1}. \quad (16.80)$$

We also measure the size of the order parameter ρ in units of ρ_0 , and introduce the reduced field strength

$$\bar{\rho} \equiv \rho/\rho_0 = |\varphi|/|\varphi_0|. \quad (16.81)$$

Then (16.78) takes the form

$$\left[-\left(\partial_{\bar{r}}^2 + \frac{1}{\bar{r}}\partial_{\bar{r}} - \frac{n^2}{\bar{r}^2}\right) + (\bar{\rho}^2 - 1)\right]\bar{\rho}(\bar{r}) = 0. \quad (16.82)$$

For small $\bar{r} \ll 1$, this is dominated by the terms in the first parentheses, leading to a differential equation of the Bessel type for $\bar{\rho}(\bar{r})$. Thus, close to the origin, the solution is

$$\bar{\rho}(\bar{r}) = A_n J_n(\bar{r}) \propto \bar{r}^n, \quad (16.83)$$

where $J_n(\bar{r})$ is the standard Bessel function. Multiplying this with the phase factor

$$e^{in\gamma} = e^{in \tan^{-1}(x_2/x_1)}, \quad (16.84)$$

we see that the complex field $\varphi(x)$ has the following small- $|\mathbf{x}|$ behavior:

$$\varphi(\mathbf{x}) \propto \bar{r}^n e^{in \tan^{-1}(x_2/x_1)} = (x_1 + ix_2)^n, \quad (16.85)$$

exhibiting a zero of n -th order in the complex plane $x_1 + ix_2$.

For large $\bar{r} \gg 1$, $\bar{\rho}(\bar{r})$ approaches the asymptotic value $\bar{\rho} = 1$. In fact, from (1.44) we can extract the $1/\bar{r}$ expansion,

$$\bar{\rho}_n(\bar{r}) = 1 - \frac{n^2}{2\bar{r}^2} - \left(n^2 + \frac{1}{8}n^4\right) \frac{1}{\bar{r}^4} - \left(8 + 2n^2 + \frac{1}{16}n^4\right) \frac{n}{\bar{r}^6} - O\left(\frac{1}{\bar{r}^8}\right). \quad (16.86)$$

Integrating the differential equation numerically inward, we find the solution displayed in Fig. 16.7. What is the energy of these vortex lines? In order to find a

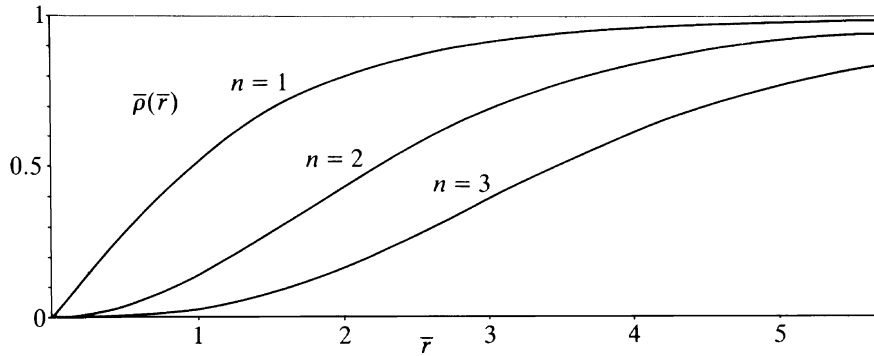


FIGURE 16.7 Reduced order parameter $\bar{\rho} = |\varphi|/|\varphi_0|$ around a vortex line of strength $n = 1, 2, 3, \dots$ as a function of the reduced distance $\bar{r} = r/\xi$, where r is the distance from the axis and ξ the healing length.

convenient expression for it we use the fact that, if $\varphi(\mathbf{x})$ is a solution of the differential equation (16.73), the rescaled solution

$$\varphi_\delta(\mathbf{x}) \equiv e^\delta \varphi(\mathbf{x}) \quad (16.87)$$

must extremize the energy as a function of δ at $\delta = 0$. In terms of the reduced quantities of Eqs. (16.79) and (16.81), the energy is given by

$$E = E_c \int d^3\bar{x} \left[|\nabla \bar{\varphi}|^2 - |\bar{\varphi}|^2 + |\bar{\varphi}|^4 \right], \quad (16.88)$$

where

$$E_c = \frac{\mu^2}{4g} \quad (16.89)$$

is the condensation energy. Inserting the reduced version of (16.87) into (16.88), we obtain

$$E = E_c \int d^3\bar{x} \left[e^{2\delta} |\nabla \bar{\varphi}|^2 - e^{2\delta} |\bar{\varphi}|^2 + e^{4\delta} |\bar{\varphi}|^4 \right]. \quad (16.90)$$

Setting the derivative with respect to δ equal to zero gives, at $\delta = 0$,

$$E_c \int d^3\bar{x} \left[|\nabla \bar{\varphi}|^2 - |\bar{\varphi}|^2 + 2|\bar{\varphi}|^4 \right] = 0. \quad (16.91)$$

Subtracting this from (16.90) at $\delta = 0$, we find that the energy of a solution of the field equation is simply given by

$$E = -E_c \int d^3\bar{x} |\bar{\varphi}|^4. \quad (16.92)$$

Most of this energy is due to the asymptotic value $|\bar{\varphi}| \rightarrow 1$, where E is equal to the negative condensation energy $-E_c$. Subtracting this from (16.90) at $\delta = 0$, we find the *additional energy* of the vortex line as

$$E_v = E_c \int d^3x (1 - |\bar{\varphi}|^4). \quad (16.93)$$

Going over to cylindrical coordinates $\bar{r}, \theta, z$, the integral becomes, for a vortex line of length L along the z -direction:

$$E_v = E_c 2\pi \bar{L} \int_0^x d\bar{r} \bar{r} \left[1 - \bar{\rho}^4(\bar{r}) \right]. \quad (16.94)$$

Before inserting the numerical solutions for $\bar{\rho}(\bar{r})$ shown in Fig. (16.7), we note that due to the factor $\bar{r}$, the additional energy comes mainly from the large $\bar{r}$ regime, i.e., from the far zone. In fact, if we insert the leading asymptotic behavior (16.86), we obtain an integral

$$E_v = E_c 4\pi n^2 \bar{L} \int^\infty \frac{d\bar{r}}{\bar{r}}, \quad (16.95)$$

which diverges logarithmically for large $\bar{r}$. An immediate conclusion is that a single vortex line can have a finite energy only in a container of finite size. In a cylindrical container of finite length L and finite radius R , the r -integral no longer diverges, and we obtain

$$E_v = E_c 4\pi n^2 \bar{L} \log(R/\xi). \quad (16.96)$$

Consider now the energy in the small- $\bar{r}$ regime, where Eq. (16.83) tells us that $\bar{\rho}(\bar{r})$ behaves like $\bar{r}^n$. Hence, $1 - \bar{\rho}^4 \approx 1$, and the energy of a thin cylindrical section of

radius r grows like r^2 . For increasing r , the rate of growth slows down rapidly and settles at the asymptotic rate $4\pi n^2 L \times \log(\bar{r}/\xi)$, where ξ is the coherence length. The proper inclusion of the non-asymptotic behavior gives simply a finite correction to the asymptotic energy, and the energy of a vortex line in a container of radius R becomes

$$E_v = E_c 4\pi n^2 \bar{L} [\log(R/\xi) + c]. \quad (16.97)$$

This is the same result that would have been obtained by replacing in (16.94) the integrand $\bar{r}[1 - \bar{\rho}^4(\bar{r})]$ by the asymptotic form $2n^2/\bar{r}$, and performing the integral from the radius $r_0 = \xi e^{-c}$ to R .

The precise numerical evaluation of the differential equation (16.82) and the integral (16.94) shows that for the lowest vortex line, c has the value

$$c = 0.385. \quad (16.98)$$

Hence the energy of the vortex line becomes

$$E_v = E_c \bar{L} 4\pi n^2 [\log(R/\xi) + 0.385]. \quad (16.99)$$

The logarithmic divergence of the energy has a simple physical origin. In order to see this, let us calculate the energy once more in another way, using the original expression (16.88), i.e. without invoking the virial theorem. It reads, for the radial solutions,

$$E_v = E_c 4\pi \bar{L} \int d\bar{r} \bar{r} \left[(\partial_{\bar{r}} \bar{\rho})^2 + \frac{1}{2}(1 - \bar{\rho}^2)^2 + \frac{n^2}{\bar{r}^2} \bar{\rho}^2 \right]. \quad (16.100)$$

The first two terms are rapidly convergent. Thus the energy of the far zone resides completely in the last term

$$\frac{n^2}{\bar{r}^2} \bar{\rho}^2 \approx \frac{n^2}{\bar{r}^2}. \quad (16.101)$$

This energy is a consequence of the angular behavior of the condensate phase $\gamma = n \tan^{-1}(x_2/x_1)$ around a vortex line. It comes entirely from the *azimuthal part* of the gradient energy $(\hbar^2/2M^2)|\varphi|^2(\nabla\gamma)^2$, i.e., the term which describes the *Nambu-Goldstone modes*. This is not surprising. We have discussed before that the *long range properties* of the system are dominated by these modes. A phase of the field φ which behaves like $\gamma = n \tan^{-1}(x_2/x_1)$ can be viewed as a coherent pile-up of these modes determining the energy in the far zone.

The dominance of the energy carried by the phase gradient can also be described in a different and more physical way. In the last section we identified the gradient $(\hbar/M)\nabla\gamma$ with the superfluid velocity. For the vortex line at hand, the superfluid velocity is found, far away from the line, to be

$$\mathbf{v}_s = \frac{\hbar}{M} n \nabla \tan^{-1} \left(\frac{x_2}{x_1} \right) = \frac{\hbar}{M} \frac{n}{r^2} (-x_2, x_1, 0) = \frac{\hbar}{M} n \frac{1}{r} \mathbf{e}_\phi, \quad (16.102)$$

where $\mathbf{e}_\phi$ is the unit vector in the azimuthal direction. Thus, around every vortex line, there is a circular flow of the superfluid whose velocity decreases like the inverse distance from the line. The hydrodynamic energy density of this flow is

$$\mathcal{E}(\mathbf{x}) = \frac{\rho_s}{2} \mathbf{v}_s^2 = \frac{\rho_s}{2} \frac{\hbar^2}{M^2} \frac{n^2}{r^2}. \quad (16.103)$$

This is precisely the dominant third term in the energy integral (16.100). Thus the energy of the vortex line is indeed mainly due to the hydrodynamic energy of the superflow around the line. For a major part of the volume, the hydrodynamic limits in expression (16.103) give an excellent approximation. Only in the neighborhood of the line, i.e., for small radii $r \leq \xi$, the energy density differs from (16.103) due to gradients in the size of the field $|\varphi|$. It is therefore suggestive to idealize the superfluid and assume the validity of the pure gradient energy density

$$\mathcal{E}(\mathbf{x}) = \frac{\rho_s}{2} \mathbf{v}_s^2 = \frac{\sigma}{2} (\nabla \gamma)^2, \quad \sigma \equiv \rho_s \frac{\hbar^2}{M^2}, \quad (16.104)$$

everywhere in space, where ρ_s is the *superfluid density*.

The deviations from this law, which become significant only very close to a vortex line, i.e., at distances of the order of the coherence length ξ , are treated approximately by simply cutting off the energy integration at a radius ξ away from a vortex line. In other words, we pretend as though there is no superflow at all within the thin tubes of radius ξ , with a sudden onset of idealized flow outside ξ , moving with the limiting velocity (16.102).

Although the internal part of the thin tube carries no superflow, it does carry rotational energy. Within the present approximation, this energy is associated with the number 0.385 in (16.99). This piece is called the *core energy*. The core energy has a physical interpretation. At distances smaller than the coherence length, the different parts of the liquid can no longer slip past each other freely. Hence the core of a vortex line is expected to rotate roughly like a solid rod, rather than with the diverging velocity $v_s \sim 1/r$. Indeed, if we use the approximation for a line of vortex strength n ,

$$v_s \propto n \begin{cases} \frac{1}{r}, & r > \xi, \\ \frac{r}{\xi^2}, & r \leq \xi, \end{cases} \quad (16.105)$$

the energy density behaves like r^2 , for small r , as observed before. Moreover, the energy integration gives

$$n^2 \left[\int_1^{R/\xi} d\bar{r}/\bar{r} + \int_0^1 d\bar{r} \bar{r}^3 \right] = n^2 [\log(R/\xi) + 0.25], \quad (16.106)$$

and we see that the number for the core energy, 0.25, emerges with the right order of magnitude.

In order to complete our discussion of the hydrodynamic picture, let us calculate the circulation of the superfluid velocity field around the vortex lines:

$$\kappa \equiv \oint_B d\mathbf{x} \cdot \mathbf{v}_s = \frac{\hbar}{M} n \oint_B d\mathbf{x} \cdot \nabla \gamma = \frac{\hbar}{M} 2\pi n = n \frac{h}{M} = n\kappa_1. \quad (16.107)$$

This integral is the same for any size and shape of the circuit B around the vortex line. Thus the circulation is quantized. It always appears in multiplets of $\kappa_1 = h/M \approx 10^{-3} \text{ cm}^2/\text{sec}$. The number n is called *vortex strength*.

The integral (16.107) can be transformed into a surface integral via Stokes' theorem:

$$\int_{S^B} d\mathbf{S} \cdot (\nabla \times \mathbf{v}_s) = \frac{\hbar}{M} 2\pi n, \quad (16.108)$$

where S^B is some surface spanned by the circuit B in (16.107), and $d\mathbf{S}$ is the surface element. This integral is the same for any size and shape of S^B . From this result we conclude that the third component of the curl of $\mathbf{v}_s$ must vanish everywhere, except at the origin. There it must have a singularity of such a strength that the two-dimensional integral gives the correct vortex strength. Hence

$$\nabla \times \mathbf{v}_s = \frac{\hbar}{M} 2\pi n \delta^{(2)}(\mathbf{x}_T) \hat{\mathbf{z}}, \quad (16.109)$$

where $\hat{\mathbf{z}}$ is the unit vector along the z -axis and $\mathbf{x}_T \equiv (x_1, x_2)$ are the coordinates orthogonal to the vortex line.

If the nonlinearities of the field equation are taken into account, the $\delta^{(2)}$ -function is really smeared out over a circle whose radius is of order ξ . As an example, let us replace $1/r^2$ in (16.103) by $1/(r^2 + \varepsilon^2)$. Then the rotation of the superfluid velocity becomes

$$\nabla \times \mathbf{v}_s = \frac{\hbar}{M} n \frac{2\varepsilon^2}{(r^2 + \varepsilon^2)^2} \hat{\mathbf{z}}. \quad (16.110)$$

The right-hand side is non-zero only within a small radius $r \neq \varepsilon$, where it diverges with the total strength

$$\int d^2x \frac{2\varepsilon^2}{(r^2 + \varepsilon^2)^2} = 2\pi\varepsilon^2 \int_0^\infty dr \frac{2r}{(r^2 + \varepsilon^2)^2} = 2\pi. \quad (16.111)$$

This shows that (16.110) is, indeed, a smeared out version of the δ -function relation (16.109).

Because of their rotational properties, vortex lines can be generated experimentally by rotating a vessel with an angular velocity m . Initially, the lack of friction will cause the superfluid part of the liquid to remain at rest. This situation cannot, however, persist forever since it is not in a state of thermal equilibrium. After some time, vortex lines form on the walls. They migrate into the liquid and distribute

themselves evenly. This goes on until their total number is such that the rotational Helmholtz free energy

$$F_{\Omega} = F - \Omega \cdot \mathbf{L} \approx \int d^3x \left(\frac{\rho_s}{2} \mathbf{v}_s^2 - \Omega \cdot \mathbf{x} \times \rho_s \mathbf{v}_s \right) \quad (16.112)$$

is minimal. This equilibration process has been observed in the laboratory and has even been photographed directly using the property that vortex lines trap ions which can be accelerated against a photographic plate. Integrating (16.112) with $\mathbf{v}_s$ from (16.102), we find that in a cylindrical vessel of radius R , the first vortex line $n = 1$ appears at a critical angular velocity

$$\Omega_c = \frac{\kappa_1}{\pi R^2} \log \frac{R}{\xi} \quad (16.113)$$

and settles on the axis of rotation.

Note that vortex lines of higher n are all unstable. Since the energy increases quadratically with n , it is favorable for a single line of higher n to decay into n lines of unit strength. When generating vortex lines by stirring a vessel, one may nevertheless be able to create, for a short time, such unstable lines, and observe their decay.

Notes and References

For more information on vortex lines see the review articles by

A.L. Fetter, *Quantum Theory of Superfluid Vortices*, Phys. Rev. **162**, 1437 (1967); *Rotating Trapped Bose-Einstein Condensates*, Rev. Mod. Phys. **81**, 647 (2009).

See also the textbook

H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I: *Superflow and Vortex Lines*, World Scientific, 1989 (<http://klnrt.de/b1>),

as well as:

H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4 -Theories*, World Scientific, Singapore 2001 (<http://klnrt.de/b8>);

H. Kleinert, *Multivalued Fields in Condensed Matter, Electromagnetism, and Gravitation*, World Scientific, Singapore 2009, pp. 1–497 (<http://klnrt.de/b11>).

*A complex system that works is invariably found
to have evolved from a simple system that works.*

JOHN GALL

17

Scalar Quantum Electrodynamics

In nature, there exist scalar particles which are charged and are therefore coupled to the electromagnetic field. In three spatial dimensions, an important nonrelativistic example is provided by superconductors. The phenomenon of zero resistance at low temperature can be explained by the formation of so-called *Cooper pairs* of electrons of opposite momentum and spin. These behave like bosons of spin zero and charge $q = 2e$, which are held together in some metals by the electron-phonon interaction. Many important predictions of experimental data can be derived from the *Ginzburg-Landau theory* of superconductivity [1]. The relativistic generalization of this theory to four spacetime dimensions is of great importance in elementary particle physics. In that form it is known as *scalar quantum electrodynamics* (scalar QED).

17.1 Action and Generating Functional

The Ginzburg-Landau theory is a three-dimensional euclidean quantum field theory containing a complex scalar field

$$\varphi(\mathbf{x}) = \varphi_1(\mathbf{x}) + i\varphi_2(\mathbf{x}) \quad (17.1)$$

coupled to a magnetic vector potential $\mathbf{A}$. The scalar field describes bound states of pairs of electrons, which arise in a superconductor at low temperatures due to an attraction coming from elastic forces. The detailed mechanism will not be of interest here; we only note that the pairs are bound in an *s*-wave and a spin singlet state of charge $q = 2e$. Ignoring for a moment the magnetic interactions, the ensemble of these bound states may be described, in the neighborhood of the superconductive transition temperature T_c , by a complex scalar field theory of the φ^4 -type, by a euclidean action

$$\mathcal{A}_E = \int d^3x \left[\frac{1}{2} \nabla \varphi^* \nabla \varphi + \frac{m^2}{2} \varphi^* \varphi + \frac{g}{4} (\varphi^* \varphi)^2 \right]. \quad (17.2)$$

The mass parameter depends on the temperature like $m^2 \propto (T - T_c)/T_c$. Above the transition temperature, the parameter m^2 is positive, below it is negative. As

a consequence, the system exhibits a spontaneous symmetry breakdown discussed in Chapter 16. The symmetry group that is broken, is given by the U(1) phase transformation

$$\varphi(x) \rightarrow e^{-i\alpha} \varphi(x) \quad (17.3)$$

under which $\mathcal{A}_E$ is obviously invariant. Alternatively we may write

$$\begin{aligned} \varphi_1 &\rightarrow \cos \alpha \varphi_1 + \sin \alpha \varphi_2, \\ \varphi_2 &\rightarrow -\sin \alpha \varphi_1 + \cos \alpha \varphi_2, \end{aligned} \quad (17.4)$$

so that we may equally well speak of an O(2)-symmetry.

The action (17.2) is the euclidean version of a relativistic field theory in $D = 2+1$ dimensions, with an action

$$\mathcal{A}_E = \int d^D x \left[\frac{1}{2} \partial_\mu \varphi^* \partial^\mu \varphi - \frac{m^2}{2} \varphi^* \varphi - \frac{g}{4} (\varphi^* \varphi)^2 \right]. \quad (17.5)$$

For the sake of generality, we shall discuss this theory for arbitrary D . Most formulas will be written down explicitly in $D = 4$ dimensions, to emphasize analogies with proper QED discussed in Chapter 12.

The phenomenon of spontaneous symmetry breakdown in this system has been studied in detail in Chapter 16. For $T > T_c$, where the mass term is positive, small oscillations around $\varphi = 0$ consist of two degenerate modes carried by φ_1, φ_2 , both of mass m^2 . For $T < T_c$, where the mass is negative, the energy is minimized by a field φ with a real non-vanishing vacuum expectation value, say

$$\langle \varphi(\mathbf{x}) \rangle \equiv \varphi_0. \quad (17.6)$$

Then the symmetry between φ_1 and φ_2 is broken and there are two different modes of small oscillations: one orthogonal to $\langle \varphi \rangle$, which is the massless Nambu-Goldstone mode, and one parallel to $\langle \varphi \rangle$, which has a positive mass $-2m^2 > 0$.

In order to describe the phenomena of superconductivity with the euclidean version of (17.5), we must include electromagnetism. According to the minimal substitution rules described in Chapter 12, we simply replace $\partial_\mu \varphi$ in (17.5) by the covariant derivative

$$\partial_\mu \varphi \rightarrow D_\mu \varphi \equiv (\partial_\mu - iqA_\mu) \varphi. \quad (17.7)$$

The extra vector potential $A^\mu(x)$ is assumed to be governed by Maxwell's electromagnetic action [see (12.3)]:¹

$$\mathcal{A}_\gamma = -\frac{1}{4} \int d^D x F_{\mu\nu}(x) F^{\mu\nu}(x). \quad (17.8)$$

The combined action becomes

$$\mathcal{A}_{\text{se}}[\varphi, \varphi^*, A] = \int d^D x \left\{ \frac{1}{2} |D_\mu \varphi|^2 - \frac{m^2}{2} |\varphi|^2 - \frac{g}{4} |\varphi|^4 - \frac{1}{4} F_{\mu\nu}^2 \right\}. \quad (17.9)$$

¹In this chapter we use natural units with $\hbar = c = 1$.

where $F_{\mu\nu}^2$ is short for $F_{\mu\nu}F^{\mu\nu}$. This action is invariant under local gauge transformations

$$\varphi(x) \rightarrow e^{iq\Lambda(x)}\varphi(x), \quad A_\mu(x) \rightarrow A_\mu(x) + \partial_\mu\Lambda(x). \quad (17.10)$$

A functional integration leads to the generating functional of scalar QED:

$$Z[\lambda, \lambda^*, j] = \int \mathcal{D}\varphi \mathcal{D}\varphi^* \int_{\text{phys.}} \mathcal{D}A^\mu e^{i\{A_{\text{se}}[\varphi, \varphi^*, A^\mu] - \int_x \lambda^* \varphi - \int_x \varphi^* \lambda - \int_x j^\mu A_\mu\}}, \quad (17.11)$$

where the symbol $\int_x$ abbreviates the volume integral $\int d^4x$, and $\lambda(x)$, $\lambda^*(x)$ are the sources of the complex scalar fields $\varphi^*(x)$ and $\varphi(x)$. The vector $j^\mu(x)$ is an external electromagnetic current coupled to the vector gauge field $A^\mu(x)$. To preserve the gauge invariance, the current is assumed to be a conserved quantity and satisfy $\partial_\mu j^\mu(x) = 0$. The functional integration over the vector field $\int_{\text{phys.}} \mathcal{D}A^\mu$ assumes that a Faddeev-Popov gauge fixing factor is inserted, together with a compensating determinant (recall the general discussion in Section 14.16):

$$\int_{\text{phys.}} \mathcal{D}A^\mu \equiv \int \mathcal{D}A^\mu \Phi^{-1}[A] F[A]. \quad (17.12)$$

For $m^2 > 0$, we may choose [recall (14.353)]

$$F[A] = F_4[A] = e^{-\frac{1}{2\alpha} \int_x (\partial_\mu A^\mu)^2}, \quad (17.13)$$

and derive from (17.11) the Feynman rules for perturbation expansions. The gauge-fixed photon propagator was given in Eq. (14.373):

$$\text{wavy line } q \quad G_{0\mu\nu}(x-y) = - \int \frac{d^D k}{(2\pi)^D} e^{-ik(x-y)} \frac{i}{k^2} \left[g_{\mu\nu} - (1-\alpha) \frac{k_\mu k_\nu}{k^2} \right]. \quad (17.14)$$

We have seen in Chapter 12 that in QED all scattering amplitudes are independent of the gauge parameter α .

In addition, the perturbation expansion derived from the generating functional (17.11) employs propagators of scalar particles represented by lines

$$\text{straight line } p \quad e^{-ik(x-y)} \quad G_0(x-y) = \int \frac{d^D k}{(2\pi)^D} e^{-ik(x-y)} \frac{i}{k^2 - m^2} \quad (17.15)$$

and vertices

$$\begin{array}{c} \text{left-hand diagram: a horizontal straight line with momentum } p \text{ entering from the left and } p' \text{ exiting to the right. A vertical wavy line with momentum } k \text{ enters the line from above.} \\ \text{right-hand diagram: a horizontal straight line with momentum } p \text{ entering from the left and } p' \text{ exiting to the right. Two wavy lines with momenta } k \text{ and } k' \text{ enter the line from above at different points.} \end{array} \quad (17.16)$$

Since the scalar field is complex, the particle carries a charge, and the charged particle lines in the Feynman diagrams carry an orientation. The coupling of the scalar field to the vector potential does not only give rise to a three-point vertex of the type (12.95) in QED [left-hand diagram in (17.16)], but also to a four-vertex in which two photons are absorbed or emitted by a scalar particle [right-hand diagram in (17.16)]. This diagram is commonly referred to as *seagull diagram*.

17.2 Meissner-Ochsenfeld-Higgs Effect

The situation is drastically different for $T < T_c$ where $m^2 < 0$. At the classical level, the lowest energy state of the pure φ theory is reached at $\varphi = \varphi_0$ with $|\varphi_0| = \phi_0 = \sqrt{-m^2/g}$, i.e.,

$$\varphi_0 = \phi_0 e^{-i\gamma_0} = \sqrt{\frac{-m^2}{g}} e^{-i\gamma_0}. \quad (17.17)$$

Now the photon part of the action (17.9) reads

$$\mathcal{A}_\gamma = \int d^D x \left(-\frac{1}{4} F_{\mu\nu}^2 - \frac{q^2 m^2}{2g} A_\mu^2 \right). \quad (17.18)$$

Extremization of this leads to the Euler-Lagrange equation

$$\partial^2 A_\mu - \partial_\mu \partial A - \frac{q^2 m^2}{g} A_\mu = 0. \quad (17.19)$$

Note that we could have chosen as well

$$\varphi = \phi_0 e^{-i\gamma_0(x)} = \sqrt{\frac{-m^2}{g}} e^{-i\gamma_0(x)}, \quad (17.20)$$

with an arbitrary spacetime-dependent phase $\gamma_0(x)$. Then the photon Lagrangian would read

$$\mathcal{A}_\gamma = \int d^D x \left[-\frac{1}{4} F_{\mu\nu}^2 - \frac{q^2 m^2}{2g} (A_\mu - \partial_\mu \gamma_0)^2 \right], \quad (17.21)$$

with the Euler-Lagrange equation

$$\partial^2 A_\mu - \partial_\mu (\partial A) - q^2 \frac{m^2}{g} (A_\mu - \partial_\mu \gamma_0) = 0. \quad (17.22)$$

The extremal field is reached at

$$A_\mu(x) = \partial_\mu \gamma_0(x). \quad (17.23)$$

Of course, the two results (17.19) and (17.22) are equivalent by a gauge transformation $A_\mu \rightarrow A_\mu + \partial_\mu \gamma_0(x)$, and the physical content of (17.21) is independent of the particular choice of $\gamma_0(x)$.

Consider now the fluctuation properties of this theory. The generating functional has the form (17.11) in which the measure sums over all φ and physical A^μ configurations orthogonal to the gauge degrees of freedom. If we decompose φ into radial and azimuthal parts

$$\varphi(x) = \rho(x) e^{-i\gamma(x)}, \quad (17.24)$$

the path integral takes the form

$$Z[\lambda, \lambda^*, j] = \int \rho \mathcal{D}\rho \mathcal{D}\gamma \int_{\text{phys}} \mathcal{D}A^\mu e^{i\{A_{\text{se}}[\varphi, \varphi^*, A^\mu] - \int_x \lambda^* \varphi - \int_x \varphi^* \lambda - \int_x j^\mu A_\mu\}}. \quad (17.25)$$

But from the structure of the covariant derivative it is obvious that no matter what the fluctuating $\gamma(x)$ configuration is, it can be absorbed into $A(x)$ as a longitudinal degree of freedom. Thus we have the option of considering complex fields $\varphi(x)$ together with physical transverse A^μ fluctuations, or real ρ together with transverse *and* longitudinal $A^\mu(x)$ -fluctuations. This may be expressed by rewriting the functional integral (17.25) as

$$Z[\lambda, \lambda^*, j] = \int \rho \mathcal{D}\rho \int_{\text{all}} \mathcal{D}A^\mu e^{i\{A_{\text{se}}[\rho, A^\mu] - \int_x \lambda^* \varphi - \int_x \varphi^* \lambda - \int_x j^\mu A_\mu\}}, \quad (17.26)$$

with the action

$$\mathcal{A}[\rho, A^\mu] = \int d^D x \left[\frac{1}{2} (\partial_\mu \rho)^2 + \frac{q^2}{2} \rho^2 A_\mu^2 - \frac{m^2}{2} \rho^2 - \frac{g}{4} \rho^4 + \frac{1}{4} F_{\mu\nu}^2 \right]. \quad (17.27)$$

Due to the second term in the exponent, the formerly irrelevant gauge degree of freedom in the vector potential $A^\mu(x)$ has now become a physical one.

Let us describe the situation more precisely in terms of a gauge-fixing functional $F[A]$ of (17.13) and a compensating Faddeev-Popov determinant $\Phi^{-1}[A]$ of Eq. (14.354). Whereas all former gauge conditions involve only the $A^\mu(x)$ -field itself, this is no longer true here. Now the transformations of A_μ and φ are coupled with each other by a gauge transformation which involves the two fields (or any other field of the system). The gauge condition will be some functional

$$F[A_\mu, \varphi] = 0, \quad (17.28)$$

which has to be compensated by some functional $\Phi[A_\mu, \varphi]$ depending on both fields. The latter is determined by the integral over the gauge volume as in (14.354):

$$\Phi[A_\mu, \varphi] = \int \mathcal{D}\Lambda F[A^\Lambda, \varphi^\Lambda]. \quad (17.29)$$

It is most conveneient to choose a gauge condition which ensures the reality of the complex scalar field φ via the δ -functional:

$$F[A_\mu, \varphi] = \delta[\varphi_2(x)], \quad (17.30)$$

where $\varphi_2(\mathbf{x}) = \text{Im } \varphi(\mathbf{x})$. Since the gauge transformations change

$$\varphi \rightarrow e^{-i\Lambda(x)} \varphi = [\cos \Lambda(x) \varphi_1 + \sin \Lambda(x) \varphi_2] + i [-\sin \Lambda(x) \varphi_1 + \cos \Lambda(x) \varphi_2], \quad (17.31)$$

we see that

$$\Phi[A_\mu, \varphi] = \int \mathcal{D}\Lambda \delta[-\sin \Lambda \varphi_1 + \cos \Lambda \varphi_2]. \quad (17.32)$$

The result must be independent of the choice of gauge and can therefore be obtained at $\varphi = (|\varphi|, 0)$, where we find

$$\Phi[A_\mu, \varphi] = \frac{1}{|\varphi(x)|}. \quad (17.33)$$

Note that Φ involves no derivative terms as in the earlier gauges. For this reason it does not require Faddeev-Popov ghost fields. Setting $\varphi = \rho(x)e^{-i\gamma(x)}$, we arrive precisely at the functional integral (17.27). The Faddeev-Popov determinant $\Phi = \rho(x)$ turns out to be responsible for bringing the integral at each point to a form expected from the radial-azimuthal decomposition $\varphi = \rho e^{-i\gamma}$, and the associated integration measure $d\varphi d\varphi^* = d\varphi_1 d\varphi_4 = \rho d\rho d\gamma$.

The generating functional (17.26) may now be used for perturbation expansions below T_c . Inserting into (17.27)

$$\rho(x) = \rho_0 + \rho'(x) = \sqrt{-\frac{m^2}{g}} + \rho'(x), \quad (17.34)$$

we can rewrite

$$\begin{aligned} \mathcal{A} = \int d^D x \left[\frac{1}{2} (\partial_\mu \rho')^2 - \frac{(-2m^2)}{2} \rho'^2 - \frac{g}{4} \rho'^4 - \frac{3}{2} g \rho_0 \rho'^3 \right. \\ \left. - \frac{1}{4} F_{\mu\nu}^2 + \frac{\mu^2}{2} A_\mu^2 + q^2 \rho_0 \rho' A_\mu + \frac{q^2}{2} \rho'^2 A_\mu^2 \right], \end{aligned} \quad (17.35)$$

with

$$\mu^2 \equiv -q^2 \frac{m^2}{g}. \quad (17.36)$$

This is the mass by which the Nambu-Goldstone theorem is violated. The model exhibits a spontaneous breakdown of the continuous U(1)-symmetry which by Noether's theorem should produce a massless excitation. But the mixing of this excitation with the field of the massless electromagnetic field has absorbed the would-be Nambu-Goldstone boson into the longitudinal part of the vector field, making it massive. This process is described more vividly by saying that the photon has “eaten up” the would-be Nambu-Goldstone boson and grown “fat”.

The same mechanism has been used to unify the theories of electromagnetic and weak interactions. Then the scalar field φ possesses more components than the real and imaginary parts of the complex field φ , and the associated Lagrangian has a higher symmetry than U(1). In that case the analog to the ρ -mass

$$m_\rho^2 = \frac{-2m^2}{2} \quad (17.37)$$

is referred to as the Higgs mass [see Eq. (27.99)], and the mass (17.36) of the fat vector field is referred to as the vector boson mass. This will be discussed in detail in Chapter 27.

From the quadratic part in ρ' we deduce the massive ρ' propagator

$$\overline{\rho'(x)}\rho'(0) = \int \frac{dq}{(2\pi)^4} e^{-iqx} \frac{i}{q^2 - (-2m^2) + i\eta}. \quad (17.38)$$

The ρ' -field has cubic ρ'^3 - and quadratic ρ'^4 -interactions. The originally massless Goldstone field γ has disappeared. It has been “eaten up” by the photon, making it massive, and giving it one more polarization degree of freedom.

In the action (17.35) there are electromagnetic vertices in which one or two particles couple to two photons

$$q^2 \rho_0. \quad (17.39)$$

The most important new feature is found in the propagator of the photon field. Given the quadratic photon part of the action in momentum space

$$\mathcal{A} = -\frac{1}{2} \int \frac{d^D k}{(2\pi)^4} A_\mu(-k) \left[k^\mu k^\nu - g^{\mu\nu} (k^2 - \mu^2) \right] A_\nu(k), \quad (17.40)$$

where the kinetic matrix between the fields is

$$M^{\mu\nu} = k^\mu k^\nu - g^{\mu\nu} (k^2 - \mu^2) \quad (17.41)$$

$$= - \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2} \right) (k^2 - \mu^2) + \mu^2 \frac{k^\mu k^\nu}{k^2}. \quad (17.42)$$

By inverting this we find the matrix

$$M_{\mu\nu}^{-1} = G_{\mu\nu}(k) = -\frac{g^{\mu\nu} - k^\mu k^\nu / k^2}{k^2 - \mu^2} + \frac{1}{\mu^2} \frac{k^\mu k^\nu}{k^2} = -\frac{g^{\mu\nu} - k^\mu k^\nu / \mu^2}{k^2 - \mu^2} \quad (17.43)$$

so that the massive propagator becomes

$$G_{\mu\nu}(x) = \int \frac{dk}{(2\pi)^4} e^{-ikx} G_{\mu\nu}(k) = \int \frac{dk}{(2\pi)^4} e^{-ikx} \frac{-i}{k^2 - \mu^2} \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right). \quad (17.44)$$

The photon has acquired a mass and can no longer propagate over a long range. The dramatic experimental consequence is known as the Meissner-Ochsenfeld effect [2]: If a superconductor is cooled below T_c , the magnetic field lines are expelled and can invade only a thin surface layer of penetration depth $1/\mu$.

At $k^2 = \mu^2$, there is a massive particle pole. Since the propagator $G_{\mu\nu}(k)$ at this pole is purely transverse, it satisfies

$$k^\mu G_{\mu\nu}(k) = 0. \quad (17.45)$$

The massive particles have three internal degrees of freedom corresponding to the three orientations of their spin. This has to be contrasted with the massless gauge invariant theory for $T > T_c$, where gauge invariance permits to choose, say, $A^0 = 0$

while still satisfying (17.45) at the pole, thereby eliminating one more degree of freedom in the asymptotic states. Only two transverse photon polarizations remain far away from the interaction. There is no contradiction in the number of degrees of freedom since for $T > T_c$ there are two modes carried by the complex φ fields. The third photon degree is a consequence of absorbing, into the vector field, the phase oscillations, i.e., the former Nambu-Goldstone degrees of freedom.

Certainly, the same theory can also be calculated with the earlier gauge fixing Lagrangian

$$\mathcal{L}_{\text{GF}} = -\frac{1}{2\alpha} (\partial^\mu A_\mu)^2, \quad (17.46)$$

in which case the quadratic piece of the action is

$$\begin{aligned} \mathcal{A}^{\text{quad}} = \int d^D x \left[\frac{1}{2} (\partial_\mu \rho')^2 - \frac{(-2m^2)}{2} \rho'^2 \right. \\ \left. - \frac{1}{4} F_{\mu\nu}^2 + \frac{\mu^2}{2} \left(A_\mu - \frac{1}{q} \partial_\mu \gamma \right)^2 - \frac{1}{2\alpha} (\partial_\mu A^\mu)^2 \right]. \end{aligned} \quad (17.47)$$

Recalling the Faddeev-Popov determinant Φ_4^{-1} of (14.365), we have to add for this gauge the Faddeev-Popov ghost action corresponding to (14.418):

$$\mathcal{A}_{\text{ghost}} = -\frac{1}{2\alpha} \int d^D x \partial_\mu c^* \partial^\mu c. \quad (17.48)$$

The generating functional is obtained by integrating the exponential $e^{i\{\mathcal{A}_{\text{se}} + \mathcal{A}_{\text{ghost}} - \lambda^* \varphi - \varphi^* \lambda - j^\mu A_\mu\}}$ over all $A_\mu(x)$, all complex $\varphi(x)$, and all ghost configurations $c^*(x), c(x)$:

$$Z[\lambda, \lambda^*, j] = \int \mathcal{D}c \mathcal{D}c^* \int \mathcal{D}\varphi \mathcal{D}\varphi^* \int \mathcal{D}A_\mu e^{i\{\mathcal{A}_{\text{se}} + \mathcal{A}_{\text{ghost}} - \lambda^* \varphi - \varphi^* \lambda - j^\mu A_\mu\}}. \quad (17.49)$$

What is the particle content of this theory? Since the Faddeev-Popov ghosts do not interact with the other fields in the action, they can be ignored. As far as the photon is concerned, let us split the vector potential as

$$A_\mu = A_\mu^t + A_\mu^l, \quad (17.50)$$

where A^t is the transverse part satisfying the Lorenz gauge condition $\partial^\mu A_\mu^t = 0$, and A^l is the longitudinal part $A_\mu^l = \partial^{-2} \partial_\mu \partial_\nu A^\nu$, which is a pure gauge field.² Then the transverse part has the propagator

$$\overline{A_\mu^t(x) A_\nu^t(0)} = \int \frac{d^D k}{(2\pi)^D} \frac{-i}{k^2 - \mu^2} \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right). \quad (17.51)$$

²As in (14.370), the letters l and t stand for longitudinal and transverse to the *four*-vector field $A_\mu(x)$.

The gauge-like pieces, on the other hand, are coupled via the would-be Nambu-Goldstone mode. In terms of the pure gradient field $A_\mu = k_\mu \Lambda$, and using the scalar field $\gamma' \equiv (1/q)\gamma$, we find the quadratic Lagrange density in energy-momentum space

$$\frac{\mu^2}{2}(\Lambda, \gamma') \begin{pmatrix} k^2 - \alpha^{-1}k^4 & -k^2 \\ -k^2 & k^2 \end{pmatrix} \begin{pmatrix} \Lambda \\ \gamma' \end{pmatrix}, \quad (17.52)$$

which has the determinant $-\mu^4/4\alpha k^6$, and eigenvalues

$$\lambda_k = \frac{\mu^2 k^2}{2} \left[1 - \frac{1}{2\alpha} \frac{k^2}{\mu^2} \pm \sqrt{1 + \left(\frac{k^2}{2\alpha\mu^2} \right)^2} \right]. \quad (17.53)$$

Both vanish at $k^2 = 0$ (and only there). Thus there are two more massless asymptotic states in Hilbert space. At first sight, this formulation describes a physical situation different from the previous one. We do know, however, that the generating functionals are the same. In the previous formulation, there were only two types of particles. Therefore all additional zero-mass asymptotic states found in the present gauge must be such that, if a scattering process takes place with the two physical particles coming in, the unphysical ones can never be produced. Physical and unphysical states should have no mutual interaction. We may say that the S -matrix is irreducible on the space of physical states. For the Faddeev-Popov ghost fields this is trivial to see. With respect to the other states, however, it is not so obvious, and the path integral is the only efficient tool for convincing us of the correctness of this statement, as demonstrated in Section 14.16. The irreducibility of the S -matrix becomes most transparent by using a particular gauge due to 't Hooft in which physical and unphysical parts of the Hilbert space receive a clear distinction which depends on the gauge parameter. Consider the gauge condition

$$F[A, \varphi] = \exp \left[-\frac{1}{2\alpha} \left(\partial_\mu A^\mu - \frac{\mu^2}{q} \alpha \gamma \right)^2 \right]. \quad (17.54)$$

For $\alpha \rightarrow 0$ this enforces the Lorenz gauge. The exponent has the pleasant advantage that, when added to the free part of the Lagrangian a term mixing γ with the gauge-like components of A_μ disappears, so that no further diagonalization is required in (17.52). Therefore, postponing the calculation of $\Phi^{-1}[A, \varphi]$ to Eq. (17.60), the gauge-fixed free action reads

$$\begin{aligned} \mathcal{A}^{\text{free}} = \int d^D x \left\{ \frac{1}{2} (\partial \rho')^2 - \frac{2m^2}{2} \rho'^2 - \frac{1}{4} F_{\mu\nu}^2 + \frac{\mu^2}{2} A_\mu^2 \right. \\ \left. + \frac{\mu^2}{2q^2} [(\partial_\mu \gamma)^2 - \alpha \mu^2 \gamma^2] - \frac{1}{2\alpha} (\partial_\mu A^\mu)^2 \right\}. \end{aligned} \quad (17.55)$$

Thus the photon has a quadratic piece

$$\frac{1}{2} A^\mu(-k) \left[- (k^2 - \mu^2) g_{\mu\nu} + k_\mu k_\nu - \frac{1}{\alpha} k_\mu k_\nu \right] A^\nu(k)$$

$$= \frac{1}{2} A^\mu(-k) \left[- (k^2 - \mu^2) \left(q_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) - \frac{k^2 - \alpha\mu^2}{\alpha} \frac{k^\mu k^\nu}{k^2} \right] A^\nu(k), \quad (17.56)$$

which by inversion of the matrix between the fields leads to a propagator

$$G_{\mu\nu}(x) = \int \frac{d^D k}{(2\pi)^4} e^{-ikx} \left[-\frac{i}{k^2 - \mu^2} \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) - \frac{i\alpha}{k^2 - \alpha\mu^2} \frac{k^\mu k^\nu}{k^2} \right]. \quad (17.57)$$

Apart from the physical propagator, there is a ghost-like state in $A^\mu(k)$ parallel to k^μ .

The new feature of this gauge is that the would-be Nambu-Goldstone mode $\gamma(x)$ has acquired a mass term $\alpha\mu^2\gamma^2(x)$. The reason for this lies in the fact that the gauge fixing term destroys explicitly also the global invariance of the Lagrangian

$$\varphi(x) \rightarrow e^{-i\Lambda} \varphi(x), \quad \gamma(x) \rightarrow \gamma(x) + \Lambda, \quad A_\mu \rightarrow A_\mu, \quad (17.58)$$

under which the gauge pieces transform as

$$-\frac{1}{2\alpha} \left(\partial_\mu A^\mu - \frac{\mu^2}{q} \alpha \gamma \right)^2 \rightarrow -\frac{1}{2\alpha} \left[\partial_\mu A^\mu - \frac{\mu^2}{q} \alpha (\gamma + \Lambda) \right]^2. \quad (17.59)$$

Therefore, pure phase transformations change the energy, and this results in a mass term.

Let us now take a look at the functional $\Phi[A, \varphi]$ in order to see that this does not modify the Lagrangian (17.55). According to (14.354), we have to integrate

$$\begin{aligned} \Phi[A, \varphi] &= \int \mathcal{D}\Lambda \exp \left[-\frac{1}{2\alpha} \left(\partial^\mu A_\mu^\Lambda - \frac{\mu^2}{q} \alpha \gamma \Lambda \right)^2 \right] \\ &= \int \mathcal{D}\Lambda \exp \left[-\frac{1}{2\alpha} \left(\partial^\mu A_\mu + \partial^2 \Lambda - \frac{\mu^2 \alpha}{q} (\gamma + \Lambda) \right)^2 \right] \\ &= \int \mathcal{D}\Lambda \exp \left[-\frac{1}{2\alpha} \left(\partial^\mu A_\mu - \frac{\mu^2}{q} \alpha \gamma + \left(\partial^2 - \frac{\mu^2}{q} \alpha \right) \Lambda \right)^2 \right] \end{aligned} \quad (17.60)$$

which, after a shift of the integration variable, gives the trivial constant

$$\Phi[A, \varphi] = \det \left(-\partial^2 + \frac{\mu^2}{q} \alpha \right) / \sqrt{\alpha}. \quad (17.61)$$

This can be expressed in terms of Faddeev-Popov ghost fields as

$$\Phi^{-1}[A, \varphi] = \int \mathcal{D}c \mathcal{D}c^* \exp \left[\frac{i}{\sqrt{\alpha}} \int dx \left(\partial c^* \partial c + \frac{\mu^2}{q} \alpha c^* c \right) \right]. \quad (17.62)$$

The situation is similar to that of the last gauge condition: There are three additional kinds of asymptotic states: Faddeev-Popov ghosts, ghost-like poles in the gauge part

of the photon field and a state carried by the would-be Nambu-Goldstone field. But contrary to the previous case, all these states now have a mass which depends on the gauge parameter α . This proves that they must be artifacts of the gauge choice and cannot contribute to physical processes. In particular, by letting the parameter α tend to infinity, all these particles become infinitely heavy and are thus eliminated from the physical Hilbert space.

17.3 Spatially Varying Ground States

The theory of a complex scalar field interacting with a photon has another interesting feature. The ground state must not necessarily be uniform. There are certain ranges of mass and external source where the system prefers to be filled with string-like field configurations, and others where the fields have spatially periodic structures of the hexagonal type. In order to see how this comes about and to be able to compare results with experimental data we consider the euclidean three-dimensional scalar QED, which is the Ginzburg-Landau theory of superconductivity [1]. Superconductivity arises if electrons in a crystal are attracted so strongly by the effects of the elastic forces that the attraction overcomes the Coulomb repulsion. Then they form Cooper pairs which can form a condensate very similar to the bosonic helium atoms. In the absence of electric fields, the mean-field approximation to the effective action is

$$\frac{1}{T}\Gamma[\Phi] = - \int d^3x \left[\frac{1}{2}\mathbf{H}^2 + \frac{1}{2}(\mathbf{D}\Phi)^* \mathbf{D}\Phi + \frac{m^2}{2}|\Phi|^2 + \frac{g}{4}|\Phi|^4 \right]. \quad (17.63)$$

Since the charge carriers are electron pairs, the charge of the field is twice the electronic charge, and the covariant derivative (17.7) becomes

$$\mathbf{D} = \nabla - iq\mathbf{A} = \nabla - i\frac{2e}{\hbar c}\mathbf{A}. \quad (17.64)$$

The first expression is written down in natural units with $\hbar = c = 1$, the second in physical CGS-units. The curl of the vector potential is the magnetic field:

$$\mathbf{H}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x}). \quad (17.65)$$

The time-independent equations of motion are

$$(-i\nabla - q\mathbf{A})^2 \Phi + m^2\Phi + g|\Phi|^2\Phi = 0, \quad (17.66)$$

and the curl of the magnetic field yields

$$\nabla \times \mathbf{H} = \mathbf{j}, \quad (17.67)$$

where $\mathbf{j}$ is the current density of the matter field

$$\mathbf{j} = \frac{q}{2i}\Phi^* \overleftrightarrow{\nabla} \Phi - q^2|\Phi|^2\mathbf{A}. \quad (17.68)$$

In order to describe superconductivity in the lower neighborhood of the critical temperature, we insert a temperature dependent mass term

$$m^2 = \mu^2 \left(\frac{T}{T_c} - 1 \right) = -\mu^2 \tau, \quad (17.69)$$

thereby choosing the minus sign to focus upon the regime below T_c .

17.4 Two Natural Length Scales

Before proceeding it is useful to introduce reduced field quantities and define

$$\psi = \frac{\Phi}{|\Phi_0|}, \quad (17.70)$$

with

$$|\Phi_0| = \sqrt{-\frac{\mu^2}{g}} = \frac{\mu}{\sqrt{g}} \sqrt{\tau} \quad (17.71)$$

being the nonzero vacuum expectation of the φ -field for $T < T_c$. We also define a length scale associated with the massive fluctuations of the Φ -particle

$$\xi(\tau) = \frac{1}{\mu\sqrt{2}}. \quad (17.72)$$

A second length scale characterizes the range of the photon, after it has “eaten up” the Nambu-Goldstone boson:

$$\lambda(\tau) = \frac{1}{q|\Phi_0|} = \frac{\sqrt{g}}{q\mu\sqrt{\tau}} = \frac{\sqrt{g}}{q} \xi(\tau). \quad (17.73)$$

The first length scale is usually referred to as coherence length, the second as penetration depth, for reasons which will become plausible soon. The ratio of the two length scales is an important temperature-independent material constant, called the Ginzburg-Landau parameter and denoted by κ :

$$\kappa \equiv \frac{\lambda(\tau)}{\xi(\tau)} = \frac{\sqrt{g}}{q}, \quad (17.74)$$

which measures the ratio between the coupling strength g with respect to q^2 . The coherence length may be used to introduce a reduced dimensionless vector potential

$$\mathbf{a} \equiv q\xi(\tau)\mathbf{A} \quad (17.75)$$

and a reduced magnetic field

$$\mathbf{h} = \kappa \nabla \times \mathbf{a} = q\kappa\lambda(\tau) \nabla \times \mathbf{A}. \quad (17.76)$$

In the absence of a magnetic field, the action may then be expressed as

$$\frac{1}{T}\Gamma[\Phi] = -4f_c \xi^3 \bar{F}, \quad (17.77)$$

where f_c is the so-called condensation energy density:

$$f_c = \frac{\Phi_0^2 m^2}{4} = -\frac{m^4}{4g} = -\frac{\mu^4}{4g}\tau, \quad (17.78)$$

and $\bar{F}$ is the reduced free energy

$$\bar{F} = \frac{1}{\xi^3} \int d^3x \left[\frac{1}{2} |\xi(\tau)(\nabla - i\mathbf{a})\psi|^2 - \frac{1}{2} |\psi|^2 + \frac{1}{4} |\psi|^4 + \frac{1}{2} \lambda^2(\tau) \mathbf{h}^2 \right]. \quad (17.79)$$

Note that h measures the magnetic field in units of

$$H_0 = \sqrt{2}H_c \equiv \frac{1}{q\lambda\xi} = \sqrt{m^2\Phi_0^2} = 2\sqrt{f_c}, \quad (17.80)$$

where H_c is the value at which the magnetic energy density $H_c^2/2$ equals the condensation energy density f_c .

If we agree to measure all lengths x in multiples of the coherence length ξ , the reduced free energy $\bar{F}$ becomes simply

$$\bar{F} = \int d^3x \left[\frac{1}{2} |(\nabla - i\mathbf{a})\psi|^2 - \frac{1}{2} |\psi|^2 + \frac{1}{4} |\psi|^4 + \mathbf{h}^2 \right]. \quad (17.81)$$

In the reduced variables, the equations of motion are simply

$$(i\nabla + \mathbf{a})^2 \psi = \psi - |\psi|^2 \psi, \quad (17.82)$$

$$\kappa \nabla \times \mathbf{h} = \kappa^2 \nabla \times (\nabla \times \mathbf{a}) = \kappa^2 [\nabla^2 \mathbf{a} - \nabla (\nabla \cdot \mathbf{a})] = \mathbf{j}, \quad (17.83)$$

where $\mathbf{j}$ is the current (17.68) in natural units

$$\mathbf{j} = \frac{1}{2i} \psi^* \overleftrightarrow{\nabla} \psi - |\psi|^2 \mathbf{a}. \quad (17.84)$$

Let us also write down these equations in the polar field decomposition

$$\psi(x) = \rho(x) e^{i\gamma(x)}. \quad (17.85)$$

It is convenient to absorb the gradient of $\gamma(\mathbf{x})$ into the vector potential, and to go over to the field

$$\mathbf{a} \rightarrow \mathbf{a} - \nabla \gamma. \quad (17.86)$$

This brings $\bar{F}$ to the simple form

$$\bar{F} = \int dx \left\{ \frac{1}{2} |(\nabla - i\mathbf{a})\rho|^2 - \frac{1}{2} \rho^2 + \frac{1}{4} \rho^4 + (\nabla \times \mathbf{a})^2 \right\}, \quad (17.87)$$

and the field equations (17.82) and (17.83) become

$$(-\nabla^2 + \mathbf{a}^2 - 1 + \rho^2)^2 \rho = 0, \quad (17.88)$$

$$\kappa \nabla \times \mathbf{h} = \kappa^2 \nabla \times (\nabla \times \mathbf{a}) = \kappa^2 [\nabla^2 \mathbf{a} - \nabla (\nabla \cdot \mathbf{a})] = -\rho^2 \mathbf{a}. \quad (17.89)$$

These will be most suitable for upcoming discussions.

17.5 Planar Domain Wall

As mentioned earlier, it has been known for a long time that superconductors have the tendency of expelling magnetic fields (Meissner-Ochsenfeld effect) [2]. Let us study what the free energy (17.87) has to say about this magnetic phenomenon. In order to get some rough ideas it is useful to consider a material sample in a magnetic field that points in the x -direction. Let us allow for variations of the system only along the z -coordinate. We may choose the vector potential $\mathbf{a}_0$ to point purely into the x -direction. If we denote the x -component of $a(z) \equiv a_0(z)$, the fields are

$$h_y(z) = \kappa a'(z), \quad h_x = h_y = 0. \quad (17.90)$$

The reduced free energy density reads

$$\bar{f} = \frac{1}{2}\rho'^2 - \frac{1}{2}\rho^2 + \frac{1}{4}\rho^4 + a^2\rho^2 + \kappa^2 a'^2. \quad (17.91)$$

Its extremization yields the equation of motion for $\rho(z)$:

$$-\rho'' + a^2\rho = \rho - \rho^3, \quad (17.92)$$

and for $a(z)$:

$$\kappa^2 a'' = a\rho^2. \quad (17.93)$$

Differentiating (17.93) and inserting (17.90), we obtain

$$\kappa^2 \rho^2 \frac{d}{dz} \left(\frac{1}{\rho^2} \frac{dh}{dz} \right) = \kappa^2 \left(h'' - \frac{2h'\rho'}{\rho} \right) = h\rho^2. \quad (17.94)$$

Inserting (17.93) into (17.92) yields

$$-\rho'' + \kappa^2 \frac{h'^2}{\rho^3} = \rho - \rho^3. \quad (17.95)$$

The last two equations can be used as coupled differential equations for h and ρ .

If these two fields are known, the vector potential may be calculated from (17.93) as

$$a = \frac{a''}{\rho^2} = \frac{h'}{\rho^2}. \quad (17.96)$$

This equation gives an immediate result: A constant magnetic field can exist only for $\rho = 0$, i.e., if the system has no spontaneous symmetry breakdown. If we assume, conversely, that $\rho = \text{const.} \neq 0$, then Eq. (17.92) shows that also a^2 is a constant, namely $a^2 = (1 - \rho^2)/\rho$. From Eq. (17.96) we see that then also h' is a constant. There is no contradiction if and only if $\rho = 1$, in which case (17.92) gives $a = 0$, and

(17.96) enforces $h' = 0$. After this, Eq. (17.94) shows that only $h = 0$ is a consistent solution. Therefore, constant solutions have only the two alternatives

$$h = \text{const} \neq 0, \quad \rho = 0, \quad \text{normal phase} \quad (17.97)$$

$$h = 0, \quad \rho = 1, \quad \text{superconductive phase.} \quad (17.98)$$

The second alternative exhibits the experimentally observed Meissner-Ochsenfeld effect [2], implying that the superconductive state does not permit the presence of a magnetic field.

Consider now z -dependent field configurations. In order to simplify the discussion let us first look at two limiting situations:

Case I: $\kappa \ll 1/\sqrt{2}$

This corresponds to a very short penetration depth of the magnetic field which may propagate only over length scales $\lambda(T) = \kappa\xi(\tau)$ or, in natural units, $z \sim 1$, i.e., it has a unit range. For very small κ , Eq. (17.95) becomes

$$\rho'' \approx \rho(1 - \rho^2), \quad (17.99)$$

which can be integrated by multiplying it with ρ' to find

$$-\rho'^2 \approx \frac{1}{2}(1 - \rho^2)^2 + E. \quad (17.100)$$

If the system is in the superconductive state for large z , the field satisfies the boundary condition corresponding to the alternative (17.97), such that $\rho \rightarrow 1$ for $z \rightarrow \infty$. Inserting this into (17.100) we see that the constant of integration E must be zero. Integrating the resulting equation further gives

$$z = \sqrt{2} \int \frac{d\rho}{1 - \rho^2} = \sqrt{2} A \tanh \rho, \quad (17.101)$$

or

$$\rho(z) = \tanh \frac{z}{\sqrt{2}}. \quad (17.102)$$

The field configuration is displayed on the right-hand side of the upper part of Fig. 17.1.

For $z < 0$, the solution (17.102) becomes meaningless, since $\rho > 0$ by definition. We can continue the solution into this regime by matching it with the trivial solution (17.97):

$$h = \text{const}, \quad \rho = 0, \quad (17.103)$$

which is shown as the left-hand branch in the upper part of Fig. 17.1.

The size of the constant magnetic field in the first case is determined by the fact that the free energy density must be the same at large positive and negative z .

Otherwise, there would be energy flow. Inserting (17.100) for $E = 0$ into (17.91), it becomes approximately

$$\hat{f} \approx -\frac{1}{4} + \frac{1}{2}a^2\rho^2 + \frac{1}{2}h^2. \quad (17.104)$$

For large z where $h = a = 0$ and $\rho = 1$, this is equal to $-1/4$. For large negative z , $\bar{f}$ is equal to h^2 . Hence the constant h in the normal phase is equal to

$$h = h_c = \frac{1}{\sqrt{2}}. \quad (17.105)$$

Within the region around $z \approx 0$, the magnetic field h drops to zero over a unit length scale determined by (17.93), which is very short compared with the length $1/\kappa$ over which ρ varies (this is precisely the coherence length). If we plot the transition region against z , the field h jumps abruptly to zero from $h = h_c$ while ρ has a smooth increase. The full approximate solution plotted in Fig. 17.1 is

$$h(z) \approx h_c \Theta(-z), \quad (17.106)$$

$$\rho(z) \approx \tanh \frac{z}{\sqrt{2}}. \quad (17.107)$$

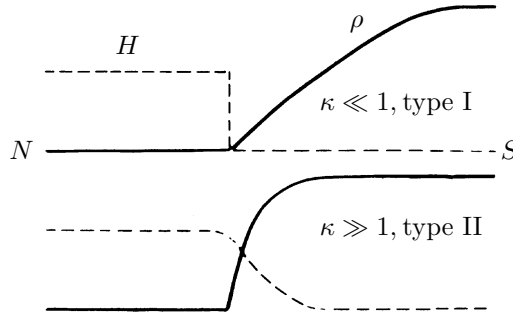


FIGURE 17.1 Dependence of order parameter ρ and magnetic field H on the reduced distance z between normal and superconductive phases. The magnetic field points parallel to the domain wall.

Case II: $\kappa \gg 1/\sqrt{2}$

Consider now the opposite limit of a very large penetration depth. Here we approximate (17.95) by

$$\kappa^2 h'^2 \approx \rho^4 (1 - \rho^2), \quad (17.108)$$

implying that we may omit the gradient term ρ'' in Eq. (17.92):

$$a^2 \rho \approx \rho (1 - \rho^2). \quad (17.109)$$

Let us calculate ρ again by starting out with $\rho = 1$ at $z = \infty$. Then h must decrease for positive z and we have to take the positive square-root

$$\kappa h' = \rho^2 \sqrt{1 - \rho^2}. \quad (17.110)$$

From Eq. (17.94), on the other hand, we obtain

$$h \approx \kappa^2 \frac{d}{dz} \left(\frac{1}{\rho^2} \frac{d}{dz} h \right) = -\kappa \frac{d}{dz} \sqrt{1 - \rho^2}. \quad (17.111)$$

It is convenient to introduce the abbreviation

$$u \equiv \sqrt{1 - \rho^2}, \quad (17.112)$$

such that (17.111) becomes

$$h = -\kappa u', \quad (17.113)$$

and (17.110) turns into the simple differential equation

$$\kappa^2 u'' = (1 - u^2) u. \quad (17.114)$$

After multiplying this with u' , and integrating, we find

$$\kappa^2 u'^2 = u^2 \left(1 - \frac{u^2}{2} \right) + \text{const.} \quad (17.115)$$

Imposing the asymptotic condition that, at large z , the order field ρ goes against 1, the function $u(z)$ must vanish in this limit, fixing the constant to zero. The equation is then solved by

$$z - z_0 = \kappa \int \frac{du}{u} \frac{1}{\sqrt{1 - u^2/2}} = \kappa \tanh^{-1} \frac{1}{\sqrt{1 - u^2/2}} \quad (17.116)$$

or

$$u(z) = \frac{\sqrt{2}}{\cosh[(z - z_0)/\kappa]}. \quad (17.117)$$

From (17.112) we find

$$\rho = \sqrt{1 - \frac{2}{\cosh^2[(z - z_0)/\kappa]}}. \quad (17.118)$$

As z comes in from large positive values, ρ decreases. We can arrange it to become zero at $z = 0$ if we choose z_0 such that

$$\sinh(z_0/\kappa) = 1. \quad (17.119)$$

From Eq. (17.113), the magnetic field is then:

$$h(z) = \frac{\sqrt{2} \sinh[(z - z_0)/\kappa]}{\cosh^2[(z - z_0)/\kappa]}. \quad (17.120)$$

It is zero at $z = \infty$, and becomes gradually stronger as it approaches $z = 0$, where it reaches the value

$$h = h_c = \frac{1}{\sqrt{2}}, \quad (17.121)$$

as before. From there on we may again match the trivial solution continuously by setting

$$h \equiv h_c, \quad \rho \equiv 0; \quad z < 0. \quad (17.122)$$

The full solution shown in Fig. 17.1 is then

$$\rho(z) = \Theta(z) \sqrt{1 - \frac{2}{\cosh^2[(z - z_0)/\kappa]}}, \quad (17.123)$$

$$h(z) = \Theta(-z)h_c + \Theta(z) \frac{\sqrt{2} \sinh[(z - z_0)/\kappa]}{\cosh^2[(z - z_0)/\kappa]}. \quad (17.124)$$

The ranges, over which h and ρ vary, are of equal order κ , or in physical units of order $\lambda = \kappa\xi$.

Case III: $\kappa = 1/\sqrt{2}$

For this κ -value, a trial ansatz

$$h = \frac{1}{\sqrt{2}} (1 - \rho^2) \quad (17.125)$$

can be inserted into (17.94), and leads to the second-order differential equation

$$(1 - \rho^2) \rho^2 = -\rho \rho'' + \rho'^2. \quad (17.126)$$

This, in turn, happens to coincide with the other equation (17.95), thus confirming the correctness of the ansatz (17.125). For $z = \infty$, the fields start out with $\rho = 1$ and $h = 0$, and go to $\rho = 0$, and $h = h_c = 1/\sqrt{2}$ for $z \rightarrow -\infty$.

Equation (17.126) takes a particularly appealing form if we consider the auxiliary function $\sigma(z)$ defined by $\rho(z) \equiv e^{\sigma(z)/2}$. Then

$$\rho' = \frac{1}{2} \sigma' e^{\sigma/2}, \quad \rho'' = \frac{1}{2} \sigma'' e^{\sigma/2} + \frac{1}{k} \sigma'^2 e^{\sigma/2}, \quad (17.127)$$

and we may rewrite (17.126) as

$$-(1 - e^\sigma) = \frac{\rho''}{\rho} - \frac{\rho'^2}{\rho^2} = \frac{1}{2} \sigma''. \quad (17.128)$$

This can be integrated to

$$e^\sigma - 1 - \sigma = \frac{\sigma'^2}{4}, \quad (17.129)$$

which has the solution

$$z = -\frac{1}{2} \int_a^\sigma \frac{d\sigma'}{\sqrt{e^{\sigma'} - 1 - \sigma'}}. \quad (17.130)$$

For $z \rightarrow \infty$, the solution $\sigma(z)$ goes to zero like $e^{-z/\sqrt{2}}$, such that $\rho \rightarrow 1$. For $z \rightarrow -\infty$, it becomes more and more negative like $\sigma(z) \sim -z^2/4$, such that $\rho(z)$ goes to zero exponentially fast in z .

For intermediate values κ , the solutions have to be found numerically. They all look qualitatively similar. The ratio κ of penetration depth to coherence length determines how far the magnetic field invades into the superconductive region relative to the coherence length.

17.6 Surface Energy

Consider the energy per unit length for these classical fields as they follow from Eq. (17.91). Inserting the equations of motion and performing one partial integration renders the much simpler expression for the energy per area $\bar{A}$, both in natural units:

$$\frac{\bar{F}}{\bar{A}} = \int dz f = \int dz \left(-\frac{1}{4} \rho^4 + \frac{1}{2} h^2 \right). \quad (17.131)$$

Obviously, the classical solution with an absolute minimum is $h = 0, \rho = 1$. In order to enforce the previously discussed configurations, an external magnetic field is needed, and we must minimize the reduced *magnetic enthalpy* per unit length area

$$\frac{\bar{G}}{\bar{A}} = \int dz \left[-\frac{1}{4} \rho^4 + \frac{1}{2} h^2 - h h_{\text{ext}} \right], \quad (17.132)$$

where we have subtracted a term

$$m h_{\text{ext}} = h h_{\text{ext}}, \quad (17.133)$$

in which the reduced magnetization $m \equiv \partial_h \bar{G} / \bar{A} = h$ is coupled to the reduced external magnetic field. Such a term does change the differential equations (17.92) and (17.93) for a and ρ , since it is a pure surface term $h_{\text{ext}} \partial_z a$.

For $z \rightarrow -\infty$, where $\rho \rightarrow 0$ and $h \rightarrow h_c$, the enthalpy goes asymptotically against

$$\frac{\bar{G}}{\bar{A}} \approx \int dz \left[\frac{1}{2} h_c^2 - h_c h_{\text{ext}} \right]. \quad (17.134)$$

For $z \rightarrow \infty$, on the other hand, where the size of the order field goes to 1 and $h \rightarrow 0$, the asymptotic value is

$$\frac{\bar{G}}{\bar{A}} \approx \int dz \left(-\frac{1}{4} \right). \quad (17.135)$$

Thus both asymptotic regimes have the same magnetic enthalpy for the particular external field $h_{\text{ext}} = h_c = 1/\sqrt{2}$. If the energy would be smaller in one regime, the wall between superconductive and normal phase would start moving towards that side, such as to decrease the energy. This would go on until the system is uniform. Thus we conclude: For $h > h_c$, the system is uniformly normal, for $h < h_c$ it is uniformly super-conductive.

We now calculate the energy stored in the finite region around $z = 0$ at the critical magnetic field $h_{\text{ext}} = h_c$. There the density deviates only slightly from the asymptotic form, and we must evaluate the expression

$$\frac{\bar{G} - \bar{G}_{as}}{\bar{A}} = \int_{-\infty}^{\infty} dz \left(-\frac{1}{4}\rho^4 + \frac{1}{2}h^2 - \frac{1}{\sqrt{2}}h + \frac{1}{4} \right). \quad (17.136)$$

Note the special properties of the case $\kappa = 1/\sqrt{2}$: Inserting (17.125), the surface energy is seen to vanish.

When inserting the $\kappa \gg 1$ -solutions (17.123) and (17.124) into (17.136), we find, using Eqs. (17.112) and (17.113), the negative energy

$$\begin{aligned} \frac{\bar{G} - \bar{G}_{as}}{\bar{A}} &= \int_{-\infty}^{\infty} dz \left[u^2 \left(1 - \frac{u^2}{2} \right) - \frac{1}{\sqrt{2}}u \left(1 - \frac{u^2}{2} \right)^{1/2} \right] \\ &= \int_{-\infty}^{\infty} dz \left[u \sqrt{1 - \frac{u^2}{2}} - \frac{1}{\sqrt{2}} \right] \frac{du}{dz} = \left(-\frac{2}{3}\sqrt{2} - \frac{1}{2} \right) < 0. \end{aligned} \quad (17.137)$$

And the same sign holds for all $\kappa > 1/\sqrt{2}$.

For $\kappa \ll 1$, on the other hand, the enthalpy (17.136) vanishes in the superconducting phase for $z > 0$, where $\rho = 1$ and $h = 0$. In the normal phase, where $h = h_c$ by Eq. (17.105), we find

$$\frac{\bar{G} - \bar{G}_{as}}{\bar{A}} = \int_{-\infty}^0 dz \frac{1}{4} (1 - \rho^4) = \frac{1}{2\sqrt{2}} \int_0^1 d\rho (1 + \rho^2), \quad (17.138)$$

which is positive for all $\kappa < 1/\sqrt{2}$.

Thus we conclude: In superconductors with $\kappa > 1/\sqrt{2}$, it is energetically more favorable to form a wall in which the magnetic field develops from zero up to h_c , instead of a uniform field configuration. For $\kappa < 1/\sqrt{2}$, the opposite is true. The first case is referred to as a soft or type-II superconductor, the second as a hard type-I superconductor.

17.7 Single Vortex Line and Critical Field H_{c1}

Consider now a type-II superconductor in a small external magnetic field H_{ext} , where it is in the state of a broken symmetry with a uniform order field $\Phi = \Phi_0$. When increasing H_{ext} , there will be a critical value H_{c1} where the field lines first begin to invade the superconductor. We expect this to happen in the form of a quantized

magnetic *flux tubes*. When increasing H_{ext} further, more and more flux tubes will perforate the superconductor, until the critical magnetic field H_c is reached, where the sample becomes normally conducting. The regime between H_{c1} and H_c is called the *mixed state* of the type-II superconductor.

The quantum of flux carried by each flux tube is

$$\Phi_0 = \frac{ch}{2e} \approx 2 \times 10^{-7} \text{ gauss cm}^2. \quad (17.139)$$

Such a flux tube may be considered as a line-like defect in a uniform superconductor. It forms a *vortex line* of supercurrent, very similar to the vortex lines in superfluid helium discussed in Section 16.4. The two objects possess, however, quite different physical properties, as we shall see.

Suppose the system is in the superconductive state without an external voltage so that there is no net-current $\mathbf{j}$. Suppose a flux tube runs along the z -axis. Then we can use the current (17.84) to find the vector potential

$$\mathbf{a} = -\frac{\mathbf{j}}{|\psi|^2} + \frac{1}{2i} \frac{1}{|\psi|^2} \psi^\dagger \overleftrightarrow{\nabla} \psi. \quad (17.140)$$

Far away from the flux tube, the state is undisturbed, the current $\mathbf{j}$ vanishes, and we have the relation

$$\mathbf{a} = \frac{1}{2i} \frac{1}{|\psi|^2} \psi^\dagger \overleftrightarrow{\nabla} \psi. \quad (17.141)$$

In the polar decomposition of the field $\psi(\mathbf{x}) = \rho(\mathbf{x})e^{i\gamma(\mathbf{x})}$, the derivative of $\rho(\mathbf{x})$ cancels, and $\mathbf{a}(\mathbf{x})$ becomes the gradient of the phase of the order parameter:

$$\mathbf{a}(\mathbf{x}) = \nabla \gamma(\mathbf{x}). \quad (17.142)$$

Here we can compare the discussion with that of vortex lines in superfluid helium in Section 16.4. There the superflow velocity was proportional to the gradient of the phase angle variable $\gamma(\mathbf{x})$. The periodicity of $\gamma(\mathbf{x})$ led to the quantization rule that, when taking the integral over $d\gamma(\mathbf{x})$ along a closed circuit around the vortex line, it had to be an integral multiple of 2π [recall Eq. (16.107)]. The same rule applies here:

$$\oint_B d\gamma(\mathbf{x}) = \oint_B d\mathbf{x} \cdot \nabla \gamma(\mathbf{x}) = 2\pi n. \quad (17.143)$$

By Stokes' theorem, this is equal to the integral $\int d\mathbf{S} \cdot \nabla \times \mathbf{a}$, where $d\mathbf{S}$ is a surface element of the area enclosed by the circuit. Since $\mathbf{h} = \kappa(\nabla \times \mathbf{a})$ is the magnetic field in natural units [recall (17.86)], the integral (17.143) is directly proportional to the magnetic flux through the area of the circuit

$$\bar{\Phi} = \int_{S_B} d\mathbf{S} \cdot \mathbf{h} = \kappa \int d\mathbf{S} \cdot (\nabla \times \mathbf{a}) = \kappa \oint_B d\mathbf{x} \cdot \mathbf{a} = \kappa \oint_B d\mathbf{x} \cdot \nabla \gamma = 2\pi n \kappa. \quad (17.144)$$

This holds in natural units, indicated by a bar on top of Φ , in which $\hbar = c = 1$. The vector potential is given by (17.75), and $\mathbf{x}$ is measured in units of the coherence length.

The quantization condition in physical CGS-units follows from the same argument, after it is applied to the original current (17.68). Remembering the equality

$$q = \frac{2e}{\hbar c} \quad (17.145)$$

if Eq. (17.64) is expressed in CGS-units, the relation (17.141) reads

$$\mathbf{A} = \frac{2e}{2i\hbar c} \frac{1}{|\psi|^2} \psi^\dagger \overleftrightarrow{\nabla} \psi, \quad (17.146)$$

and (17.142) becomes

$$\mathbf{A}(\mathbf{x}) = \frac{\hbar c}{2e} \nabla_i \gamma(\mathbf{x}) = \frac{\Phi_0}{2\pi} \nabla_i \gamma(\mathbf{x}). \quad (17.147)$$

The magnetic flux integral in CGS-units is therefore

$$\Phi = \int_{S_B} d\mathbf{S} \cdot \mathbf{H} = \int d\mathbf{S} \cdot (\nabla \times \mathbf{A}) = \oint_B d\mathbf{x} \cdot \mathbf{A} = \frac{\Phi_0}{2\pi} \oint_B d\mathbf{x} \cdot \nabla \gamma = n\Phi_0, \quad (17.148)$$

and thus an integer multiple of the fundamental flux (17.139).

It is instructive to perform the circuit integral (17.144) once more around a circle close to the flux tube, where the current in Eq. (17.140) no longer vanishes. The angular integral $\oint d\mathbf{x} \cdot \nabla \gamma$ still has to be equal to $2\pi n$, and we find the quantization rule

$$\oint_B d\mathbf{x} \cdot \left(\mathbf{A} + \frac{\mathbf{j}}{|\psi|^2} \right) = 2\pi n, \quad (17.149)$$

or

$$\bar{\Phi} + \frac{1}{|\psi|^2} \oint_B d\mathbf{x} \cdot \mathbf{j} = 2\pi n\kappa. \quad (17.150)$$

This shows that a smaller circuit, which encloses fewer magnetic field lines, contains an increasing contribution of the supercurrent around the center of the vortex line. The sum of the two contributions in (17.150) remains equal to $2\pi n\kappa$. This shows that the flux tube is also a vortex line with respect to the supercurrent. The circular current density must be inversely proportional to the distance. This behavior will be derived explicitly in Eq. (17.192).

Quantitatively, we can find the properties of a vortex line by solving the field equations (17.88) and (17.89) in cylindrical coordinates. Inserting the second into the first equation, we find

$$-\frac{1}{r} \frac{d}{dr} r \frac{d\rho}{dr} + \frac{\kappa^2}{\rho^3} \left(\frac{dh}{dr} \right)^2 - (1 - \rho^2)\rho = 0, \quad (17.151)$$

where h denotes the z -component of $\mathbf{h}$. Forming the curl of the second equation gives the cylindrical analogue of (17.96), i.e.,

$$h = \kappa^2 \frac{1}{r} \frac{d}{dr} \frac{r}{\rho^2} \frac{d}{dr} h. \quad (17.152)$$

For $r \rightarrow \infty$, we have the boundary condition $\rho = 1$, $h = 0$ (superconductive state with Meissner effect [2]) and $\mathbf{j} = 0$ (no current). Since $\mathbf{j}$ is proportional to $\nabla \times \mathbf{h}$ by Eq. (17.83), the last condition implies that

$$h'(r) = 0, \quad r \rightarrow \infty. \quad (17.153)$$

In cylindrical coordinates, the flux quantization condition (17.144) can be written in the form

$$\bar{\Phi} = 2\pi \int_0^\infty dr r h(r) = 2\pi n \kappa. \quad (17.154)$$

Inserting here Eq. (17.152) yields

$$\bar{\Phi} = 2\pi \kappa^2 \left[\frac{r}{\rho^2} h'(r) \right]_0^\infty = -2\pi \kappa^2 \left[\frac{r}{\pi^2} h'(r) \right]_{r=0}, \quad (17.155)$$

so that the quantization condition turns into a boundary condition at the origin:

$$h' \rightarrow -\rho^2 \frac{n}{\kappa} \frac{1}{r}, \quad \text{for } r \rightarrow 0. \quad (17.156)$$

Inserting this condition into (17.151) we see that, close to the origin, $\rho(r)$ satisfies the equation

$$-\frac{1}{r} \frac{d}{dr} r \frac{d}{dr} \rho(r) + \frac{n^2}{r^2} \rho - (1 - \rho^2) \rho \approx 0, \quad (17.157)$$

implying the small- r behavior of $\rho(r)$:

$$\rho(r) = c_n \left(\frac{r}{\kappa} \right)^n + \mathcal{O}(r^{n+1}). \quad (17.158)$$

Reinserting this back into (17.156) we have

$$h(r) = h(0) - \frac{c_n^2}{2\kappa} \left(\frac{r}{\kappa} \right)^{2n}. \quad (17.159)$$

For large r , where $\rho \rightarrow 1$, the differential equation (17.152) is solved by the modified Bessel function K_0 , with some proportionality factor α :

$$h(r) \rightarrow \alpha K_0 \left(\frac{r}{\kappa} \right), \quad r \rightarrow \infty. \quad (17.160)$$

More explicitly, the limit is

$$h(r) \rightarrow \alpha \sqrt{\pi\kappa/2r} e^{-r/\kappa}, \quad r \rightarrow \infty. \quad (17.161)$$

Consider now the deep type-II regime where $\kappa \gg 1/\sqrt{2}$. There $\rho(r)$ goes rapidly to unity, as compared to the length scale over which $h(r)$ changes, which is κ in our natural units. Therefore, the behavior (17.160) holds very close to the origin. We can determine α by matching (17.160) to (17.156) from which we find (using the small- r behavior $K'_0(r) = -K_1(r) \approx -l/r$):

$$\alpha = \frac{n}{\kappa}. \quad (17.162)$$

In general, $h(r)$ and $\rho(r)$ have to be evaluated numerically. A typical solution for $n = 1$ is shown in Fig. 17.2 for $\kappa = 10$.

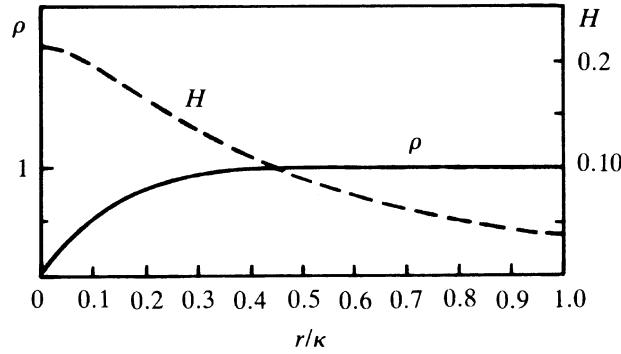


FIGURE 17.2 Order parameter ρ and magnetic field h for an $n = 1$ vortex line in a deep type-II superconductor with $K = 10$.

The energy of a vortex line is obtained from Eq. (17.87). Inserting the equations of motion (17.88) and (17.89), and subtracting the condensation energy, we obtain from (17.131)

$$\Delta \bar{F}_{\text{vort}} = \bar{F}_{\text{vort}} - \bar{F}_c = \frac{1}{2} \int d^3x \left[\frac{1}{2}(1 - \rho^4) + h^2 \right]. \quad (17.163)$$

For $\kappa \gg 1/\sqrt{2}$, we may neglect the small radius $r \leq 1$, over which ρ increases quickly from zero to its asymptotic value $\rho = 1$. Above $r \approx 1$ the magnetic field for $r \leq \kappa$ is given by (17.160). Inserting this into (17.151) with (17.158), we find

$$\rho(r) \approx 1 - \frac{n^2}{2r^2}. \quad (17.164)$$

Thus the region $1 \leq r \leq \kappa$ yields an energy per unit length

$$\frac{1}{L} \bar{F}_{\text{vort}} = \frac{1}{2} 2\pi \int_1^\kappa dr r \left[\frac{1}{2}(1 - \rho^4) + h^2 \right] = \pi n^2 \int_1^\kappa dr r \left[\frac{1}{r^2} + \frac{1}{\kappa^2} K_0^2 \left(\frac{r}{\kappa} \right) \right]. \quad (17.165)$$

For $\kappa \rightarrow \infty$, the second integral becomes a constant, as a consequence of the integral $\int_0^\infty dx x K_0^2(x) = 1/2$. The first integral, on the other hand, has a logarithmic divergence, so that we find

$$\frac{1}{L} \bar{F}_{\text{vort}} \approx \pi n^2 [\log \kappa + \text{const.}]. \quad (17.166)$$

A more careful evaluation of the integral yields $\pi n^2 (\log \kappa + 0.08)$.

Let us now see at which external magnetic field such vortex lines can form. For this we consider again the magnetic enthalpy (17.132), and subtract from $\bar{G}_{\text{vort}}/L$ the magnetic $\bar{G}_{\text{vort}}/L$ coupling $h h^{\text{ext}}$ so that, per unit length,

$$\frac{1}{L} \bar{G}_h = \pi n^2 (\log \kappa + 0.08) - 2\pi \int_0^\infty dr r h h^{\text{ext}}. \quad (17.167)$$

But the integral over h is simply the flux quantum (17.144) associated with the vortex line, such that

$$\frac{1}{L} \bar{G}_h = \pi n^2 (\log \kappa + 0.08) - 2\pi n \kappa h^{\text{ext}}. \quad (17.168)$$

When this quantity is smaller than zero, a vortex line invades the superconductor along the z -axis. The associated critical magnetic field is, in natural units,

$$h_{c1} = \frac{n \log \kappa + 0.08}{2\kappa}. \quad (17.169)$$

For large κ , this field can be quite small. In Fig. 17.3 we compare the asymptotic result with a numerical solution of the differential equation for $n = 1, 2, 3, \dots$ in Fig. 17.3.

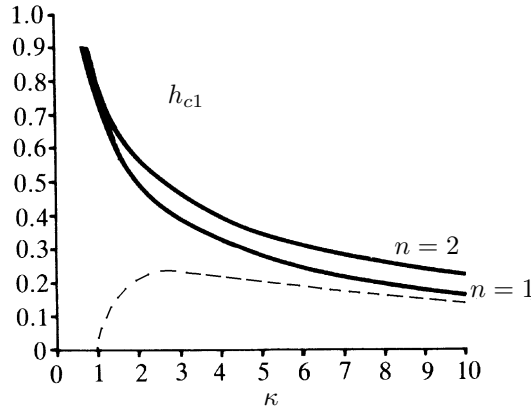


FIGURE 17.3 Critical field h_{c1} where a vortex line of strength n begins invading a type-II superconductor, as a function of the parameter κ . The dotted line indicates the asymptotic result $(1/2\kappa) \log \kappa$ of Eq. (17.169). The magnetic field h is measured in natural units, which are units of $\sqrt{2}H_c$ where H_c is the magnetic field at which the magnetic energy equals the condensation energy.

For a comparison with experiment one expresses this field in terms of the critical magnetic field $h_c = 1/\sqrt{2}$ and measures the ratio

$$\frac{H_{c1}}{H_c} = \frac{n}{\sqrt{2}\kappa}(\log \kappa + 0.08). \quad (17.170)$$

If the magnetic field is increased above H_{c1} , more and more flux tubes invade the type-II superconductor. These turn out to repel each other. The repulsive energy between them can be minimized if the flux tubes form a hexagonal array, as shown in Fig. 17.4. The tubes will perform thermal fluctuations, which may be so violent that the superflow experiences dissipation. The taming of these fluctuations is one of the main problems in high-temperature superconductors. It is usually done by introducing lattice defects at which the vortex lines are pinned.

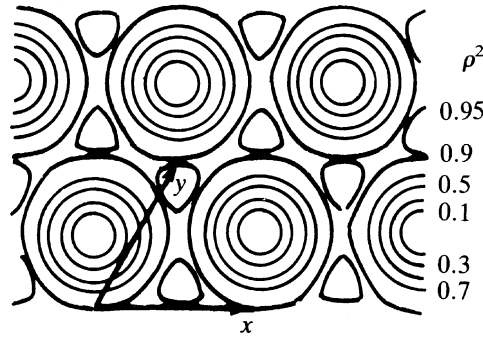


FIGURE 17.4 Spatial distribution magnetization of the order parameter $\rho(\mathbf{x})$ in a typical mixed state in which the vortex lines form a hexagonal lattice [3].

17.8 Critical Field H_{c2} where Superconductivity is Destroyed

In the study of planar z -dependent field configurations we found that, for $H > H_c$, the order parameter vanishes, so that the magnetic field pervades the superconductor. Experimentally this is not quite true. The symmetric field inside the sample can increase markedly only up to a certain larger field value H_{c2} which, however, may lie far above H_c in a deep type-II superconductor. In fact, by allowing a more general space dependence, a non-zero field ρ can exist up to a magnetic field

$$H_{c2} = \kappa\sqrt{2}H_c > H_c \quad \text{for} \quad \kappa > 1/\sqrt{2}. \quad (17.171)$$

Only for $H > H_{c2}$ the field $\rho(\mathbf{x})$ is forced to be zero in the entire system, which then behaves like a normal conductor.

In order to calculate the size of H_{c2} , we observe that, for H very close to H_{c2} , the order parameter must be very small. Hence we can linearize the field equation (17.82), writing it approximately as

$$(i\nabla + \mathbf{a})^2 \psi \approx \psi. \quad (17.172)$$

For a uniform magnetic field in the z -direction, we may choose different forms of the vector potential $\mathbf{a}$ which differ by gauge transformations. A convenient form is

$$\mathbf{a} = \frac{h}{\kappa} (0, x, 0). \quad (17.173)$$

Then ψ satisfies the Schrödinger equation

$$\left[-\partial_x^2 + \left(i\partial_y + \frac{h}{\kappa}x \right)^2 - \partial_z^2 \right] \psi = \psi. \quad (17.174)$$

This may be solved by a general ansatz

$$\psi(x, y, z) = e^{ik_z z + ik_y y} \chi(x), \quad (17.175)$$

where $\chi(x)$ satisfies the differential equation

$$\left\{ -\frac{d^2}{dx^2} + \left[\left(-k_y + \frac{h}{\kappa}x \right)^2 - (1 - k_z^2) \right] \right\} \chi(x) = 0. \quad (17.176)$$

This is the Schrödinger equation of a linear oscillator of frequency $\omega = h/\kappa$, with the potential centered at

$$x_0 = \frac{\kappa k_y}{h}. \quad (17.177)$$

In fact, Eq. (17.176) can be written as

$$-\chi_{xx}(x) + \omega^2 (x - x_0)^2 \chi(x) = (1 - k_z^2) \chi(x). \quad (17.178)$$

This equation has a solution $\chi(x)$, which goes to zero for $x \rightarrow \infty$, if

$$\frac{1}{2} (1 - k_z^2) \equiv E_n = \omega \left(n + \frac{1}{2} \right) = \frac{h}{\kappa} \left(n + \frac{1}{2} \right). \quad (17.179)$$

The energy $E_n = \frac{1}{2}(1 - k_z^2)$ is bounded by 1 from above. Hence, there cannot be solutions for arbitrarily large h . The highest h is supported by the ground state solution, where $n = 0$. But also this ceases to exist as h reaches the critical value h_{c2} given by

$$\frac{\omega}{2} = \frac{h}{2\kappa} = \frac{1}{2}, \quad (17.180)$$

where

$$h_{c2} = \kappa. \quad (17.181)$$

Going back to physical magnetic fields, this amounts to

$$H_{c2} = \kappa \sqrt{2} H_c. \quad (17.182)$$

The wave functions of these solutions are strongly concentrated around $x \approx x_0$, implying that the system is normal almost everywhere, except for a sheet of thickness $\sqrt{\kappa/h}$, in units of the coherence length.

This sheet carries a supercurrent. Let us study its properties. If we insert $\psi(\mathbf{x})$ of Eq. (17.175) and $\mathbf{a}$ of Eq. (17.173) into Eq. (17.84), we find a supercurrent density

$$\begin{aligned} \mathbf{j} &= \frac{1}{2i} \psi^* \overleftrightarrow{\nabla} \psi - |\psi|^2 \mathbf{a} = |\chi(x)|^2 \left[(0, k_y, k_z) - \frac{h}{\kappa} (0, x, 0) \right] \\ &= -|\chi(x)|^2 \left(0, \frac{h}{\kappa} (x - x_0), k_z \right). \end{aligned} \quad (17.183)$$

The superconducting sheet is centered around the plane with $x = x_0$ parallel to the y z -plane. It carries no net charge flow along the x -axis. It consists of a double layer of current flowing in $\pm y$ directions for $x > x_0$ or $x < x_0$, respectively.

If the current along the z -axis is nonzero, the critical magnetic field is reduced to a lower value

$$h_{c2} \rightarrow \kappa (1 - k_z^2). \quad (17.184)$$

The sheet configuration is obviously degenerate with respect to the position x_0 of the sheet. Moreover, being in the regime of a linear Schrödinger equation, we can use the superposition principle to set up different spatial structures. For example, we may form an average over sheets in the rotated $(\cos \varphi \hat{x} + \sin \varphi \hat{y}, \hat{z})$ -planes, and obtain cylindrical structures. These have a definite angular momentum around the z -axis rather than a definite linear momentum k_y . Their wave function can be found directly from a vector potential

$$\mathbf{a} = \frac{h}{2\kappa} (-y, x, 0), \quad (17.185)$$

which reads in cylindrical coordinates

$$a_\varphi = \frac{h}{2\kappa} \rho, \quad a_r = 0, \quad a_z = 0. \quad (17.186)$$

The linearized field equation now becomes

$$\left[- \left(\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) + \frac{h^2}{\kappa^2} r^2 \right] \psi(z, r, \varphi). \quad (17.187)$$

It may be solved by a factorized ansatz

$$\psi(zr\varphi) = \chi(\sqrt{h/\kappa}r) e^{im\varphi} e^{ik_z z}. \quad (17.188)$$

The differential operator in (17.187) is the same as for a two-dimensional harmonic oscillator of frequency $\omega = h/\kappa$, and the solutions are well known. They may be expressed in terms of the confluent hypergeometric functions ${}_1F_1(a; b; z)$ as

$$\chi(r') = e^{-r'/2} r'^{|m|/2} {}_1F_1(-n; |m| + 1; r'), \quad (17.189)$$

where $r' = \sqrt{h/\kappa r}$. The corresponding energy eigenvalues are

$$E = \omega \left(n + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2} \right) + k_z^2. \quad (17.190)$$

They have to be equated with $1/2(1 - k_z^2)$ to obtain the highest possible magnetic field, which is again found to be

$$h_{c2} = \kappa(1 - k_z^2), \quad (17.191)$$

as in (17.184). The current carried by this cylindrical solution is found by inserting (17.185) and (17.188) into (17.83). For $n = 0$ and arbitrary $m > 0$, we obtain

$$\begin{aligned} \mathbf{j} &= \chi^2 \left(\sqrt{h/\kappa r} \right) \left[m \left(\frac{y}{r^2}, -\frac{x}{r^2}, 0 \right) + (0, 0, k_z) - \frac{h}{2\kappa} (-y, x, 0) \right] \\ &= \chi^2 \left(\sqrt{h/\kappa r} \right) \left[k_z \mathbf{e}_z + \left(\frac{m}{r^2} - \frac{h}{2\kappa} \right) \mathbf{e}_\varphi \right]. \end{aligned} \quad (17.192)$$

The wave function is non-zero within a narrow tube of diameter $\sqrt{\kappa/h}$ in units of the coherence length. Within this tube, a current is rotating clockwise around the z -axis, just as deduced before in the qualitative discussion of Eq. (17.150). In addition, there may be an arbitrary linear current that flows into the z -direction.

The magnetic enthalpy (17.132) of a type-II superconductor is always smaller than zero because of the negative interfacial energy. Thus, for H below H_{c2} , there will be states with nonzero magnetic field.

If the magnetic field is far below H_{c2} , the magnitude $\rho(\mathbf{x})$ of the order field will be so large that the quartic terms in the field equation (17.88) can no longer be neglected. The field configuration becomes inaccessible to simple analytic calculations.

The different critical magnetic fields for various superconducting materials are listed in Table 17.1.

TABLE 17.1 Different critical magnetic fields, in units of gauss, for various superconducting materials with different impurities.

material	H_c	H_{c1}	H_{c2}	T_c/K
Pb	550	550	550	4.2
0.85 Pb, 0.15 Ir	650	250	3040	4.2
0.75 Pb, 0.25 In	570	200	3500	4.2
0.70 Pb, 0.30 Tl	430	145	2920	4.2
0.976 Pb, 0.024 Hg	580	340	1460	4.2
0.912 Pb, 0.088 Bi	675	245	3250	4.2
Nb	1608	1300	2680	4.2
0.5 Nb, 0.5 Ta	252	—	1370	5.6

17.9 Order of Superconductive Phase Transition

The Ginzburg-Landau parameter κ does not only distinguish type I from type II superconductors. Its magnitude distinguishes also the order of the superconductive phase transition. If κ is very large, the effect of the electromagnetic field is extremely weak and the superconductor behaves very similar to a pure superfluid. Then the transition is certainly of second order. In the opposite limit of small κ , the mass acquired by the electromagnetic field is quite large and the penetration depth is very small. Then the transition becomes of first order. Somewhere between these limits, the order must change and it is possible to show that this happens at a tricritical value of $\kappa \approx \kappa_t \approx 0.81/\sqrt{2}$ [4, 5]. The theoretical tool for this was the development of a disorder field theory [6, 7]. In it, the relevant elementary excitations are the vortex lines whose grand-canonical ensemble is described by a fluctuating field. When vortex lines proliferate, the disorder field acquires a nonzero expectation value. Depending on the strength of the electromagnetic coupling e , the phase transition can be at the boundary of a first- and a second-order phase transition, marking a tricritical point.

17.10 Quartic Interaction and Tricritical Point

According to the action (17.9), the Ginzburg-Landau theory of superconductivity is characterized by the following free energy density:

$$\begin{aligned} f(\varphi, \nabla\varphi, \mathbf{A}, \nabla\mathbf{A}) &= \frac{1}{2} (\nabla + iq\mathbf{A})\varphi^* (\nabla - iq\mathbf{A})\varphi \\ &+ \frac{m^2}{2}|\varphi|^2 + \frac{g}{4}|\varphi|^4 \\ &+ \frac{1}{2}(\nabla \times \mathbf{A})^2, \end{aligned} \quad (17.193)$$

with the order field

$$\varphi(x) = \rho(x)e^{-i\gamma(x)}, \quad (17.194)$$

where $\rho(x)$ and $\gamma(x)$ are real variables. The electromagnetic field is represented by the vector $\mathbf{A}$, and $q = 2e/\hbar c$ accounts for the electromagnetic coupling of Cooper pairs whose charge is $2e$.³ The real constants m^2 and g parametrize the size of the quadratic and quartic terms, respectively. If the mass parameter m^2 drops below zero, the ground state of the potential

$$V(\varphi) = \frac{1}{2}m^2|\varphi|^2 + \frac{g}{4}|\varphi|^4 \quad (17.195)$$

is obtained by an infinite number of degenerate states that satisfy

$$\langle\varphi\rangle^2 = \rho_0^2 = -\frac{m^2}{g}. \quad (17.196)$$

³The Euler number is represented by the roman letter e, not to be confused with the electric charge e .

The phase transition is of second order.

If we choose the ground state to have a real field φ , i.e., if we choose $\gamma(x) = 0$ in (17.194), the free energy density becomes

$$\begin{aligned} f(\varphi, \nabla\varphi, \mathbf{A}, \nabla\mathbf{A}) &= \frac{1}{2}(\nabla\rho)^2 + V(\rho) + \frac{q^2\rho^2}{2}\mathbf{A}^2 \\ &+ \frac{1}{2}(\nabla \times \mathbf{A})^2. \end{aligned} \quad (17.197)$$

At the potential minimum, the vector field has a mass

$$m_A = q\rho_0. \quad (17.198)$$

This can be observed experimentally as a *London penetration depth* $\lambda_L = 1/m_A = 1/q\rho_0$ of the magnetic field into the superconductor.

The ratio of the two characteristic length scales of a superconductor, the coherence length $\xi = 1/\sqrt{-2m^2}$ and the penetration depth λ_L , constitutes a dimensionless material parameter of a superconductor, the so-called *Ginzburg-Landau parameter* $\kappa \equiv \lambda_L/\sqrt{2}\xi$. Using (17.196) we find for κ the value

$$\kappa = \sqrt{\frac{g}{q^2}}. \quad (17.199)$$

A first-order phase transition arises in the Ginzburg-Landau theory by including the effects of quantum corrections, which in the mean-field approximation [8] neglecting fluctuations in ρ , lead to an additional cubic term in the potential:

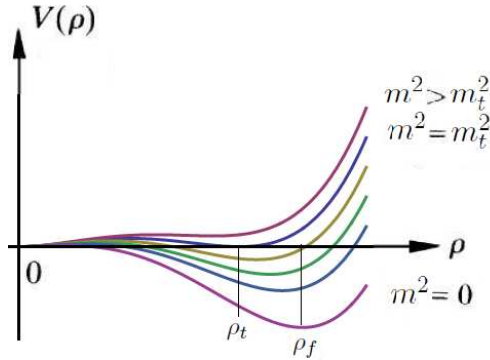


FIGURE 17.5 Effective potential for the order parameter ρ with a fluctuation-generated cubic term. For $m^2 = m_t^2$, there exist two minima of equal height $V(\rho)$, one at $\rho = 0$ and another one around ρ_t , causing a first-order transition at $m^2 = m_t^2$. When m^2 is lowered down to zero, the field has huge fluctuations around the origin without a stabilizing mass, and the fluctuations move to some larger $\rho = \rho_f > \rho_t$ with a fluctuation-generated mass m_f^2 .

$$V(\rho) = \frac{1}{2}m^2\rho^2 + \frac{g}{4}\rho^4 - \frac{c}{3}\rho^3, \quad c = \frac{q^3}{2\pi}. \quad (17.200)$$

We can see in Fig. 17.5 that the cubic term generates for $m^2 < c^2/4g$ a second minimum at

$$\rho_2 = \frac{c}{2g} \left(1 + \sqrt{1 - \frac{4m^2g}{c^2}} \right). \quad (17.201)$$

At the specific point $m_t^2 = 2c^2/9g$, the minimum lies at the same level as the origin. This happens at $\rho_t = 2c/3g$. The jump from $\rho = 0$ to ρ_t is a phase transition of first-order (tricritical point). Therefore, in this point, the coherence length of the ρ -field fluctuations becomes

$$\xi_t = \frac{1}{\sqrt{m^2 + 3g\rho_t^2 - 2c\rho_t}} = \frac{3}{c} \sqrt{\frac{g}{2}}. \quad (17.202)$$

This is the same as for the fluctuations around $\rho = 0$.

The value of the Ginzburg-Landau parameter at the tricritical point is estimated with the help of a *duality transformation* to lie close to the place where type I goes over into type II superconductivity at [4, 5, 6]

$$\kappa \approx \kappa_t = \frac{3\sqrt{3}}{2\pi} \sqrt{1 - \frac{4}{9} \left(\frac{\pi}{3} \right)} \approx \frac{0.8}{\sqrt{2}}. \quad (17.203)$$

If the mass term drops to zero, the second minimum, at which the fluctuations stabilize, has a curvature that determines a square mass

$$m_f^2 = 3g, \quad (17.204)$$

which corresponds to a coherence length $\xi_f = 1/3g$.

17.11 Four-Dimensional Version

Let us see how this result changes in the four-dimensional version of the Ginzburg-Landau theory, the Coleman-Weinberg model. Setting again $\varphi(x) = \rho(x)e^{-i\gamma(x)}$ as in (17.194) (see also the $O(N)$ -model in Chapter 22 for $N = 2$), the effective potential of the Coleman-Weinberg model at one-loop level is [9]

$$V(\rho) = \frac{1}{2}m^2\rho^2 + \frac{g}{4}\rho^4 + \frac{3q^4}{64\pi^2}\rho^4 \left(\log \frac{\rho^2}{\mu^2} - \frac{25}{6} \right), \quad (17.205)$$

where the magnitude of the scalar (spin-0) field is represented by $\rho(x) = \sqrt{\Phi^2}$. Here g gives the strength of the quartic term, and μ is the value of ρ at which the renormalization is done. We shall assume g to be of the same order as q^4 , which is very small. For this reason we can neglect, in the one-loop approximation (17.205), the purely scalar higher-loop corrections since these are of the order g^2 , which would

be extremely small $\propto q^8$. To see this clearly we define a new scale parameter M by setting

$$\frac{g}{4} = \frac{3q^4}{64\pi^2} \left(\log \frac{\mu^2}{M^2} + \frac{11}{3} \right), \quad (17.206)$$

which turns the effective potential into

$$V(\rho) = \frac{1}{2}m^2\rho^2 + \frac{3q^4}{64\pi^2}\rho^4 \left(\log \frac{\rho^2}{M^2} - \frac{1}{2} \right). \quad (17.207)$$

If the theory is massless, i.e., if $m^2 = 0$, the potential (17.207) has a minimum at the field value

$$\rho = \rho_f \equiv M^2. \quad (17.208)$$

There the potential has a nonzero curvature (see Fig. 17.6).

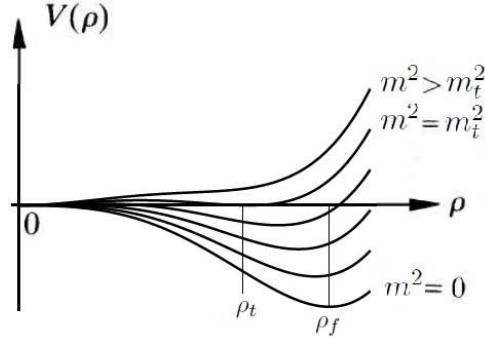


FIGURE 17.6 Effective potential for the order parameter ρ in four spacetime dimensions according to Eq. (17.205). As in three dimensions, a new second minimum develops around ρ_t causing a first-order transition for $m^2 = m_t^2$. For $m = 0$, the effective potential has a minimum at some $\rho = \rho_f > \rho_t$ with a fluctuation-generated mass term m_f^2 .

The curvature implies a nonzero mass generated by fluctuations:

$$m_f^2 = m^2(\rho_f) = \left. \frac{\partial^2 V}{\partial \rho^2} \right|_{m=0, \rho=\rho_c} = \frac{q^4 \rho_f^2}{16\pi^2} \left(9 \log \frac{\rho_f^2}{M^2} + 6 \right) = \frac{6q^4 M^2}{16\pi^2}. \quad (17.209)$$

As described in [9, 10], the effective potential has, for a positive m^2 , both a maximum and a minimum as long as $m^2 < 2m_1^2/e^{1/2} \equiv 3q^4 M^2 e^{-1}/16\pi^2$. The minimum of the potential lies at the same level as the origin if $m^2 = m_t^2 \equiv 3q^4 M^2 e^{-1/2}/32\pi^2$ with $\rho_t^2 = M^2 e^{-1/2}$. This is the tricritical point, and the scalar mass at that point is

$$\begin{aligned} m^2(\rho_t) &= \left. \frac{\partial^2 V}{\partial \rho^2} \right|_{\rho=\rho_t} = m_t^2 + \frac{q^4 \rho_t^2}{16\pi^2} \left(9 \log \frac{\rho_t^2}{M^2} + 6 \right) = \frac{3q^4 M^2}{16\pi^2 e^{1/2}} \\ &= \frac{\lambda}{\alpha} \rho_t^2, \end{aligned} \quad (17.210)$$

where

$$\alpha = \left(\log \frac{\mu^2}{M^2} + \frac{11}{3} \right) \quad (17.211)$$

parametrizes the fluctuation scale M . A Ginzburg-Landau parameter may be defined for the four-dimensional theory, as in three dimensions, by the ratio of the two characteristic length scales of the theory [compare (17.199)]

$$\kappa = \frac{\lambda_L}{\sqrt{2}\xi} = \frac{1}{\sqrt{2}} \frac{m(\rho_t)}{q\rho_t} = \frac{1}{\sqrt{2\alpha}} \sqrt{\frac{g}{q^2}}. \quad (17.212)$$

The result has the same form as the previously obtained 3-dimensional result in (17.199). It becomes exactly the same with an appropriate choice (17.211) of the renormalization scale M .

The above U(1)-gauge-invariant framework is still far from the full description of the electroweak interaction, where the true symmetry group is $SU(2)_L \times U(1)_Y$ (see Chapter 27 and Ref. [12]).

17.12 Spontaneous Mass Generation in a Massless Theory

The most interesting property of the Coleman-Weinberg model is that it illustrates how fluctuations are capable of spontaneously converting a classically massless theory into a massive theory. This is best seen by looking at the set of effective classical potentials for various mass terms $m^2\rho^2/2$, shown in Fig. 17.6. If $m^2 = 0$, the curvature of the quadratic term in the field $\partial V(\rho)/\partial\rho^2$ at $\rho = 0$ is zero and the theory is massless. The effect is that the field fluctuations around $\rho = 0$ diverge and make the theory critical. The interactions of the field limit the fluctuations so that the field expectation settles at some value $\rho_f = M > \rho_t$ with a finite mass m_f . From Eq. (17.210) we see that

$$m_f^2 = \frac{3q^4M^2}{8\pi^2}. \quad (17.213)$$

Remember that after the ρ -field acquires a nonzero expectation, the vector field has a nonzero mass $m_A = qM$ given by Eq. (17.198). Inserting this into (17.213), we obtain the famous experimentally observable mass ratio caused by fluctuations of a massless theory:

$$\frac{m_f^2}{m_A^2} = \frac{3}{2\pi} \frac{q^2}{4\pi}. \quad (17.214)$$

The value of the effective potential at this new minimum is, according to Eq. (17.207),

$$V(\rho_f) = -\frac{3q^4M^4}{128\pi^2} = -\frac{3m_A^4}{128\pi^2}. \quad (17.215)$$

This is the important lesson of the Coleman-Weinberg model. Even though the classical theory has a scalar field of zero mass, the fluctuations produce a nonzero mass m_f via the nonzero field expectation value $\rho_f = M$. The mass m_f is a so-called spontaneously generated mass. The origin of the mass lies in the need to introduce some nonzero mass scale μ when calculating divergent loop diagrams. The new finite mass parameter M is also referred to as the *dimensionally transmuted coupling constant* of the massless theory.

Notes and References

For more information on vortex lines see the textbooks

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*Nobody can be exactly like me.
Sometimes even I have trouble doing it.*
TALLULAH BANKHEAD (1903–1968)

18

Exactly Solvable $O(N)$ -Symmetric ϕ^4 -Theory for Large N

The functional integral representation of quantum field theory introduced in Chapter 14 has an important advantage over the operator formulation: it offers a similar freedom in changing variables of integration as ordinary integrals do. In physical applications it may often be more economic to describe the system not in terms of the most fundamental particles. In fact, many interesting phenomena in many-body systems are carried by products of fundamental fields which will be called *composite fields* or *collective fields*.

18.1 Introduction of a Collective Field

As an example we consider a scalar field theory with a ϕ^4 -self-interaction, in which the field carries an extra index $a = 1, \dots, N$ accounting for an $O(N)$ -degree of freedom that is usually referred to as *color*.

The generating functional is

$$Z[j] = \mathcal{N} \int \mathcal{D}\phi e^{i \int d^4x \left\{ \frac{1}{2}(\partial\phi_a)^2 - \frac{m_0^2}{2}\phi_a^2 - \frac{g}{4}(\phi_a^2)^2 + j_a\phi_a \right\}}, \quad (18.1)$$

where $\mathcal{N}$ is a normalization factor

$$\mathcal{N} = \left[\text{Tr} \log \left(-\partial^2 - m_0^2 \right) \right]^{1/2}. \quad (18.2)$$

We have slightly changed the convention of how the coupling constant appears in the action, replacing $g/4!$ by $g/4$, to save some numerical factors in the upcoming calculations.

The above theory of a fluctuating ϕ_a will now be transformed into another one, in which only an $O(N)$ -invariant collective field σ appears, which describes the phenomena carried by the composite ϕ_a^2 . We can achieve this by means of an auxiliary functional

$$Z_{\text{aux}} = \int \mathcal{D}\sigma e^{i \frac{1}{4g} (\sigma - g\phi_a^2)^2}. \quad (18.3)$$

The integral is of the pure Fresnel type and cannot depend on the field ϕ_a^2 . Thus it is a constant that may be multiplied with the partition function (18.1) without changing the dynamics. Note that the field $\sigma(x)$ fluctuates quadratically around $g\phi_a^2(x)$, and contains all information carried by the composite operator. In fact, the classical equation of motion is simply

$$\sigma_{\text{cl}}(x) = g\phi_a^2(x). \quad (18.4)$$

The modified expression for the generating functional

$$\begin{aligned} Z[j] &= Z_{\text{aux}} \int \mathcal{D}\phi e^{i \int d^4x \left\{ \frac{1}{2}(\partial\phi_a^2)^2 - \frac{m_0^2}{2}\phi_a^2 - \frac{g}{4}(\phi_a^2)^2 + j_a\phi_a \right\}} \\ &= \mathcal{N} \int \mathcal{D}\phi \mathcal{D}\sigma e^{i \int d^4x \left\{ \frac{1}{2}\phi_a(-\partial^2 - m_0^2 - \sigma)\phi_a + \frac{1}{4g}\sigma^2 + j_a\phi_a \right\}} \end{aligned} \quad (18.5)$$

describes exactly the same theory as before [3].

In the presence of the collective σ -field, each ϕ_a -field has a propagator

$$G_\sigma(x, x') \equiv \frac{i}{-\partial^2 - m_0^2 - \sigma}(x, x'). \quad (18.6)$$

Diagrammatically it is easy to understand why this is so. In the diagrams associated with the action in (18.5), the original four-vertex

$$\begin{array}{c} b \\ \diagdown \\ \times \\ \diagup \\ c \end{array} \quad \begin{array}{c} d \\ \diagup \\ \times \\ \diagdown \\ a \end{array} = 3!gT_{abcd} = 2g(\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}) \quad (18.7)$$

is generated by the exchange of σ . If this field is represented by a wiggly line, its interactions with the original field may be pictured by the following vertex diagram

$$\begin{array}{c} b \\ \diagdown \\ \text{---} \text{wiggly line} \text{---} \\ \diagup \\ a \end{array} \quad \sigma \quad \delta_{ab}. \quad (18.8)$$

The quadratic part of the action in the field σ is

$$\mathcal{A}_0[\sigma] = i \frac{1}{4g} \sigma^2, \quad (18.9)$$

which corresponds to a *propagator* [2]

$$G_{\sigma\sigma} = \text{---} \text{wiggly line} \text{---} = 2g. \quad (18.10)$$

The four-vertices (18.4) are then recovered, in the partition function (18.5), from the diagrams

$$(18.11)$$

An important point is to observe that the action (18.5) is quadratic in ϕ such that we can perform the Gaussian functional integral over ϕ using formula (14.26), leading to

$$Z[j] = \mathcal{N} \int \mathcal{D}\sigma e^{i \int d^4x \left\{ \frac{1}{4g} \sigma^2 + iN \frac{\hbar}{2} \text{Tr} \log(-\partial^2 - m_0^2 - \sigma) + \frac{i}{2} j \frac{i}{-\partial^2 - m_0^2 - \sigma} j \right\}}, \quad (18.12)$$

where the last term is due to the quadratic completion [3]. Note that in the last term we have omitted the repeated subscripts a .

The factor N in front of the trace log arises from the N components ϕ_a , of which each gives the same contribution. The new representation of $Z[j]$ describes the same physics in terms of a single composite field σ rather than N fundamental fields ϕ_a .

Since the main application of this formalism is in many-body problems where composite fields describe collective phenomena, the field σ is referred to as collective field, and the exponent in (18.12) as *collective action*.

Let us derive the Feynman rules for the collective field theory. The “free part” of the action is $\sigma^2/4g$ with the σ -“propagator” (18.10). The vertices are obtained from the powers σ^n in an expansion of the remaining part of the collective action. The trace of the logarithm may be expanded into loops just as shown in (22.32). In contrast to the diagrams (22.36), the loops now emit single wiggly lines for σ rather than pairs of ϕ -lines

$$(18.13)$$

Similarly, the current piece may be expanded in powers of σ as

$$\begin{aligned} -\frac{1}{2} j \frac{i}{-\partial^2 - m_0^2 - \sigma} j &= -\frac{1}{2} j \left[\frac{i}{-\partial^2 - m_0^2} + \frac{i}{-\partial^2 - m_0^2} (-i\sigma) \frac{i}{-\partial^2 - m_0^2} \right. \\ &\quad \left. + \frac{i}{-\partial^2 - m_0^2} (-i\sigma) \frac{i}{-\partial^2 - m_0^2} (-i\sigma) \frac{i}{-\partial^2 - m_0^2} + \dots \right]. \end{aligned} \quad (18.14)$$

This corresponds to the following Feynman graphs

$$(18.15)$$

in which a line connects two currents and emits any number of wiggly σ -lines along the way.

It is obvious that every fundamental graph can be recovered by connecting the σ -ends in (18.13) and (18.15) via the “propagator” $G_{\sigma\sigma} = 2g$.

18.2 The Limit of Large N

One of the most interesting features of the collective field σ is that it can be used to *solve* the full quantum field theory in the limit $N \rightarrow \infty$. While taking N to infinity, the coupling constant should be lowered simultaneously by a factor $1/N$, setting

$$g = g_1/N \quad (18.16)$$

with fixed g_1 . In order to see how this works we first rewrite the functional integral over σ , in the absence of external currents j as [4]

$$e^{iN\mathcal{A}_{\text{coll}}[\sigma]} = \int \mathcal{D}\sigma e^{iN \int d^4x \left[\frac{1}{2g_1} \sigma^2 - i\frac{\hbar}{2} \text{Tr} \log(-\partial^2 - m_0^2 - \sigma) \right]}. \quad (18.17)$$

The factor N in the exponent has the same effect as previously the factor $1/\hbar$ in the semiclassical limit. For $N \rightarrow \infty$, the exponential becomes a δ -functional around the extremum of the action which is given by

$$\Sigma(x) = 4g_1 \frac{\hbar}{2} \left(\frac{i}{-\partial^2 - m_0^2 - \Sigma} \right) (x, x). \quad (18.18)$$

Fluctuations around this solution are suppressed by a factor $1/N$ (just as previously $\hbar$). Thus, to leading order in N , the effective action is given by

$$W[j]|_{j=0} = \mathcal{A}_{\text{coll}}[\Sigma] = \int d^4x \left[\frac{1}{2g} \Sigma^2 - iN \frac{\hbar}{2} \text{Tr} \log(-\partial^2 - m_0^2 - \Sigma) \right].$$

Let us now include external currents and consider

$$e^{iW[j]} = \int \mathcal{D}\sigma \exp \left\{ iN\mathcal{A}_{\text{coll}}[\sigma] - \frac{1}{2} j \frac{i}{-\partial^2 - m_0^2 - \sigma} j \right\}. \quad (18.19)$$

Then, as $N \rightarrow \infty$, we have to allow for the possibility that the external particles contribute to leading order in N (for instance if there is one external line for each index $a = 1, \dots, N$). Then the field σ has to be chosen to extremize the full exponent which happens, say, at $\sigma = \Sigma[j]$. The extremization can be formalized by making use of a Legendre transformation. We go from $W[j]$ to the effective action and do this by introducing first an effective field as

$$\Phi_a[j] = \frac{\delta W[j]}{\delta j_a} = i \frac{1}{-\partial^2 - m_0^2 - \Sigma[j]} j_a. \quad (18.20)$$

The inverse transformation is $j_a = j_a[\Phi_a]$, and from this we derive $\Sigma[\Phi_a] = \Sigma[j_a[\Phi_a]]$. Note that there is no contribution to this from the derivative $\delta\Sigma/\delta j_a$ via the chain rule $\delta W[j]/\delta\Sigma \times \delta\Sigma/\delta j_a$, since $W[j]$ is extremal in Σ if differentiated at fixed j_a . At the end we calculate the effective action from the equation

$$\Gamma[\Phi_a] = N\mathcal{A}_{\text{coll}}[\Sigma] - \frac{1}{2} \int d^4x \Phi_a (-\partial^2 - m_0^2 - \Sigma) \Phi_a - j_a[\Phi_a] \Phi_a. \quad (18.21)$$

Here Σ is the extremal functional $\Sigma[\Phi_a]$. It is obvious that this functional can be obtained directly from minimizing (18.21) at a constant Φ_a . This is so since the extremality condition

$$K = \frac{\delta W[j]}{\delta \Sigma} = 0 \quad (18.22)$$

determines $\Sigma = \Sigma[j]$. It also implies that

$$\Gamma_\Sigma[\Phi_a] = [W[j] - \Phi_a j_a]_\Sigma = (W_{j_a}[j] - \Phi_a) \frac{\partial j_a}{\partial \Sigma} + \frac{\partial W[j]}{\partial \Sigma} = 0, \quad (18.23)$$

a relation which serves to determine $\Sigma = \Sigma[\Phi]$. Thus it is more practical to consider

$$\Gamma[\Phi_a, \Sigma] = N \mathcal{A}_{\text{coll}}[\Sigma] + \frac{1}{2} \int d^4x \Phi_a (-\partial^2 - m_0^2 - \Sigma) \Phi_a \quad (18.24)$$

as an effective action of two fields Φ_a and Σ . The physical field configurations are obtained by extremizing $\Gamma[\Phi_a, K]$ with respect to *both* arguments, thus determining, say, Φ_a^0, Σ^0 .

The calculation of higher vertex functions proceeds as follows. One expands $\Gamma[\Phi_a, \Sigma]$ around Φ_a^0, Σ^0 by writing

$$\begin{aligned} \Gamma[\Phi_a, \Sigma] &= \Gamma[\Phi_0^0 + \Phi'_a, \Sigma^0 + \Sigma'] = \Gamma[\Phi_a^0, \Sigma^0] \\ &+ \frac{1}{2} \left\{ \Gamma_{\Phi_a \Phi_b}[\Phi^0, \Sigma^0] \Phi'_a \Phi'_b + 2\Gamma_{\Sigma \Phi_a}[\Phi_a^0, \Sigma^0] \Phi'_a \Sigma' + \Gamma_{\Sigma \Sigma}[\Phi^0, \Sigma^0] \Sigma' \Sigma' \right\} \\ &+ \text{higher derivative terms.} \end{aligned} \quad (18.25)$$

In the sequel we shall often omit the subscripts a . The first derivatives vanish, the second determine propagators of Φ' and Σ' fields

$$G_{\Phi' \Phi'} = i\Gamma_{\Phi \Phi}^{-1}[\Phi^0, \Sigma^0], \quad (18.26)$$

$$G_{\Sigma' \Sigma'} = i\Gamma_{\Sigma \Sigma}^{-1}[\Phi^0, \Sigma^0]. \quad (18.27)$$

By means of the vertex functions fixed by the higher functional derivatives we may now compose all tree diagrams. Only those with external Φ' -lines survive since $\Gamma_\Sigma = 0$. But any number of internal Σ' -lines may occur.

Let us convince ourselves that these vertex functions are the same as those which would be obtained from higher functional derivatives of $\Gamma[\Phi]$ in (18.21). In order to avoid writing the two arguments of $\Gamma[\Phi, \Sigma]$ let us denote $\Gamma[\Phi] \equiv \Gamma[\Phi, \Sigma[\Phi]]$ by $F[\Phi]$ for the discussion to follow, i.e.,

$$F[\Phi] \equiv \Gamma[\Phi, \Sigma[\Phi]]. \quad (18.28)$$

As argued before, the functional $\Sigma[\Phi]$ satisfies

$$\Gamma_\Sigma[\Phi, \Sigma[\Phi]] = 0, \quad (18.29)$$

or

$$\Sigma_\Phi = -\Gamma_{\Sigma\Sigma}^{-1}\Gamma_{\Sigma\Phi}. \quad (18.30)$$

This relation can be used when deriving the higher vertex functions from (18.28):

$$F_\Phi = \Gamma_\Phi + \Gamma_\Sigma \Sigma_\Phi = \Gamma_\Phi - \Gamma_\Sigma \Gamma_{\Sigma\Sigma}^{-1} \Gamma_{\Sigma\Phi}. \quad (18.31)$$

This may be represented graphically as

$$\text{diagram} = \text{diagram} - \text{diagram}. \quad (18.32)$$

An open blob with two double legs stands for the second functional derivative of $\Gamma[\Sigma, \Phi]$ with respect to Σ , which is $-i$ times the propagator of the Σ' -field (with the notation of Wick-contractions in Section 10.8):

$$\text{diagram} = \Gamma_{\Sigma\Sigma}^{-1} = -i \overline{\Sigma' \Sigma'}. \quad (18.33)$$

The grey blobs are the vertices of the two-argument effective action $\Gamma[\Phi, \Sigma]$. They have single or double legs emerging, the latter representing the Σ' -field. Differentiating this with respect to Φ adds one more single leg:

$$\frac{\delta}{\delta\Phi} \text{diagram} = \text{diagram}. \quad (18.34)$$

A differentiation with respect to Σ adds one more double leg:

$$\frac{\delta}{\delta\Sigma} \text{diagram} = \text{diagram}. \quad (18.35)$$

Since $\delta\Gamma_{\Sigma\Sigma}^{-1}/\delta\Phi = \Gamma_{\Sigma\Sigma}^{-3}\Gamma_{\Sigma\Phi}$ we see that differentiating (18.33) with respect to Φ produces a three- Σ' vertex:

$$\frac{\delta}{\delta\Phi} \text{diagram} = \text{diagram}. \quad (18.36)$$

Differentiating (18.31) further we find

$$F_{\Phi\Phi} = \Gamma_{\Phi\Phi} - \Gamma_{\Phi\Phi}\Gamma_{\Sigma\Sigma}^{-1}\Gamma_{\Sigma\Phi} - \Gamma_{\Sigma}\Gamma_{\Sigma\Sigma}^{-1}\Gamma_{\Sigma\Phi\Phi} - \Gamma_{\Phi\Sigma}\Gamma_{\Sigma\Sigma}^{-3}\Gamma_{\Sigma\Sigma\Sigma}\Gamma_{\Sigma\Phi}\Gamma_{\Sigma}, \quad (18.37)$$

which has the graphical form

$$\text{Diagrammatic equation (18.38)} \quad (18.38)$$

The procedure can be continued via the chain rule of differentiation. A blob with n legs stands for the n th functional derivative of (18.28):

$$F_{\Phi\Phi\dots\Phi} = \text{Diagram of a blob with } n \text{ legs} \quad (18.39)$$

Let us restore the color labels a in the effective action and write it as

$$\Gamma[\Phi_a, \Sigma] = N\mathcal{A}_{\text{coll}}[\Sigma] + \frac{1}{2} \int d^4x \Phi_a (-\partial^2 - m_0^2 - \Sigma) \Phi_a. \quad (18.40)$$

We can now simplify the algebraic treatment of the graphical rules. We set $\gamma[\Sigma] \equiv N\mathcal{A}_{\text{coll}}[\Sigma]$, and obtain the simple vertex functions

$$\Gamma_{\Phi_a\Phi_b} = (-\partial^2 - m_0^2 - \Sigma) \delta_{ab} \quad (18.41)$$

$$\Gamma_{\Sigma\Phi_a} = -\Phi_a, \quad (18.42)$$

$$\Gamma_{\Sigma\Phi_a\Phi_b} = -\delta_{ab}, \quad (18.43)$$

$$\Gamma_{\Sigma\Phi_{a_1}\dots\Phi_{a_n}} = 0, \quad n \geq 2, \quad (18.44)$$

$$\Gamma_{\Sigma_1\dots\Sigma_n\Phi_a} = 0, \quad n \geq 2, \quad (18.45)$$

$$\Gamma_{\Sigma_1\dots\Sigma_n} = \gamma_{\Sigma_1\dots\Sigma_n} \quad n \geq 2. \quad (18.46)$$

Then the second functional derivative (18.37) becomes

$$\Gamma_{\Phi_a\Phi_b} = -\partial^2 - m_0^2 - \Sigma - \Phi_a \gamma_{\Sigma\Sigma}^{-1} \Phi_b + \Gamma_{\Sigma} \gamma_{\Sigma\Sigma}^{-1} - \Gamma_{\Sigma\Sigma}^{-3} \gamma_{\Sigma\Sigma\Sigma} \Phi^2 \Gamma_{\Sigma}. \quad (18.47)$$

This has to be evaluated at the extremum, where $\Gamma_{\Sigma_a} = 0$. We therefore obtain the propagator of the Φ_a -field

$$G_{ab} = iF_{\Phi_a\Phi_b}^{-1} = i \left[(-\partial^2 - m_0^2 - \Sigma) \delta_{ab} - \Phi_a \gamma_{\Sigma\Sigma}^{-1} \Phi_b \right]^{-1}. \quad (18.48)$$

We best exhibit the extremization of (18.40) graphically, and replace the vertices Eqs. (18.41) and (18.42) by the following diagrams $\Gamma_{\Sigma\Phi}$ and $\Gamma_{\Sigma\Phi\Phi}$:

$$\Gamma_{\Sigma\Phi_a} = \text{diagram of a shaded circle with a double line on the left and a single line on the right labeled } a = - \text{diagram of a square box labeled } \Phi_a \quad , \quad \Gamma_{\Sigma\Phi_a\Phi_b} = \text{diagram of a shaded circle with two double lines on the left labeled } a \text{ and } b = - \text{diagram of a square box labeled } \delta_{ab} . \quad (18.49)$$

Then the differential equation (18.36) can be rewritten as

$$\frac{\delta}{\delta\Phi_a} \text{diagram of a circle with a double line on the left} = \text{diagram of a circle with a double line on the left connected to a shaded circle which is connected to a circle with a double line on the right, and a square box labeled } \Phi_a \text{ is connected to the top of the shaded circle} , \quad (18.50)$$

and (18.38) takes the form:

$$\begin{aligned} a \text{diagram of a circle with a diagonal line} b &= - \text{diagram of a square box labeled } \Phi_a \text{ connected to a circle with a double line on the right, which is connected to a square box labeled } \Phi_b \\ &+ \text{diagram of a shaded circle connected to a circle with a double line on the right, which is connected to a square box labeled } \delta_{ab} - \text{diagram of a square box labeled } \Phi_a \text{ connected to a circle with a double line on the right, which is connected to a shaded circle, which is connected to a circle with a double line on the right, which is connected to a square box labeled } \Phi_b . \end{aligned} \quad (18.51)$$

A functional differentiation of $\Gamma_{\Sigma\Sigma\dots\Sigma}$ with more than one Σ -leg with respect to Φ gives

$$\frac{\delta}{\delta\Phi_a} \text{diagram of a shaded circle with four double lines} = \text{diagram of a shaded circle with four double lines, where one double line is connected to a circle with a double line on the right, which is connected to a square box labeled } \Phi_a . \quad (18.52)$$

Let us finally write down the propagators and vertices of the Σ' -field explicitly. For this we consider the Taylor series of the trace log term in (18.17):

$$\begin{aligned} &N \frac{i}{2} \text{Tr} \log \left(-\partial^2 - m_0^2 - \Sigma^0 - \Sigma' \right) \\ &= N \frac{i}{2} \left[\text{Tr} \log \left(-\partial^2 - m_0^2 - \Sigma^0 \right) + \text{Tr} \log \left(1 + \frac{i}{-\partial^2 - m_0^2 - \Sigma^0} i \Sigma' \right) \right] \\ &= N \frac{i}{2} \sum_{n=1}^{\infty} \frac{1}{n} \left[\frac{i}{-\partial^2 - m_0^2 - \Sigma^0} (-i \Sigma') \right]^n . \end{aligned} \quad (18.53)$$

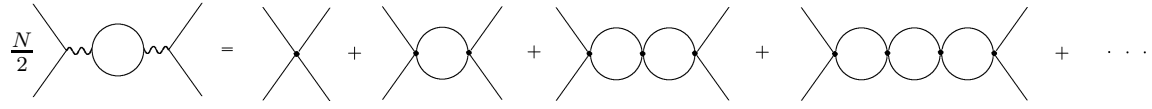
Reading off the quadratic terms

$$\frac{N}{4} \left[\frac{1}{g_1} \Sigma'^2 + i \text{Tr} \left(\frac{i}{-\partial^2 - m_0^2 - \Sigma^0} \Sigma' \right) \right] , \quad (18.54)$$

we find in momentum space the Wick rotated propagator

$$G_{\Sigma'\Sigma'}(q') \equiv i\Gamma_{\Sigma\Sigma}^{-1} = \delta^{(4)}(q - q') \frac{2}{N} i \left\{ \frac{1}{g_1} \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 - m_0^2 - \Sigma^0} \frac{1}{(q - k)^2 - m_0^2 - \Sigma^0} \right\}^{-1}. \quad (18.55)$$

This propagator is a non-perturbative object. Expanding it in powers of g_1 , we may write the interaction caused by it as a series of ordinary Feynman diagrams



$$\frac{N}{2} \text{ (wavy line with blob)} = \text{four-point vertex} + \text{bubble} + \text{two-bubbles} + \text{three-bubbles} + \dots \quad (18.56)$$

where the wiggle with a blob represents the propagator (18.55) of the Σ' -field, a line the simple Φ' propagator

$$G_{\Phi'\Phi'} = \frac{i}{-\partial^2 - m_0^2 - \Sigma^0}, \quad (18.57)$$

and a dot the fundamental ϕ^4 -vertex g_1 .

It should be pointed out that the higher terms in the bubble sum in (18.56) do not carry the same multiplicity factors as in the original perturbation expansion of the ϕ^4 -theory in (10.6.1). The factors in that expansion are $4g/4!$, $(4!4!/2)(g/4!)^2$ for zero- and one-bubble diagrams. After exchanging $g/4! \rightarrow g/4$ these become $6g$, $24g^2$. In the σ exchange between two Φ' -lines, only one third of the contractions are done, so that the factor $6g$ is reduced to $2g = 2g_1/N$. This explains the first term in the propagator (18.56). For N components, the second multiplicity receives a factor $T_I = (N + 8)/9$ [recall (11.233) and (11.248)], which in the limit $N \rightarrow \infty$ becomes $N/9$. Thus the second terms carries a factor $\frac{2}{N}g^2 = g_1$, in agreement with the second term in (18.56).

The n -point vertex functions for the Σ' field are given by

$$-\frac{N}{2} i \frac{i}{n} \left[\frac{i}{-\partial^2 - m_0^2 - \Sigma^0} (-i\Sigma') \right]^n \quad (18.58)$$

which are the one-loop diagrams (18.13) with Φ' lines emerging from the circle. In this way every n -point vertex function of the original field theory has been reduced, in the limit $N \rightarrow \infty$, to a finite sum of tree diagrams involving Σ' propagators

and Σ' -vertices, all of which consist of one-loop diagrams of the Φ' field. For the four-point function we obtain

$$\begin{aligned}
 & \text{Diagram with four external lines } a, b, c, d \text{ meeting at a central shaded circle} \\
 &= -3 \left[\text{Diagram with two internal lines, each with a double line and a box labeled } \delta_{ab} \text{ and } \delta_{cd} \right] \\
 & - \left[\text{Diagram with a central shaded circle and four external lines, each with a box labeled } \Phi_a, \Phi_b, \Phi_c, \Phi_d \right] \\
 & - 3 \left[\text{Diagram with a central shaded circle and four external lines, each with a box labeled } \Phi_a, \Phi_b, \Phi_c, \Phi_d \right] \\
 & - 3 \left[\text{Diagram with a central shaded circle and four external lines, each with a box labeled } \Phi_a, \Phi_b, \Phi_c, \Phi_d \right] \\
 & - 3 \left[\text{Diagram with a central shaded circle and four external lines, each with a box labeled } \Phi_a, \Phi_b, \Phi_c, \Phi_d \right]
 \end{aligned} \tag{18.59}$$

plus terms which contain Γ_Σ at the end of one double line and vanish at the extremum. We now see that the rules derived in this algebraic fashion are indeed just the Feynman rules for tree diagrams of the theory with propagators

$$G_{\Sigma'\Sigma'} = i\gamma_{\Sigma\Sigma'}^{-1}. \tag{18.60}$$

The double lines either end on a field Φ_a or on a Kronecker δ_{ab} .

18.3 Variational Equations

We have seen in Section 13.9 that the effective action can be used as a basis for variational calculations of a field theory. As an application we study here a simple exactly solvable field-theoretic model which permits us to see the effect of all loop corrections. The simplest model is a ϕ_a^4 -theory with N fields $\phi_1, \dots, \phi_N$ in the limit $N \rightarrow \infty$. In statistical mechanics, this is known as the *spherical model*. In the last section, we have derived the effective action as a function of the classical field $\Phi_a(x)$ and the collective field $\Sigma(x)$ as

$$\begin{aligned}
 \Gamma[\Phi_a, \Sigma] = \mathcal{A}[\Phi_a] + \Gamma_{\text{coll}}[\Phi, \Sigma] &= \int d^D x \left[\frac{1}{2} (\partial \Phi_a)^2 - \frac{m_0^2}{2} \Phi_a^2 - \frac{1}{2} \Sigma \Phi_a^2 + \frac{N}{4g_0} \Sigma^2 \right] \\
 &+ \frac{i}{2} N \text{Tr} \log (-\partial^2 - m_0^2 - \Sigma). \tag{18.61}
 \end{aligned}$$

To leading order in N , this is the exact effective action of the theory. For the discussion to follow it will be useful to abbreviate $m_0^2 + \Sigma(x)$ by $\lambda(x)$:

$$m_0^2 + \Sigma(x) \equiv \lambda(x), \tag{18.62}$$

since this combination appears inside the functional Tr log like a spacetime-dependent mass term. Then we write

$$\begin{aligned} \Gamma[\Phi_a, \lambda] &= \int d^D x \left[\frac{1}{2} (\partial \Phi_a)^2 - \frac{1}{2} \lambda \Phi_a^2 - \frac{N}{2g_0} m_0^2 \lambda + \frac{N}{4g_0} \lambda^2 + \frac{N}{4g_0} m_0^4 \right] \\ &+ \frac{i}{2} N \text{Tr log} (-\partial^2 - \lambda). \end{aligned} \quad (18.63)$$

According to Eq. (13.79), the effective action has to be extremal for physical values of the vacuum expectation of the fields $\Phi_a = \langle \phi_a \rangle$. We expect the ground state to be isotropic in spacetime, and look for minima of the effective potential as a function of *constant* fields λ, Φ_a , for which the functional Tr log reduces to a simple integral over phase space. Dividing out the spacetime volume, we obtain the effective potential

$$v(\Phi, \lambda) = \frac{1}{2} \lambda \Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0} \lambda^2 - \frac{N}{4g_0} m_0^4 + \frac{N}{2} \int \frac{d^D k}{(2\pi)^D} \log(k^2 + \lambda). \quad (18.64)$$

The momentum integral can be done using formula (11.134) and we obtain

$$v(\Phi, \lambda) = \frac{1}{2} \lambda \Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0} \lambda^2 - \frac{N}{4g_0} m_0^4 + \frac{1}{2} N S_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \frac{2}{D} \lambda^{D/2}. \quad (18.65)$$

To find the extrema of this we distinguish two cases:

1. Case

$$\frac{\partial v}{\partial \Phi_a} = \lambda \Phi_a = 0. \quad (18.66)$$

This equation allows two possible solutions:

- a) $\Phi_a = 0$,
- b) $\Phi_a \neq 0, \quad \lambda = 0$.

2. Case

$$\frac{\partial v}{\partial \lambda} = \Phi_a^2 + \frac{N m_0^2}{g_0} - \frac{N}{g_0} \lambda + N S_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \lambda^{D/2-1} = 0. \quad (18.67)$$

The extremum 1a) corresponds to a normal ground state possessing the same $O(N)$ -symmetry as the original action. The ground state 1b) associated with the other extremum, on the other hand, breaks the $O(N)$ -symmetry of the action. This phenomenon is called *spontaneous symmetry breakdown*. It is a universal phenomenon in many-body systems, where it is observed in the form of ordered phases. The most widely known systems of this type are ferromagnets, which display a spontaneous magnetization at sufficiently low temperature. The magnetization vector may be identified with the field at an expectation Φ_a for $N = 3$. The magnetized state is

not rotationally invariant, thus violating spontaneously the rotational invariance of the Hamilton operator of the system. Above a critical temperature, called *Curie- or Néel-temperature*, the system loses its magnetization and becomes rotationally symmetric. This is the normal state.

In the $O(N)$ -symmetric solution 1a), the second equation (18.67) determines λ :

$$\frac{Nm_0^2}{g_0} = \frac{N}{g_0}\lambda - NS_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \lambda^{D/2-1}. \quad (18.68)$$

In solution 1b), it determines the field strength in the ground state:

$$\Phi_a^2 = -\frac{Nm_0^2}{g_0}. \quad (18.69)$$

We have seen before that the functional integral is stable only for $g_0 > 0$. The state with spontaneously broken $O(N)$ -symmetry can exist only for $m_0^2 < 0$.

Observe the following important physical property of the theory. For a negative m_0^2 , the theory without self-interaction possesses excitations which in Minkowski spacetime propagate faster than the speed of light. These are called *tachyons*, and many authors have speculated about the consequences of their possible existence. The ϕ^4 -theory presented here gives a simple no-go answer to this possibility. If m_0^2 is negative, the system undergoes a phase transition into a new ground state with $\Phi_a \neq 0$ around which the excitations have a speed lower than light velocity. More about this will be discussed on pages 1134, 1294, and 1311.

18.3.1 Non-trivial Ground States

The solutions to the above equations depend on the dimension of spacetime, and will now be discussed.

Dimension $D = 4$

Setting $D = 4 - \epsilon$ and using (11.163) to expand

$$\frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) = -\frac{1}{\epsilon} + \mathcal{O}(\epsilon),$$

equation (18.67) becomes

$$\Phi_a^2 = \frac{N}{g_0} (\lambda - m_0^2) + NS_D \mu^{-\epsilon} \lambda \frac{1}{\epsilon} - NS_D \mu^{-\epsilon} \lambda \log \frac{\lambda}{\mu^2}. \quad (18.70)$$

This is renormalized by introducing the physical masses and coupling constants m and g :

$$\frac{1}{g} \equiv \frac{1}{g_0 \mu^\epsilon} + S_D \frac{1}{\epsilon}, \quad (18.71)$$

$$\frac{m^2}{g} \equiv \frac{m_0^2}{g_0}, \quad (18.72)$$

with an arbitrary mass parameter μ . Then we can take the limit $\epsilon \rightarrow 0$ in (18.70), and find

$$\Phi_a^2 = \frac{N}{g} (\lambda - m^2) - NS_4 \frac{1}{2} \lambda \log \frac{\lambda}{\mu^2}, \quad (18.73)$$

where $S_4 = 1/8\pi^2$. The corresponding potential is

$$v(\Phi_a, \lambda) = \frac{1}{2} \lambda \Phi_a^2 + \frac{N}{2g} m^2 \lambda - \frac{N}{4g} \lambda^2 - \frac{N}{4g_0} m_0^4 + NS_4 \frac{1}{8} \lambda \left(\log \frac{\lambda}{\mu^2} - \frac{1}{2} \right). \quad (18.74)$$

Consider the ground state with a spontaneous symmetry breakdown, where the minimum of $n(\Phi_a, M)$ lies at $\Phi_a \neq 0$ with $\lambda = 0$. From (18.69) and (18.72), this minimum lies at

$$\Phi_a^2 = -\frac{Nm^2}{g}. \quad (18.75)$$

For a positive renormalized coupling constant g , this ground state requires a regular m^2 . Let us see how $v(\Phi_a, M)$ behaves in the neighborhood of $m^2 = 0$. For $m^2 > 0$, Φ_a^2 necessarily increases since the logarithm in (18.74) is negative. Its slope in λ is initially infinite, being given by

$$\frac{\partial v(\Phi_a, \lambda)}{\partial \lambda} = \frac{1}{2} \left[\Phi_a^2 + \frac{Nm^2}{g} - \frac{N}{2g} \lambda - NS_4 \frac{1}{4} \left(\log \frac{\lambda}{\mu^2} + \frac{1}{2} \right) \right]. \quad (18.76)$$

If we insert (18.73) back into the potential (18.74), we find

$$v_{\min} = \frac{1}{4} \lambda \left(\Phi_a^2 + \frac{Nm^2}{g} \right) - NS_4 \frac{1}{16} \lambda^2. \quad (18.77)$$

Then, for increasing small λ , the potential increases. This goes on until $v_{\min}$ reaches a maximum which is determined by

$$\Phi_{a \max}^2 + \frac{Nm^2}{g} = NS_4 \frac{1}{2} \lambda_{\max}. \quad (18.78)$$

Together with (18.73), this implies

$$\log \frac{\lambda_{\max}}{\mu^2} = -1 + \frac{2}{gS_4}. \quad (18.79)$$

If we want to calculate Φ_a for a value $\Phi_a^2 > \Phi_{a \max}^2$, we have to choose a complex λ , so that also the potential becomes complex indicating an instability of the corresponding state. Even though this field configuration can be reached only via an external current, there are disastrous consequences as we shall see later when discussing the Green functions of the theory.

Dimension $D = 3$

Here the equation (18.67) reads

$$\Phi_a^2 = \frac{N}{g_0} (m^2 - m_0^2) + N\mathcal{S}_3 M, \quad (18.80)$$

where $\mathcal{S}_3 = 1/2\pi^2$. With this regularization, neither m_0^2 nor g_0 need to be renormalized, so that they can be replaced by m^2 and g . The potential becomes

$$v(\Phi_a, M) = \frac{1}{2} \left(\Phi_a^2 + \frac{Nm^2}{g} \right) - \frac{N}{4g} \lambda^2 - N\mathcal{S}_3 \frac{\pi}{6} \lambda^{3/2}. \quad (18.81)$$

Again, as λ increases from zero, $\Phi_a^2 + Nm^2/g$ moves to positive values. The potential at the extremum g in λ is

$$\begin{aligned} v_{\text{ext}} &= \lambda \left(\Phi_a^2 + \frac{Nm^2}{g} \right) \left(\frac{1}{2} - \frac{1}{D} \right) - \frac{N}{4g} \left(1 - \frac{4}{D} \right) \lambda^2 \\ &= \frac{1}{6} \lambda \left(\Phi_a^2 + \frac{Nm^2}{g} \right) + \frac{1}{12} \frac{N}{g} \lambda^2. \end{aligned} \quad (18.82)$$

There is now an important difference with respect to the previous $D = 4$ case. The potential increases monotonously for $\Phi_a^2 > -Nm^2/g$ and does not become complex for any large positive Φ^2 . For $\Phi_a^2 < -Nm^2/g$, however, the situation is in some respect similar to $D = 4$, but in an important aspect it is different. To see most easily what happens we may express λ from (18.67) in terms of $\Phi_a^2 + Nm^2/g$, and have

$$\sqrt{\lambda} = -\frac{g}{4} \mathcal{S}_3 \pi + \left[\left(\frac{g\mathcal{S}_3 \pi}{4} \right)^2 + \frac{g}{N} \left(\Phi_a^2 + \frac{Nm^2}{g} \right) \right]. \quad (18.83)$$

As long as $\Phi_a^2 > -Nm^2/g$, the solution has $\sqrt{\lambda} > 0$. Below this value, the square-root becomes negative. Thus there is again a complex value of the auxiliary field λ , just as for $D = 4$. The difference with respect to that case lies in the fact that in spite of λ being complex, $v(\Phi_a, \lambda)$ remains real and increases with $\Phi^2 < -Nm^2/g$. It therefore has a proper minimum at $\Phi^2 = -Nm^2/g$. Thus the theory is consistent and displays a spontaneous breakdown of $O(N)$ -symmetry.

Dimension $D = 2$

In two dimensions everything changes drastically. Here the potential becomes for $D = 2 + \epsilon$ [using $\Gamma(D/2)\Gamma(1 - D/2)2/D \approx -2/\epsilon + 1$]:

$$v = \frac{1}{2} \lambda \Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0} \lambda^2 - \frac{N}{4g_0} m_0^4 - \frac{1}{4} N \mathcal{S}_2 \lambda \left(\log \frac{\lambda}{\nu^2} - 1 \right), \quad (18.84)$$

so that Eq. (18.67) becomes

$$\Phi_a^2 = \frac{N}{g_0} (\lambda - m_0^2) + N S_D \frac{1}{\epsilon} + \frac{1}{2} N \mu^2 S_D \log \frac{\lambda}{\mu^2}. \quad (18.85)$$

We can again renormalize the mass by introducing

$$m^2 = m_0^2 - g_0 S_D \frac{1}{\epsilon}. \quad (18.86)$$

For the coupling constant there is no need of renormalization, i.e., $g = g_0$. Then the finite equation reads

$$\Phi_a^2 = \frac{N}{g} (\lambda - m^2) + \frac{1}{2} N S_2 \log \lambda / \mu^2, \quad (18.87)$$

where $S_2 = 1/2\pi$. The potential at the minimum is given by

$$v_{\min} = \frac{1}{2} \lambda \left(\Phi_a^2 + \frac{N m^2}{g} \right) - \frac{N}{4g} \lambda^2 + N \frac{1}{4} S_2 \lambda \left[\log \left(\frac{\lambda}{\mu^2} \right) - 1 \right]. \quad (18.88)$$

At the minimum, the value of Φ_a^2 as a function of λ behaves quite differently from the previous cases. There is no finite value of Φ_a^2 for which λ can be equal to zero, since for $\lambda \rightarrow 0$, the square field Φ_a^2 should go to $-\infty$, which is impossible. Thus there can be no spontaneous symmetry breakdown in two dimensions. The condensation energy behaves exceptionally for $N = 2$. In two dimensions there exist no ordered ground state, which is merely quasi-ordered. A related situation holds for $N = 1$.

Dimension $D = 1$

Also in one dimension, there can be no spontaneous symmetry breakdown. This is obvious since the system is equivalent to quantum mechanics of a particle at the time-dependent position $\phi(t)$, i.e., the Hamiltonian

$$H = \frac{1}{2} (\partial \phi_a)^2 - \frac{m_0^2}{2} \phi_a^2 - \frac{g_0}{4N} (\phi_a^2)^2 \quad (18.89)$$

may be interpreted as that of a mass point in N -dimensional space moving in an $O(N)$ -invariant potential. The quantum mechanical ground state is unique, and there can be no degeneracy, hence no spontaneous symmetry breakdown. Contrary to the case $D = 2$, this argument also holds for any N , also for $N = 2$ and $N = 1$. Certainly, Eq. (18.67) has to reflect this feature, and indeed does so. There is now no need for renormalization, so that we can omit the subscripts zero and find for $D = 1$ with $S_1 = 1/\pi$:

$$\Phi_a^2 = \frac{N}{g} (\lambda - m^2) - (\lambda)^{-1/2}, \quad (18.90)$$

$$v_{\min} = -\frac{1}{2} \lambda \left(\Phi_a^2 + \frac{N m^2}{g} \right) + \frac{N}{4g} \lambda^2. \quad (18.91)$$

Again there is no solution for $\lambda \rightarrow 0$, since this would imply $\Phi_a^2 \rightarrow -\infty$.

18.4 Special Features of Two Dimensions

The impossibility of a spontaneous breakdown of a continuous symmetry in two spacetime dimensions is related to the fact that such a phase would contain massless Nambu-Goldstone bosons in two dimensions. But it can easily be shown that massless fields $\phi(x)$ cannot exist in this reduced spacetime. The reason is basically that the associated propagator

$$G(x) = \langle \phi(x)\phi(0) \rangle = \int \frac{d^2q}{(2\pi)^2} \frac{i}{q^2} e^{iqx} \quad (18.92)$$

is divergent for all $\mathbf{x}$, due to the singularity at $q = 0$. To have such a propagator, one needs a small- q cutoff or, equivalently, an infinitesimally small mass μ . If that were present, the D dimensional propagator would read, according to (7.145),

$$\begin{aligned} G(x) &= \int \frac{d^Dq}{(2\pi)^D} \frac{i}{q^2 - \mu^2} e^{iqx} \\ &= \frac{1}{(2\pi)^{D/2}} \left(\frac{\mu}{|x|} \right)^{D/2-1} K_{D/2-1}(\mu|x|), \end{aligned} \quad (18.93)$$

where $|x| \equiv \sqrt{-(x-x')^2}$. For $|x| \ll 1/\mu$, which due to the smallness of μ means almost everywhere, we use the small-argument limit of the Bessel function

$$K_\nu(z) \approx \Gamma(\nu) \frac{1}{2} \left(\frac{2}{z} \right)^\nu, \quad (18.94)$$

to obtain the approximations

$$G(x) \approx \begin{cases} \Gamma(D/2 - 1) \frac{1}{4\pi^{D/2} |x|^{D-2}}, & D > 2 \\ -\frac{1}{2\pi} \log \frac{\mu\sqrt{-x^2}}{2e^{-\gamma}}, & D = 2. \end{cases} \quad (18.95)$$

Here $\gamma = 0.577\dots$ is Euler's number. The two-dimensional expression diverges logarithmically in the limit $\mu \rightarrow 0$. This behavior has given rise to a physical feature of two-dimensional systems, formulated as a theorem, which in many-body physics is known as the *Mermin-Wagner theorem*, and in quantum field theory as *Coleman's no-go theorem* [5]. Notwithstanding this theorem, the systems in which one would have expected massless Nambu-Goldstone modes, do have a characteristic feature: They show what are called *quasi-long-range correlations*. These lead to physical observations which are quite similar to those of proper long-range fluctuations [6]. There are experiments which measure correlation functions of the exponential of such fields, and these have a power-like behavior. Let us calculate this. By Eq. (18.95) we have

$$\begin{aligned} C(x) \equiv \langle e^{ia\phi(x)} e^{-ib\phi(0)} \rangle &= e^{-\frac{1}{2} \langle [a\phi(x) - b\phi(0)]^2 \rangle} = e^{-\frac{1}{2} \langle a^2 \phi^2(x) - 2ab\phi(x)\phi(0) + b^2 \phi^2(0) \rangle} \\ &= e^{-\frac{1}{2} (a-b)^2 G(0)} e^{ab[G(x) - G(0)]}. \end{aligned} \quad (18.96)$$

Since $G(0)$ is positively infinite, the prefactor vanishes unless $a = b$, in which case it is equal to unity, and we obtain

$$\langle e^{ia\phi(x)} e^{-ia\phi(0)} \rangle = e^{-\frac{a^2}{2}\langle [\phi(x)-\phi(0)]^2 \rangle} = e^{a^2[G(x)-G(0)]}. \quad (18.97)$$

The exponent contains the subtracted propagator (18.95):

$$G'(x) \equiv G(x) - G(0) \equiv \int \frac{d^2q}{(2\pi)^2} \frac{i}{q^2 - \mu^2} (e^{iqx} - 1) \approx -\frac{1}{2\pi} \log \frac{\Lambda \sqrt{-x^2}}{2e^{-\gamma}}. \quad (18.98)$$

In contrast to (18.95), this subtracted integral is infrared-finite, but ultraviolet-divergent. It contains therefore an ultraviolet cutoff Λ . The x -behavior (18.98) is correct for $|x| \gg 1/\Lambda$, which is again almost everywhere, due to the large size of Λ . After inserting (18.98) into the correlation function (18.96) with $a = b \neq 0$, we obtain the pure power falloff behavior with the distance

$$C(x) = \left(\frac{\Lambda \sqrt{-x^2}}{2e^{-\gamma}} \right)^{-a^2/2\pi}, \quad (18.99)$$

called *quasi-long-range behavior*. It is observed experimentally for many observables in two-dimensional systems as a result of the the quasi-long-range correlations functions (18.96), whenever a perfectly ordered state is forbidden by the Mermin-Wagner theorem [5].

In two dimensions, the system with the complex pair field Δ exhibits also a completely new phenomenon. There are macroscopic quantum fluctuations which produce quantum vortices and antivortices, in analogy to the vortex lines in three-dimensional superfluid helium and superconductors, discussed in Section 17.7. They attract each other by a logarithmic potential just like an electron gas with Coulomb interaction. At a temperature T_c , the long-range correlations of this Coulomb interaction are made short range by screening, caused by the dissociation of vortex pairs into free vortices. Thus there is a phase transition even though there can be no condensate [7].

18.5 Experimental Consequences

Given the effective potentials and the associated ground states and assuming that the $N \rightarrow \infty$ limit carries valid information also for finite N , we can study the radiative correction to field expectation values like

$$\langle \phi^2(x) \rangle \quad (18.100)$$

and the susceptibility

$$\begin{aligned} (2\pi)^D \delta^{(D)}(q+q') \chi^{-1}(q) &\equiv \langle T \phi_a(q) \phi_b(q') \rangle_c \\ &= - \left. \frac{\delta^2 \Gamma[\Phi]}{\delta \Phi_a(q) \delta \Phi_b(q')} \right|_{\Phi=\Phi_0} = (2\pi)^D \delta^{(D)}(q-q') (m^2 + \lambda - q^2) \delta_{ab}, \end{aligned} \quad (18.101)$$

where the subscript c indicates the connected Green function. In mean-field theory, the first quantity behaves like

$$\langle \phi^2(x) \rangle = 0, \quad \text{for } m^2 > 0, \quad (\tau > 0), \quad (18.102)$$

$$\langle \phi^2(x) \rangle = -\frac{Nm^2}{g} \sim -\frac{N\mu^2}{g}\tau, \quad \text{for } m^2 < 0, \quad (\tau < 0). \quad (18.103)$$

The inverse susceptibility is, for $T > T_c$,

$$\chi(q) = m^2 + \mathbf{q}^2 - q_0^2 = \mu^2\tau + \mathbf{q}^2 - q_0^2, \quad (18.104)$$

and for $T < T_c$:

$$\begin{aligned} \chi_{\parallel}(q) &= \mathbf{q}^2 - q_0^2, \\ \chi_{\perp}(q) &= -2m^2 + \mathbf{q}^2 - q_0^2 = -2\mu^2\tau + \mathbf{q}^2 - q_0^2. \end{aligned} \quad (18.105)$$

These behaviors can be modified considerably by the radiative corrections calculated in the last section. Consider first the cases of one and two-dimensions where there is no spontaneous symmetry breakdown. Here the susceptibility remains isotropic and finite for all temperatures. We calculate

$$\begin{aligned} \chi^{-1}(0) &= \lambda \\ \chi^{-1}(q) &= \lambda + \mathbf{q}^2 - q_0^2 \end{aligned} \quad (18.106)$$

and see that far above T_c , χ^{-1} approaches the mean field value since there $\lambda \sim m^2 \sim \mu^2 T_c$. Close to T_c , however, $\chi_{\perp}^{-1}(0)$ no longer goes to zero. It smoothly becomes flatter and tends to zero like

$$\begin{aligned} \chi_{\perp}^{-1}(0) &\sim \mu^2 e^{\tau\mu^2 4\pi/g} & D=2, \\ \chi_{\perp}^{-1}(0) &\sim \frac{g^2}{4\mu^4} \tau^{-1} & D=1. \end{aligned}$$

This rapid falloff may be seen as a washed-out remnant of the original anisotropic vanishing of $\chi_{\perp}^{-1}(0)$ due to the Nambu-Goldstone modes. Here it is due to large *isotropic* pretransitional fluctuations. The expectations of $\langle \phi^2(x) \rangle$ can be obtained as follows: Differentiate the generating functional $Z[j]$ with respect to the mass square in the functional picture. Then we see that

$$2i \frac{\partial}{\partial m^2} Z[j] = \int \mathcal{D}\phi \left(\int d^D x \phi^2 \right) e^{i\mathcal{A}[\phi] + i \int d^D x j(x) \phi(x)}. \quad (18.107)$$

But this is, up to the normalization factor $Z[j]$, the Green function in the presence of the external field j :

$$\int d^D x \langle T \phi(x) \phi(x) \rangle_j. \quad (18.108)$$

Explicitly, we obtain

$$\int d^D x \langle \phi^2(x) \rangle_j = Z^{-1}[j] 2i \frac{\partial}{\partial m^2} Z[j]. \quad (18.109)$$

From this, the desired quantity $\langle 0|\phi^2(x)|0\rangle \equiv \langle \phi^2(x) \rangle_{j=0}$ can be calculated as

$$\langle 0|\phi^2(x)|0\rangle = \frac{1}{VT} Z^{-1}[0] 2i \frac{\partial}{\partial m^2} Z[0]. \quad (18.110)$$

Using the effective action, this becomes

$$\langle 0|\phi^2(x)|0\rangle = -\frac{1}{VT} 2 \frac{\partial}{\partial m^2} \Gamma[\Phi], \quad (18.111)$$

or, expressed in terms of the effective potential:

$$\langle 0|\phi^2(x)|0\rangle = 2 \frac{\partial}{\partial m^2} v(\Phi). \quad (18.112)$$

Inserting the previous results in one and two dimensions we find

$$\langle 0|\phi^2(x)|0\rangle = \frac{1}{g}(\lambda - m^2). \quad (18.113)$$

For large m^2 , where $\lambda \rightarrow m^2$, this tends to zero, i.e., to the mean-field result. As m^2 goes to zero, however, the function remains smooth (and positive). When the temperature drops far below T_c ($m^2 \rightarrow -\infty$), then λ tends to zero and the behavior becomes again mean-field like.

We can summarize: In one- and two-dimensional systems, the expectation value $\langle \phi^2(x) \rangle$ interpolates smoothly between the mean-field limits above and below T_c . The susceptibility $\xi^{-1}(0)$ does the same interpolation, and remains isotropic for decreasing T .

Consider now the cases of $D = 3$ and $D = 4$ dimensions, for which the only ground states with real potential $v(\Phi, \lambda)$ were found at $\lambda = 0$ and $\Phi_{0a} \neq 0$. In order to calculate the susceptibilities at zero energy-momentum q , we write v in the form

$$v(\Phi, \lambda) = \frac{1}{2} \lambda \Phi_a^2 - \gamma_D(\lambda), \quad (18.114)$$

where in 3 dimensions

$$-2\gamma_3(\lambda) = -\frac{N}{2g} \lambda^2 + \frac{Nm^2}{g} \lambda + N \frac{\pi}{3} \mathcal{S}_3 \lambda^{3/2}, \quad (18.115)$$

and in 4 dimensions

$$-2\gamma_4(\lambda) = -\frac{N}{2g} \lambda^2 + \frac{Nm^2}{g} \lambda + \frac{N}{4} \mathcal{S}_4 \lambda^2 \left(\log \frac{\lambda}{\mu^2} - \frac{1}{2} \right). \quad (18.116)$$

Let us now form the derivatives

$$v_{\Phi_a} = \lambda \Phi_a + \left[\frac{1}{2} \Phi_a^2 - \gamma'_D(\lambda) \right] \lambda_{\Phi_a}, \quad (18.117)$$

$$v_{\Phi_a \Phi_b} = \lambda \delta_{ab} + \{ [\Phi_a \lambda_{\Phi_b} + (a \leftrightarrow b)] - \gamma''(\lambda) \lambda_{\Phi_a} \lambda_{\Phi_b} \} + \left[\frac{1}{2} \Phi_a^2 - \gamma(\lambda) \right] \lambda_{\Phi_a \Phi_b}. \quad (18.118)$$

We use the equation of state $\Phi^2 = 2\gamma'(\lambda)$ and its derivative $\Phi_a = \gamma''(\lambda) \lambda_{\Phi_a}$ to simplify (18.117), and write it as

$$v_{\Phi_a \Phi_b} = \lambda \delta_{ab} + \frac{\Phi_a \Phi_b}{\gamma''(\lambda)} = \lambda \left(\delta_{ab} - \frac{\Phi_a \Phi_b}{\Phi_c^2} \right) + \frac{\Phi_a \Phi_b}{\Phi_c^2} \left[\lambda + \frac{1}{\gamma''(\lambda)} \right] \Phi_c^2. \quad (18.119)$$

Thus we can identify the transverse inverse correlation length of the susceptibility as

$$\xi_{\perp}^{-1}(0) = \lambda, \quad (18.120)$$

and the longitudinal one as

$$\xi_{\parallel}^{-1}(0) = \left[\lambda + \frac{1}{1/\gamma''(\lambda)} \right] \Phi_c^2 = 2 \left[\lambda + \frac{1}{\gamma''(\lambda)} \right] \gamma'(\lambda). \quad (18.121)$$

Actually, we could have obtained the result (18.118) from our earlier equations (18.47) where the full inverse Green function was derived. Inserting there

$$m_0^2 + \Sigma = \lambda, \quad \gamma(\Sigma) \rightarrow \gamma(\lambda), \quad (18.122)$$

we immediately verify (18.119).

For spontaneously broken symmetry, λ vanishes and we find

$$\xi_{\perp}^{-1}(0) = 0 \quad (18.123)$$

just as in mean-field theory, since this is a rigorous consequence of the Nambu-Goldstone theorem. For the longitudinal component we obtain

$$\chi_{\parallel}^{-1}(0) = 2\gamma'(0)/\gamma''(0). \quad (18.124)$$

Inserting (18.115) we have in 3 and 4 dimensions

$$\chi_{\parallel}^{-1}(0) = 0. \quad (18.125)$$

Thus, contrary to the mean field case where $\xi_{\parallel}^{-1}(0) = -2m^2 > 0$, the longitudinal susceptibility diverges. In particle physics this is a direct consequence of the *Nambu-Goldstone theorem*. A zero-mass excitation implies an infinite correlation length. In many-body physics, this divergence has also been formulated as a theorem, attributed to *Hugenholtz and Pines* [8].

18.6 Correlation Functions for Large N

We have argued in Chapter 13 that the set of all vertex functions can be obtained from a finite number of tree diagrams which follow from the effective action $\Gamma[\Phi_0 + \Phi', \Sigma_0 + \Sigma']$ considered as a functional of Φ', Σ' [see the equations after (6.194)]. Let us therefore set

$$\lambda_0 = m_0^2 + \Sigma_0, \quad (18.126)$$

and inserting into the effective action (18.61) the field decomposition $\Sigma = \Sigma_0 + \Sigma'$ to expand

$$\begin{aligned} \Gamma[\Phi, \Sigma_0 + \Sigma'] &= \frac{1}{2}(\partial\Phi)^2 - \frac{1}{2}\lambda_0\Phi^2 - \frac{1}{2}\Sigma'\Phi^2 + \frac{i}{2}N\text{Tr} \log(-\partial^2 - \lambda_0 - \Sigma') \\ &+ \frac{N}{4g_0} \int d^D x \Sigma'^2 + \frac{N}{2g_0} (\lambda_0 - m_0^2) \int d^D x \Sigma' + \frac{N}{4g_0} (\lambda_0 - m_0^2)^2. \end{aligned} \quad (18.127)$$

The value of Σ_0 is determined by solving

$$\Gamma_{\Sigma'}[\Phi_{0a}, \Sigma_0] = 0. \quad (18.128)$$

This eliminates all graphs with a Σ' line ending in the vacuum (tadpole graphs). The same rules hold for $m^2 < 0$ in one and two dimensions, where there is no spontaneous symmetry breakdown.

Consider now the non-trivial cases of $m^2 < 0$ in three and four dimensions. Again we can remove the Σ' tadpoles by going to the extremum. Contrary to (18.128), this lies now at

$$\Sigma_0 = \lambda_0 = 0, \quad (18.129)$$

with a non-zero value of Φ given by

$$\Phi_a^2 = \gamma'(0) = -\frac{N}{g_0}m_0^2. \quad (18.130)$$

Thus we may write the effective action as

$$\begin{aligned} \Gamma[\Phi, \Sigma_0 + \Sigma'] &= \frac{1}{2}(\partial\Phi_a)^2 - \frac{1}{2}\Sigma'[\Phi_a^2 - (\Phi_{0a})^2] \\ &+ \frac{1}{2}\Sigma'\Gamma^{(2)}\Sigma' - i\frac{N}{2}\text{Tr} \sum_{n=3}^{\infty} \left(-\frac{i}{-\partial^2}\Sigma'\right)^n \frac{1}{n} + \frac{N}{4g}m_0^4. \end{aligned} \quad (18.131)$$

This action is free of linear terms in Σ' if, instead of the fields Φ_a , one uses the shifted fields $\Phi'_a = \Phi_a - \Phi_{0a}$. The components of Φ_a parallel to Φ_{0a} will be denoted by $\Phi_{\parallel}$. In order to find the eigenmodes we have to diagonalize the fluctuation matrix, which reads for euclidean momenta:

$$\begin{pmatrix} q^2 & \Phi_0 \\ \Phi_0 & \Gamma^{(2)}(q) \end{pmatrix}, \quad (18.132)$$

where $\Phi_0 \equiv \sqrt{\Phi_{0a}^2}$. Let us write down $\Gamma^{(2)}(q)$ explicitly as

$$\Gamma^{(2)}(q) = -\frac{1}{2}N \left[\frac{1}{g} + I(q) \right], \quad (18.133)$$

with

$$I(q) = \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2(k+q)^2}. \quad (18.134)$$

In D dimensions, this was calculated in (5.135):

$$I(q) = S_D \frac{1}{2} \Gamma(2 - \epsilon/2) \Gamma(\epsilon/2) \mu^{-\epsilon} \int_0^1 d^D x \frac{\mu^\epsilon}{[q^2 x(1-x)]^{\epsilon/2}}. \quad (18.135)$$

Consider the case of $D = 3$ dimensions. Then $S_3 = 1/2\pi^2$, and the integral is finite

$$I(q) = \frac{1}{8\pi} \frac{\mu}{(q^2)^{1/2}} \int_0^1 d^D x [x(1-x)]^{-1/2} = \frac{1}{8\sqrt{q^2}}. \quad (18.136)$$

Using this we find for the diagonalized modes

$$G_{\Phi'_\parallel \Phi'_\parallel} = \frac{q + g/8}{q(q^2 + qg/8 - 2m^2)}, \quad (18.137)$$

$$G_{\Sigma' \Sigma'} = \frac{gq^2}{N(m^2 - qg/16 - q^2/2)}. \quad (18.138)$$

In the limit $g \rightarrow 0$, the first mode corresponds to the mean-field particle of mass $-2m^2$, whereas the second mode disappears.

We are now in a position to understand the divergence of the longitudinal susceptibility for $q^2 \rightarrow 0$. From (18.137) we see that the propagator has a square-root singularity in q^2 at this point. This does not correspond to another zero-mass particle. It is generated by the possibility of the $\Phi_\parallel$ particle to decay into two massless Nambu-Goldstone bosons if fluctuations are taken into account. As a matter of fact, the diagonal $\Phi_\parallel$ -mode does really correspond to a proper particle: If we return from euclidean to physical values of q , the mean field pole at $q^2 = -2m^2$ is no longer visible but hides in the second sheet of a complex q^2 -plane. This is cut from $q^2 = 0$ to $q^2 = \infty$. The physical region lies right above the cut, in accordance with the usual $-i\epsilon$ prescription for singularities (recall that according to the $-i\epsilon$ prescription, the cut has to be displaced slightly down by an imaginary amount $i\epsilon$). The pole can only be reached by passing the cut from above into the second sheet at

$$\sqrt{-q^2} = -\frac{g}{16} - \sqrt{2m^2 + \left(\frac{g}{16}\right)^2}, \quad (18.139)$$

i.e.,

$$q^2 = -2m^2 - 2\left(\frac{g}{16}\right)^2 - i\frac{g}{8}\sqrt{-2m^2 - \left(\frac{g}{16}\right)^2}.$$

There is another pole at the complex conjugate position above the axis, but this is far away from the physical region above the cut: It can only be reached by circulating anticlockwise around the branch point and going into the second sheet from below.

Let us now look at the four-dimensional situation. Here $I(q)$ becomes with $S_4 = 1/8\pi^2$ [see (11.176) and (22.49)]

$$I(q) = \frac{1}{8\pi^2} \left(\frac{1}{\epsilon} + \frac{1}{2} - \frac{1}{2} + \log \frac{q^2}{\mu^2} \right). \quad (18.140)$$

The $1/\epsilon$ -singularity is absorbed in a renormalization of $1/g_0$ as in (18.71), and we have

$$\Gamma^{(2)}(q) = -\frac{N}{2} \left[\frac{1}{g} + \frac{1}{16\pi^2} \left(1 - \log \frac{q^2}{\mu^2} \right) \right], \quad (18.141)$$

such that the diagonalized propagators become

$$G_{\Phi'_{\parallel}\Phi'_{\parallel}} = \frac{1}{2} \frac{1/g + (1 - \log q^2/\mu^2)/16\pi^2}{-m^2/g + (q^2/2)[1/g + (1 - q^2/\mu^2)/16\pi^2]}, \quad (18.142)$$

$$G_{\Sigma'\Sigma'} = -\frac{1}{N} \frac{q^2}{-m^2/g + (q^2/2)[1/g + (1 - q^2/\mu^2)/16\pi^2]}. \quad (18.143)$$

Again we observe the cut in the q^2 -plane, starting at $q^2 = 0$, which is now logarithmic rather than of the square-root type. Note that there exists a conjugate pair of poles, one near $+2m^2$ but hidden in the second sheet.

18.7 No-Tachyon Theorem

There is, however, an important difference with respect to the previous case. There is also another pole in both propagators which does not correspond to a physical particle since it lies at a large positive value of euclidean q^2 . In Minkowski spacetime, this corresponds to a particle moving with a velocity faster than light, a so-called *tachyon*. The appearance of such a pole in a correlation function indicates that the solution to the model is unphysical. The problem is resolved in nature by the system undergoing a phase transition to a state of lower energy, usually a state with another vacuum expectation value of the fields. This is the typical way how nature deals with unstable physical systems: A timber-framed house that has some eigenfrequencies with a negative square value will be unstable. Upon a small vibration, such a structure collapses. This goes on until it becomes a stable ruin. In the ruin, all frequencies have positive square values.

Notes and References

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*Any intelligent fool can make things bigger, more complex, and more violent.
It takes a touch of genius—and a lot of courage—to move in the opposite direction.*
E. F. SCHUMACHER (1911–1977)

19

Nonlinear σ -Model

Another field theoretic model that is exactly solvable in a limit $N \rightarrow \infty$ and illustrates some typical properties of such theories is the so-called *nonlinear σ -model*. It has its origin in statistical mechanics where it arises as a limit of the classical Heisenberg spin model of ferromagnetism. There it is known under the name of *spherical model*. The nonlinear σ -model yields a complementary approach to the critical phenomena described previously by the $O(N)$ -symmetric ϕ^4 -theory.

19.1 Definition of Classical Heisenberg Model

The model consists of a fluctuating field $n_a(\mathbf{x})$ of unit vectors with N components

$$n_a(\mathbf{x}) \quad (a = 1, \dots, N), \quad n_a^2(\mathbf{x}) = 1. \quad (19.1)$$

We shall discuss here the euclidean formulation in which the model is described by a partition function

$$Z = \prod_{\mathbf{x}} \left[\int \frac{d^{N-1}n_a(\mathbf{x})}{S_N} \right] \exp \left[-\frac{1}{2g} \int d^D x [\nabla n_a(\mathbf{x})]^2 \right]. \quad (19.2)$$

The constant S_N is the surface of a sphere in N dimensions covered by the directional integral $d^D n^a$. This ensures a unit integral $\int d^{N-1}n^a/S_N = 1$. Explicitly, $S_N = 2\pi^{N/2}/\Gamma(N/2)$ [recall (11.126)]. This model can be thought of as arising from the euclidean action of a previous $O(N)$ -symmetric ϕ^4 -theory in Chapter 18, where

$$\mathcal{A} = \int d^D x \left[\frac{1}{2} (\nabla \phi_a)^2 + \frac{m^2}{2} \phi_a^2 + \frac{g}{4} (\phi_a^2)^2 \right] \quad (19.3)$$

by going to the limit of very large negative m^2 . For negative m^2 , the $O(N)$ -symmetry is spontaneously broken, and the initially degenerate N field fluctuations decompose into a massive fluctuation of the field size $\phi \equiv \sqrt{\phi_a^2}$, the so-called *radial fluctuations*, and $N - 1$ fluctuation modes around the direction of the field ϕ_a , the so-called *azimuthal fluctuations*, described by the unit vectors

$$n_a \equiv \phi_a / \sqrt{\phi_a^2}. \quad (19.4)$$

These are the *Goldstone bosons* which arise whenever there is a spontaneous breakdown of a continuous symmetry (see Section 16.2). In the limit of $m^2 \rightarrow \infty$, the size fluctuations are completely frozen out. The action can be written approximately as

$$\mathcal{A} \xrightarrow{m^2 \rightarrow -\infty} \int d^D x \left[-\frac{(-m^2)^2}{4g} + \frac{1}{2} |\phi|^2 (\nabla n_a)^2 \right]. \quad (19.5)$$

Dropping the first term with the constant condensation energy, we arrive at the $O(N)$ nonlinear σ -model (19.3) with a coupling constant

$$g = \frac{1}{|\phi|^2}. \quad (19.6)$$

Readers familiar with models of statistical mechanics will recognize the intimate relation of the model (19.2) with the so-called classical $O(N)$ -symmetric *Heisenberg model of ferromagnetism*. It is defined on a lattice, where its energy is written as a sum over nearest-neighbor interactions between local D -dimensional spin vectors $\mathbf{S}_i$, which are conventionally normalized to unit length:

$$E = -\frac{J}{2} \sum_{\{i,j\}} \mathbf{S}_i \cdot \mathbf{S}_j \quad \text{with } J > 0 \quad \text{and} \quad \mathbf{S}_i^2 = 1. \quad (19.7)$$

The symbol $\{i, j\}$ denotes neighboring index pairs. If the spin vectors $\mathbf{S}_i$ are not of unit length, the length fluctuates and $\mathbf{S}_i$ represents an order field. The expectation value $\mathbf{M} \equiv \langle \mathbf{S}_i \rangle$ is often called magnetization. If $\mathbf{M}$ is nonzero, the system is said to exhibit a spontaneous magnetization. This happens only at low temperatures. Above a critical temperature T_c^{MF} , such a system becomes usually demagnetized with $\mathbf{M} = 0$. This is referred to as the *normal state*. Then T_c^{MF} is called the *Curie temperature*.

A special case of this model is the famous *Ising model* where the direction of the vector $\mathbf{S}_i$ is restricted to a single axis, pointing parallel or antiparallel to it. The phase transition of magnetic systems with strong anisotropy can be described by this model. Then $\mathbf{S}_i$ can be replaced by a scalar field with positive and negative signs, and the symmetry which is spontaneously broken in the low-temperature phase is the reflection symmetry $S(\mathbf{x}) \rightarrow -S(\mathbf{x})$.

Let us denote the lattice points by a vector $\mathbf{x}$ on a simple cubic lattice, i.e., we let $\mathbf{x}$ take the values

$$\mathbf{x}_{(m_1, m_1, \dots, m_d)} \equiv \sum_{i=1}^D m_i \mathbf{i}, \quad (19.8)$$

where $\mathbf{i}$ are the basis vectors of a D -dimensional hypercubic lattice, and m_i are integer numbers $0, \pm 1, \pm 2, \dots$.

The partition function associated with the generalized Heisenberg model is

$$Z = \sum_{\substack{\text{spin} \\ \text{configurations}}} e^{-E/k_B T}, \quad (19.9)$$

where the sum runs over all possible spin configurations. The unit spin vectors $\mathbf{S}_i$ are now identified with the unit vector fields $\mathbf{n}(\mathbf{x})$ in (19.1). The sum over products $\sum_{\{i,j\}} \mathbf{n}_i \mathbf{n}_j$ in the energy (19.7) can then be rewritten as

$$\begin{aligned} \sum_{\{i,j\}} \mathbf{n}_i \mathbf{n}_j &= \sum_{\{i,j\}} [\mathbf{n}_i(\mathbf{n}_j - \mathbf{n}_i) + 1] = 2 \sum_{\mathbf{x}} \sum_{\mathbf{i}} \{\mathbf{n}(\mathbf{x})[\mathbf{n}(\mathbf{x} + \mathbf{i}) - \mathbf{n}(\mathbf{x})] + 1\} \\ &= - \sum_{\mathbf{x}} \left\{ \sum_{\mathbf{i}} [\mathbf{n}(\mathbf{x} + \mathbf{i}) - \mathbf{n}(\mathbf{x})]^2 - 2D \right\}. \end{aligned} \quad (19.10)$$

Now we introduce *lattice gradients*:

$$\nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x}) \equiv \frac{1}{a} [\mathbf{n}(\mathbf{x} + \mathbf{i}) - \mathbf{n}(\mathbf{x})], \quad (19.11)$$

$$\bar{\nabla}_{\mathbf{i}} \mathbf{n}(\mathbf{x}) \equiv \frac{1}{a} [\mathbf{n}(\mathbf{x}) - \mathbf{n}(\mathbf{x} - \mathbf{i})], \quad (19.12)$$

where a is the lattice spacing, and we can rewrite (19.10) as

$$\sum_{\{i,j\}} \mathbf{n}_i \mathbf{n}_j = - \sum_{\mathbf{x}} \left\{ a^2 \sum_{\mathbf{i}} [\nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x})]^2 - 2D \right\}. \quad (19.13)$$

With this, the partition function (19.9) takes the form

$$Z = \prod_{\mathbf{x}} \left[\int \mathbf{n}(\mathbf{x}) \right] \exp \left[-\frac{J}{2k_B T} \sum_{\mathbf{x}} \left(\sum_{\mathbf{i}} a^2 [\nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x})]^2 - 2D \right) \right]. \quad (19.14)$$

Here We can use the lattice version of partial integration¹

$$\sum_{\mathbf{x}} \sum_{\mathbf{i}} [\nabla_{\mathbf{i}} f(\mathbf{x})] g(\mathbf{x}) = - \sum_{\mathbf{x}} \sum_{\mathbf{i}} f(\mathbf{x}) \bar{\nabla}_{\mathbf{i}} g(\mathbf{x}), \quad (19.15)$$

which is valid for all lattice functions with periodic boundary conditions, to express (19.13) in terms of a lattice version of the Laplace operator $\bar{\nabla}_{\mathbf{i}} \nabla_{\mathbf{i}}$, where repeated lattice unit vectors are summed. Then

$$\sum_{\mathbf{x}} \left\{ \sum_{\mathbf{i}} a^2 [\nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x})]^2 - 2D \right\} = - \sum_{\mathbf{x}} \left[a^2 \mathbf{n}(\mathbf{x}) \bar{\nabla}_{\mathbf{i}} \nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x}) + 2D \right]. \quad (19.16)$$

Ignoring the irrelevant constant term $\sum_{\mathbf{x}} 2D$, we can then write the sum over all spin configurations in the partition function (19.9) as a product of integrals over a unit sphere at each lattice point

$$Z = \prod_{\mathbf{x}} \left[\int \mathbf{n}(\mathbf{x}) \right] \exp \left\{ \frac{Ja^2}{2k_B T} \sum_{\mathbf{x}} \mathbf{n}(\mathbf{x}) \bar{\nabla}_{\mathbf{i}} \nabla_{\mathbf{i}} \mathbf{n}(\mathbf{x}) \right\}. \quad (19.17)$$

¹For the handling of lattice gradients see Section 2.2 in the textbook H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, World Scientific Publishing, Singapore 1995.

For small a , the sum in (19.16) has a continuum limit

$$a^{2-D} \int d^D x \left\{ [\nabla n_a(\mathbf{x})]^2 - \frac{2D}{a^2} \right\} = -a^{2-D} \int d^D x \left\{ n_a(\mathbf{x}) \nabla^2 n_a(\mathbf{x}) + \frac{2D}{a^2} \right\}. \quad (19.18)$$

After dropping the irrelevant D/a^2 term, the Boltzmann factor in the partition function (19.17) agrees with the exponential in the partition function (19.2) of the nonlinear σ -model with a coupling constant

$$g = \frac{k_B T}{J} a^{D-2}. \quad (19.19)$$

In these models, g grows with temperature, and due to the significance of the model for statistical mechanics, we find it convenient to replace the prefactor $1/g$ in (19.2) by a reduced inverse temperature $1/T$, thus discussing the model as a function of a reduced temperature rather than of the coupling strength. As we see from (19.19), the so-defined reduced temperature corresponds to the true one if that is measured in units of J/a^{D-2} .

As mentioned in the beginning of this chapter, the limit $N \rightarrow \infty$ of this model is referred to as the *spherical model*.

19.2 Spherical Model

The $N \rightarrow \infty$ -limit of the Heisenberg model was first solved by Berlin and Kac in 1952.² The solution of the model is quite simple. We liberate n_a from its constraint $n_a^2 = 1$, allowing each component to fluctuate between $-\infty$ and ∞ . The constraint is enforced by an extra functional integral over a Lagrange multiplier $\lambda(\mathbf{x})$. Thus we write the lattice partition function as

$$Z = \prod_{\mathbf{x}} \left[\int_{-i\infty}^{i\infty} \frac{d\lambda(\mathbf{x})}{4\pi iT} \int_{-\infty}^{\infty} \frac{d^N n_a(\mathbf{x})}{S_N} \right] \exp \left\{ -\frac{1}{2g} \int d^D x [(\nabla n_a)^2 + \lambda(n_a^2 - 1)] \right\}. \quad (19.20)$$

In this form, the integrals over the components n_a are Gaussian, so that they can be performed, leaving only a functional integral over $\lambda(\mathbf{x})$:

$$Z = \prod_{\mathbf{x}} \left[\int_{-i\infty}^{i\infty} \frac{d\lambda(\mathbf{x})}{4\pi iT} \right] \exp \left[-\frac{N}{2} \text{Tr} \log [-\nabla^2 + \lambda(\mathbf{x})] + \frac{1}{2T} \int d^D x \lambda(\mathbf{x}) \right]. \quad (19.21)$$

In the limit $N \rightarrow \infty$, this is the partition function of the spherical model. In this limit, the first term in the exponent grows so large that the λ fluctuations become frozen at the extremum of the action. The limit is non-trivial if we allow g^{-1} to carry a factor N . Thus we set

$$g \equiv t/N. \quad (19.22)$$

²T.H. Berlin and M. Kac, Phys. Rev. 86, 82 (1952).

Now we can go to large N , and find the partition function

$$Z \xrightarrow[N \rightarrow \infty]{} e^{-F/t}, \quad (19.23)$$

with a free energy per $O(N)$ -degree of freedom and per temperature unit equal to

$$\frac{F}{t} \xrightarrow[N \rightarrow \infty]{} \frac{1}{2} \left[\text{Tr} \log [-\nabla^2 + \lambda(\mathbf{x})] - \frac{1}{t} \int d^D x \lambda(\mathbf{x}) \right], \quad (19.24)$$

to be evaluated at the extremum where the functional derivative $\delta F / \delta \lambda(\mathbf{x})$ vanishes. Explicitly, this condition reads

$$\frac{1}{t} = [-\nabla^2 + \lambda(\mathbf{x})]^{-1}(\mathbf{x}, \mathbf{x}). \quad (19.25)$$

Each solution $\lambda_i(\mathbf{x})$ of this equation must be found, and the partition function is given by the sum over the Boltzmann factors (19.23) for all of them. In general, these solutions are hard to find. One solution, however, is straightforward: that with a constant $\lambda(\mathbf{x}) \equiv \lambda$, for which the free energy (19.24) yields

$$\frac{F}{tL^D} \xrightarrow[N \rightarrow \infty]{} \frac{1}{2} \left[\int \frac{d^D p}{(2\pi)^D} \log(\mathbf{p}^2 + \lambda) - \frac{1}{t} \int d^D x \lambda \right], \quad (19.26)$$

where L^D is the spatial volume of the system. The extremality condition (19.25) turns into the so-called *gap equation*:

$$\frac{1}{t} = \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + \lambda}. \quad (19.27)$$

Its solution will now be discussed.

19.3 Free Energy and Gap Equation in $D > 2$ Dimensions

Using formulas (11.134) and (11.137), the integrals in (19.26) and (19.27) can be done right-away in D dimensions with the result

$$\frac{F}{tL^D} \xrightarrow[N \rightarrow \infty]{} \frac{1}{2} S_D \frac{1}{D} \Gamma\left(\frac{D}{2}\right) \Gamma\left(1 - \frac{D}{2}\right) \lambda^{D/2} - \frac{\lambda}{2t} \quad (19.28)$$

for the free energy and

$$\frac{1}{t} = S_D \frac{1}{2} \Gamma\left(\frac{D}{2}\right) \Gamma\left(1 - \frac{D}{2}\right) \lambda^{D/2-1} \quad (19.29)$$

for the gap equation, where $S_D = S_D / (2\pi)^D = 2 / (4\pi)^{D/2} \Gamma(D/2)$ from Eq. (11.129). It is easy to check that the free energy (19.28) is extremal for λ satisfying (19.29).

In order to discuss the physical consequences of these equations, consider first the case of two dimensions. Letting $\epsilon \equiv D - 2$ approach zero, the equations become

$$\frac{F}{tL^D} \xrightarrow{N \rightarrow \infty} -\frac{1}{2}S_D \frac{1}{\epsilon} \frac{1}{1 + \epsilon/2} \lambda^{1+\epsilon/2} - \frac{\lambda}{2t} + \mathcal{O}(\epsilon), \quad (19.30)$$

$$\frac{1}{t} = -S_D \frac{1}{\epsilon} \lambda^{\epsilon/2} + \mathcal{O}(\epsilon). \quad (19.31)$$

Note that we use ϵ for the deviations from $D = 2$ dimensions, in contrast to ε for the deviations from $D = 4$.

The gap equation (19.31) has a solution only for *negative* t . To avoid the infinities in the limit $\epsilon \rightarrow 0$, we introduce an arbitrary mass scale μ and a renormalized temperature t_R via the defining equation for t_R :

$$\frac{1}{t} \equiv \frac{\mu^\epsilon}{t_R} - S_D \frac{1}{\epsilon} \mu^\epsilon. \quad (19.32)$$

Then we can take the limit $\epsilon \rightarrow 0$ and find

$$\frac{F}{tL^D} \xrightarrow{N \rightarrow \infty} -S_D \frac{1}{4} \lambda \left(\log \frac{\lambda}{\mu^2} - 1 \right) - \frac{\lambda}{2t_R} \quad (19.33)$$

$$\frac{1}{t_R} = -S_D \frac{1}{2} \log \frac{\lambda}{\mu^2}. \quad (19.34)$$

The renormalized gap equation is solved for $\lambda = \bar{\lambda}$ satisfying the equation

$$\frac{\bar{\lambda}}{\mu^2} = e^{-2/t_R S_D}. \quad (19.35)$$

For this value, the free energy has a maximum. It corresponds to a minimum in the λ -integrals in (19.21) which runs along the imaginary direction. Only the immediate neighborhood of this minimum contributes to the integral (see Fig. 19.1).

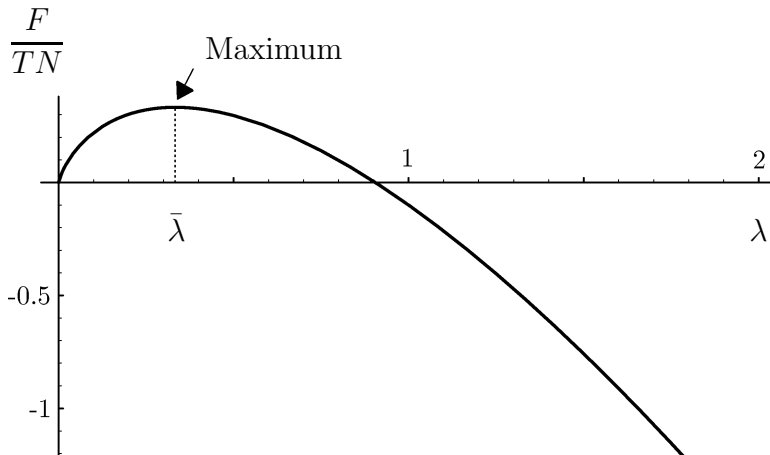


FIGURE 19.1 Free energy as a function of λ for $D = 2$ (schematically). The gap equation (19.35) determines the value $\bar{\lambda}$ of the maximum.

The value of λ at the minimum is a parameter characterizing the solution, having the dimension of a square-mass. From the role played by λ in Eq. (19.20) and in the trace of the logarithm of the fluctuations (19.24) we see that λ is the square-mass of the n_a -fluctuations. This implies that even though we had started out with a model describing $N - 1$ massless Goldstone bosons, the interacting system is no longer massless, but all N fields have acquired a nonzero mass $M = \sqrt{\lambda}$. What we witness here is the *spontaneous restoration* of the $O(N)$ -symmetry due to the violence of the directional fluctuations in two dimensions.

It is instructive to consider also the case of more than two dimensions and treat it in a way which has a smooth limit for $\epsilon \equiv D - 2 \rightarrow 0$. If ϵ is arbitrary, the free energy in $D \equiv 2 + \epsilon$ dimensions becomes

$$\frac{F(\lambda)}{tL^D} = -\frac{c_\epsilon}{2} \frac{\lambda^{1+\epsilon/2}}{1+\epsilon/2} - \frac{\lambda}{2t}, \quad (19.36)$$

where

$$c_\epsilon \equiv -\frac{S_D}{2} \Gamma\left(\frac{D}{2}\right) \Gamma\left(1 - \frac{D}{2}\right) = \frac{1}{\epsilon} S_D \frac{\pi\epsilon/2}{\sin(\pi\epsilon/2)}. \quad (19.37)$$

For small ϵ this behaves like

$$c_\epsilon \approx \frac{1}{2\pi\epsilon} + \mathcal{O}(\epsilon). \quad (19.38)$$

In order to have a smooth limit $\epsilon \rightarrow 0$ of the free energy, we write

$$\frac{F(\lambda)}{tL^D} = \left\{ -\frac{1}{2} \frac{c_\epsilon}{1+\epsilon/2} \left[\left(\frac{\lambda}{\mu^2} \right)^{\epsilon/2} - \left(1 + \frac{\epsilon}{2} \right) \right] \lambda - \frac{\lambda}{2t_R} \right\} \mu^\epsilon, \quad (19.39)$$

where t_R is the renormalized temperature defined by

$$\frac{1}{t} \equiv \frac{\mu^\epsilon}{t_R} - c_\epsilon \mu^\epsilon. \quad (19.40)$$

19.3.1 High-Temperature Phase

At high temperatures, where t_R is large, the free energy (19.36) has a maximum. Its position $\lambda = \bar{\lambda}$ of the maximum is determined by the unrenormalized gap equation as

$$\frac{1}{t} = -c_\epsilon \bar{\lambda}^{\epsilon/2}. \quad (19.41)$$

For $2 > \epsilon > 0$, i.e., between two and four dimensions, there is a solution for the bare parameter $t < 0$. Equation (19.40) implies that the renormalized temperature is, in this regime, larger than a certain critical value t_R^c given by

$$t_R^c = c_\epsilon^{-1} > 0. \quad (19.42)$$

In terms of t_R , Eq. (19.40) reads

$$\frac{1}{t} = \mu^\epsilon \left(\frac{1}{t_R} - \frac{1}{t_R^c} \right), \quad (19.43)$$

and Eq. (19.43) gives the gap $\bar{\lambda}$ as a function of $t_R > t_R^c$:

$$\bar{\lambda} = \mu^2 \left(1 - \frac{t_R^c}{t_R} \right)^{2/\epsilon}. \quad (19.44)$$

For $t_R < t_R^c$, the maximum lies at $\lambda = \bar{\lambda} = 0$. For $t_R > t_R^c$, it becomes positive (see Fig. 19.2).

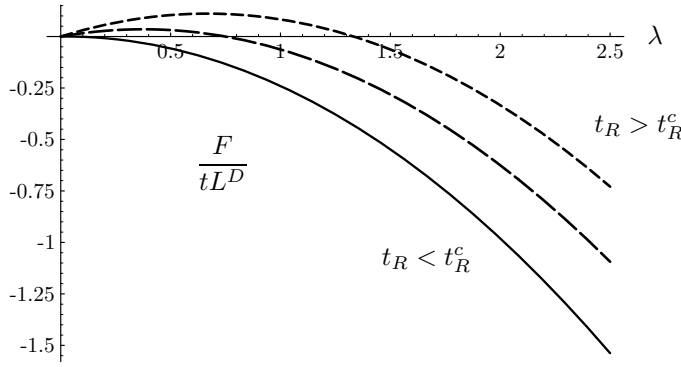


FIGURE 19.2]

Free energy as a function of λ for $D = 2$ (schematically). The value $\bar{\lambda}$ of the maximum is determined by the gap equation (19.44).

Note that in order to make the functional integral of the theory (19.20) well-defined for $t_R > t_R^c$ where $t < 0$, the n^a -integrations have to be taken along the imaginary field axis. We shall see later in Section 19.5 that this apparently unphysical condition is an artifact of the analytic continuation in the dimension D .

19.3.2 Low-Temperature Phase

In the low-temperature regime

$$t_R < t_R^c, \quad (19.45)$$

where the unrenormalized temperature is positive, the gap equation (19.41) has no solution. The reason for this is an incorrect treatment of the fluctuations at zero momentum. In order to see what went wrong in the above calculations we may proceed in two ways. One is inspired by the treatment in Subsection 2.15.3 of the ideal Bose gas at a fixed particle number N . There we observed that the equation for the particle number containing a momentum integral over the Bose distribution could be performed only down to a certain temperature, where the chemical potential

first hits zero (from the negative side). For lower temperatures, the state of zero momentum accumulates a macroscopic number of states, the so-called *condensate*. To account for its presence, it was essential to treat the system in a finite volume, where the momenta have to be summed up rather than being integrated over. Then, the zero-momentum state can be isolated and treated separately. This is a typical solution of an infrared problem of a field system. Let us do the same thing here.

If the system is enclosed in a box of volume L^D , we calculate the free energy (19.24) as

$$\frac{F}{tL^D} = \frac{1}{2L^D} \log \lambda + \frac{1}{2L^D} \sum_{\mathbf{k} \neq 0} \log (\mathbf{k}^2 + \lambda) - \frac{\lambda}{2t}. \quad (19.46)$$

The first term is responsible for generating a local maximum at a real $\lambda = \bar{\lambda}$ which is a minimum for the fluctuations in $\delta\lambda \equiv \lambda - \bar{\lambda}$ along the imaginary λ -axis. The maximum's value $\bar{\lambda}$ is determined by the gap equation

$$\frac{1}{L^D} \frac{1}{\bar{\lambda}} + \frac{1}{L^D} \sum_{\mathbf{k} \neq 0} \frac{1}{\mathbf{k}^2 + \bar{\lambda}} = \frac{1}{t}. \quad (19.47)$$

If the system has more than two dimensions, the sum over $1/(\mathbf{k}^2 + \lambda)$ with $\mathbf{k} \neq 0$ can be replaced by a phase-space integral $\int d^D k L^D / (2\pi)^D (\mathbf{k}^2 + \lambda)$. The relative error is only of order $1/\lambda L^2$, which can be calculated exactly using a D -dimensional version of the *Euler-Maclaurin approximation* to the sum in Eq. (7.693). Thus the gap equation (19.41) reads, more precisely,

$$\frac{1}{t} = \frac{1}{L^D \bar{\lambda}} - c_\epsilon \bar{\lambda}^{\epsilon/2}. \quad (19.48)$$

For $t < 0$, and a large volume L^D , this equation has the same solution $\bar{\lambda}$ as before in (19.41), since the first term $1/L^D \bar{\lambda}$ on the right-hand side can be ignored. For $t > 0$, however, this term makes an essential difference. It gives rise to a nonzero solution $\bar{\lambda}$, which is very small for a large volume L^D . In this regime, the second term in (19.48) can be neglected with respect to the first term, so that for positive t :

$$\bar{\lambda} \approx \frac{t}{L^D}. \quad (19.49)$$

The general solution for both finite and infinite volumes L^D is illustrated in Fig. 19.3. In the limit of infinite volume, the solution is

$$\begin{aligned} \bar{\lambda} &= 0, & t &\geq 0, \\ \bar{\lambda} &> 0, & t < 0. \end{aligned} \quad (19.50)$$

There is a phase transition at $t = 0$. For $t > 0$, all modes become massive and the $O(N)$ -symmetry is restored. For $t < 0$, the original $N - 1$ massless Goldstone modes survive.

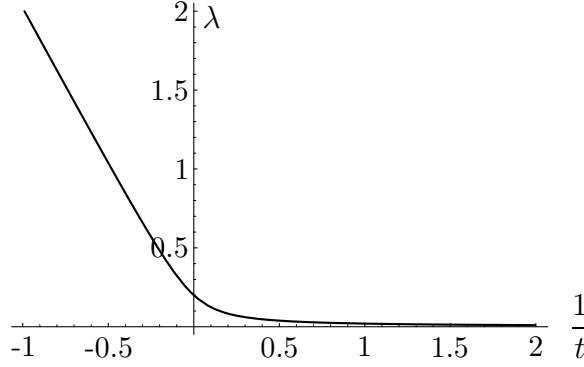


FIGURE 19.3 Solution of the gap equation (19.48) for $\epsilon = 1$ and large volume L^D . For $L \rightarrow \infty$, the right-hand part of the curve approaches more and more the abscissa.

What does this imply for renormalized quantities? Using (19.42) and (19.43), we find from (19.48) the properly renormalized gap equation correcting the previous Eq. (19.44):

$$1 - \frac{t_R^c}{t_R} = -\frac{t_R^c}{\mu^\epsilon L^D \bar{\lambda}} + \left(\frac{\bar{\lambda}}{\mu^2} \right)^{\epsilon/2}. \quad (19.51)$$

For $t_R \geq t_R^c$ and large volume L^D , we can neglect the first term on the right-hand side, and (19.51) coincides with (19.44). For $t_R < t_R^c$, on the other hand, we can neglect the second term on the right-hand side, to find for the spontaneously generated square-mass $\bar{\lambda}$ of n_a -fluctuations:

$$\bar{\lambda} \approx \frac{t_R}{(\mu L)^\epsilon L^2} \left(1 - \frac{t_R}{t_R^c} \right)^{-1}. \quad (19.52)$$

This almost zero part of the gap in the low-temperature phase is pictured by the right-hand branch in Fig. 19.3. In the thermodynamic limit of infinite volume, $\bar{\lambda}$ goes to zero. In this limit, the system has a phase transition at the critical temperature $t_R^c > 0$, where the symmetry changes as described above. The statements for $t < 0$ and $t > 0$ hold now for $t_R > t_R^c$ and $t_R < t_R^c$, respectively. This is, of course, the same transition found earlier in the $O(N)$ -symmetric ϕ^4 -theory, only in quite a different description.

In a finite volume, the square-mass $\bar{\lambda}$ is always nonzero, and there exists no phase in which the n_a -fluctuations are massless. The spontaneous breakdown of $O(N)$ -symmetry is always restored by fluctuations.

19.4 Approaching the Critical Point

It is instructive to study the way in which the mass vanishes as t_R approaches t_R^c from above. From (19.44) we know that

$$\bar{\lambda} = \mu^2 \left(1 - \frac{t_R^c}{t_R} \right)^{2/\epsilon}. \quad (19.53)$$

Since $\bar{\lambda}$ is the square-mass of all n_a -fluctuations, this implies that the correlation functions of the n^a fields fall off exponentially with

$$\langle n_a(\mathbf{x}) n_a(0) \rangle \xrightarrow{x \rightarrow \infty} e^{-|\mathbf{x}|/\xi}, \quad (19.54)$$

where $\xi = \bar{\lambda}^{-\frac{1}{2}}$ is the correlation length. As t_R approaches the critical temperature, ξ goes to infinity, according to the power law

$$\xi \sim (t_R - t_R^c)^{-\nu} \quad (19.55)$$

with

$$\nu = \frac{1}{\epsilon}. \quad (19.56)$$

This number is called the critical exponent of the correlation length. The power behavior of ξ as a function of temperature is shown in Fig. 19.4. A similar power behavior will be obtained later in Chapter 20, for finite N as well, using renormalization-group techniques, although for finite N it will no longer be possible to find an exact result.

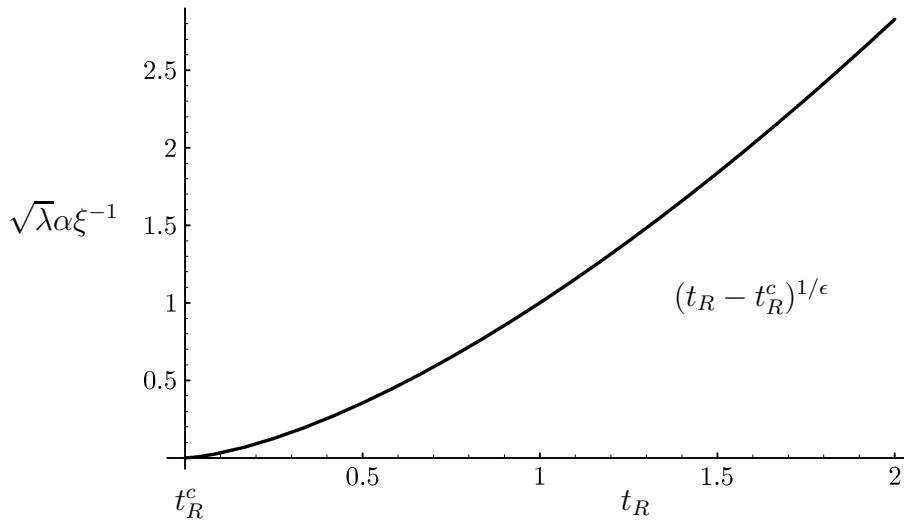


FIGURE 19.4 Temperature behavior of the correlation length.

19.5 Physical Properties of the Bare Temperature

The reader may rightfully wonder whether the entire treatment is consistent. We have observed above that the phase in which the symmetry has been restored possesses a negative bare temperature. This is not the sign of t for which the model was originally defined. Only for field integrations dn^a along the imaginary field direction

does the partition function make sense. Fortunately, this apparent inconsistency is not intrinsic to the theory, but merely a mathematical artifact of the dimensional regularization of the divergent integral. A more physical regularization would have proceeded via a cutoff Λ in momentum space. Let us verify how this would change the range of the bare temperature if the phase transition is approached from positive t .

In order to be specific, consider first the cases of $D = 2$ and 3 dimensions. Using the integrals

$$\begin{aligned} \int_{|k|<\Lambda} \frac{d^2k}{(2\pi)^2} \log(k^2 + \lambda) &= \frac{1}{4\pi} \left[(\Lambda^2 + \lambda) \log(\Lambda^2 + \lambda) - \Lambda^2 - \lambda \log \lambda \right] \\ &\xrightarrow{\Lambda \rightarrow \infty} \frac{1}{4\pi} \left[\Lambda^2 (\log \Lambda^2 - 1) + (\log \Lambda^2 + 1) \lambda - \lambda \log \lambda \right], \end{aligned} \quad (19.57)$$

$$\begin{aligned} \int_{|k|<\Lambda} \frac{d^3k}{(2\pi)^3} \log(k^2 + \lambda) &= \frac{1}{6\pi^2} \left\{ \Lambda^3 \log(\Lambda^2 + \lambda) - \frac{2}{3} \Lambda^3 + 3\Lambda\lambda - 2\lambda^{\frac{3}{2}} \arctan \frac{\Lambda}{\sqrt{\lambda}} \right\} \\ &\xrightarrow{\Lambda \rightarrow \infty} \frac{1}{6\pi^2} \left[\Lambda^3 \left(\log \Lambda^2 - \frac{2}{3} \right) + 3\Lambda\lambda - \pi\lambda^{\frac{3}{2}} \right], \end{aligned} \quad (19.58)$$

the free energy (19.24) becomes

$$\frac{F}{tL^2} = \frac{1}{2} \frac{1}{4\pi} \left[\Lambda^2 (\log \Lambda^2 - 1) + (\log \Lambda^2 + 1) \lambda - \lambda \log \lambda \right] - \frac{\lambda}{2t}, \quad (19.59)$$

$$\frac{F}{tL^3} = \frac{1}{2} \frac{1}{6\pi^2} \left[\Lambda^3 \left(\log \Lambda^2 - \frac{2}{3} \right) + 3\Lambda\lambda - \pi\lambda^{3/2} \right] - \frac{\lambda}{2t}. \quad (19.60)$$

In writing these expressions, we have assumed all momenta and masses to be dimensionless quantities. For mathematically proper expressions, all these quantities should be divided by some standard mass μ , which we have assumed to be equal to one.

The dimensionally regularized expression (19.36), on the other hand, reads for dimensions $D = 2 + \epsilon$ with small $\epsilon > 0$

$$\frac{F}{tL^2N} = -\frac{1}{4} \frac{1}{2\pi} \frac{2}{\epsilon} \lambda - \frac{1}{4} \frac{\lambda}{2\pi} \log \frac{\lambda}{\mu^2} - \frac{\lambda}{2t}, \quad (19.61)$$

and for $D = 3$:

$$\frac{F}{tL^3N} = -\frac{1}{4} \frac{1}{2\pi} \frac{2}{3} \lambda^{\frac{3}{2}} - \frac{\lambda}{2t}. \quad (19.62)$$

For $D = 2 + \epsilon$, the positively divergent cutoff expression $(\log \Lambda^2 + 1) \lambda / 8\pi$ in the second term of (19.60) is replaced by the negatively divergent $-\lambda / 4\pi\epsilon$ in the first term of (19.61). For $D = 3$, the dimensionally regularized expression in (19.61) shows no trace of the infinite linearly divergent term $\Lambda\lambda / 4\pi^2$ in (19.60). Thus the inverse temperature $1/t$ in the dimensionally regularized expressions must be thought of as being an unphysical version of the original inverse temperature $1/t$ in

the initial bare energy, from which the constants $[(\log \Lambda^2 + 1) + 2/\epsilon]/4\pi$ for $D = 2$, or $\Lambda/2\pi^2$ for $D = 3$, have been subtracted. Since these are very large quantities, there is no wonder that the dimensionally regularized discussion yields the phase with restored symmetry at a negative unphysical t .

The analytic continuation is taking advantage of the inobservability of the bare value of t in a continuous field theory. In any system in which there are well-defined physical mechanisms which regularize the short-wavelength fluctuations (for example lattice structures) and in which the bare temperature t is measurable by microscopic methods, the dimensional regularization cannot be used directly to properly represent the physical circumstances of the bare theory. This must be kept in mind when applying such a method, in particular, when dealing with the non-renormalizable $O(N)$ -lattice models of statistical mechanics, to which the present nonlinear σ -model is related in the continuum limit. This issue is discussed in the following section.

19.6 Spherical Model on Lattice

In order to illustrate the dimensional regularization issue discussed in the previous section it is instructive to go through the treatment once more in the lattice formulation of the spherical model. Then the lattice spacing a provides us with a natural short-distance cutoff, so that there is no need for introducing a momentum space cutoff Λ , nor dimensional regularization. On a simple hypercubic lattice, the partition function (19.17) reads

$$Z = \prod_{\mathbf{x}} \left[\int \frac{d\lambda(\mathbf{x}) \beta a^2}{4\pi i} \right] \prod_{\mathbf{x}} \left[\int \frac{d^D n_a(\mathbf{x})}{S_D} \right] \exp \left(-\frac{\beta a^2}{2} \sum_{\mathbf{x}} \{ [(\nabla_i n)^2 + \lambda n^2] - \lambda \} \right), \quad (19.63)$$

where the gradient term has been brought to the lattice form (19.14) omitting the irrelevant term $-2D$. The dimensionless parameter

$$\beta \equiv \frac{1}{T} = \frac{J}{k_B T} \quad (19.64)$$

is called the *stiffness* of the directional fluctuations. The free energy per lattice site is given by

$$\beta f = \frac{1}{2} \left(\int_{-\pi/a}^{\pi/a} N \frac{d^D k a^D}{(2\pi)^D} \log \left\{ \sum_{i=1}^D [2 - 2 \cos(k_i a)] + a^2 \lambda \right\} - \beta a^2 \lambda \right), \quad (19.65)$$

where $a^{-2} \sum_{i=1}^D [2 - 2 \cos(k_i a)]$ is the Fourier transform of the lattice Laplacian $-\nabla_i \bar{\nabla}_i$. Extremizing this with respect to λ yields the gap equation

$$\beta = N v_{a^2 \lambda}^D(\mathbf{0}), \quad (19.66)$$

where

$$v_{a^2 m^2}^D(\mathbf{x}) = \int_{-\pi/a}^{\pi/a} \frac{d^D k a^D}{(2\pi)^D} \frac{e^{i\mathbf{k}\mathbf{x}}}{\sum_{i=1}^D [2 - 2 \cos(k_i a)] + a^2 m^2} \quad (19.67)$$

is the dimensionless lattice Green function of mass m in D dimensions. For small β , i.e., high temperatures, the gap equation has a solution $\lambda > 0$ and the fluctuations are massive. The solution exists up to a critical β_c given by

$$\beta_c = N v_0^D(\mathbf{0}). \quad (19.68)$$

For $D = 2$, the momentum integral diverges at the origin: $v_0^2(\mathbf{0}) = \infty$. This implies $\beta_c = 0$, so that a nonzero λ exists for all temperatures T larger than zero. Here the approximation (19.68) becomes useless, and a special discussion is necessary [12].

The Green function (19.67) is the dimensionless lattice version of the Yukawa potential in D dimensions:

$$V_{m^2}^D(\mathbf{x}) = \int \frac{d^D k}{(2\pi)^D} \frac{e^{i\mathbf{k}\mathbf{x}}}{\mathbf{k}^2 + m^2}. \quad (19.69)$$

The lattice version has the Fourier representation

$$v_{a^2 m^2}^D(\mathbf{x}) = \prod_i \left[\int_{-\pi/a}^{\pi/a} \frac{d(ak_i)}{2\pi} \right] \frac{e^{i\mathbf{k}\mathbf{x}}}{\sum_{i=1}^D (2 - 2 \cos ak_i) + a^2 m^2}. \quad (19.70)$$

The denominator can be rewritten as $\int_0^\infty ds e^{-s[\sum_{i=1}^D (2 - 2 \cos ak_i) + a^2 m^2]}$, leading to the multiple integral

$$v_{a^2 m^2}^D(\mathbf{0}) = \int_0^\infty ds e^{-s(a^2 m^2 + 2D)} \prod_{i=1}^D \left[\int_{-\pi}^{\pi} \frac{d\kappa_i}{2\pi} e^{2s \cos \kappa_i} \right]. \quad (19.71)$$

The integrations over k_i can now easily be performed, and we obtain the integral representation

$$v_{a^2 m^2}^D(\mathbf{0}) = \int_0^\infty ds e^{-s(a^2 m^2 + 2D)} [I_0(2s)]^D, \quad (19.72)$$

where $I_0(2s)$ is the modified Bessel function. Integrating this numerically, we find for $D = 3, 4, \dots$ the values shown in Table 19.1.³ A power series expansion of the

TABLE 19.1 Values of the lattice Yukawa potential $v_{l^2}^D(\mathbf{0})$ of reduced mass l^2 at the origin for different dimensions and l^2 . The lower entries show the approximate values from the hopping expansion (19.74).

D	$v_0^D(\mathbf{0})$	$v_1^D(\mathbf{0})$	$v_2^D(\mathbf{0})$	$v_3^D(\mathbf{0})$	$v_4^D(\mathbf{0})$
3	0.2527	0.1710	0.1410	0.1214	0.1071
	0.2171	0.1691	0.1407	0.1214	0.1071
4	0.1549	0.1271	0.1105	0.0983	0.0888
	0.1496	0.1265	0.1104	0.0983	0.0888

³See also the Tables on pages 178 and 241 of the textbook [3].

D th power of the modified Bessel function in (19.72),

$$[I_0(2s)]^D = 1 + Ds^2 + D(2D-1)\frac{s^4}{4} + D(6D^2-9D+4)\frac{s^3}{36} + \dots, \quad (19.73)$$

leads to the so-called *hopping expansion* for $v_{a^2\lambda}^D(\mathbf{0})$:

$$v_{a^2\lambda}^D(\mathbf{0}) = \frac{1}{2D+a^2\lambda} + \frac{2D}{(2D+a^2\lambda)^3} + \frac{6D(2D-1)}{(2D+a^2\lambda)^5} + \frac{20D(6D^2-9D+4)}{(2D+a^2\lambda)^7} + \mathcal{O}(D^{-9}). \quad (19.74)$$

It converges rapidly for large D , and yields for $D = 3, 4$ the approximate values shown in the lower entries of Table 19.1. They lie quite close to the exact values in the upper entries.

The lattice potential at the origin $v_{a^2\lambda}^D(\mathbf{0})$ in the gap equation (19.66) is always smaller than the massless potential $v_0^D(\mathbf{0})$. A nonzero value for λ can therefore only be found for sufficiently small values of the stiffness β , i.e., for sufficiently high temperatures T [recall (19.64)]. The temperature T_c , at which the gap equation (19.66) has the solution $\lambda = 0$, determines the Curie point. Thus we have

$$T_c = \frac{J}{\beta_c k_B}, \quad (19.75)$$

where β_c is the critical stiffness (19.68):

$$\beta_c = N v_0^D(\mathbf{0}). \quad (19.76)$$

This result, derived for large N , turns out to be amazingly accurate even for rather small N . As an important example, take $N = 2$ where the model consists of planar spins and is referred to as XY-model. For $D = 3$, it describes accurately the critical behavior of the superfluid transition in helium near the λ -transition. From (19.76) and the value $v_0^D(\mathbf{0}) \approx 0.2527$ in Table 19.1, we estimate the critical value

$$\beta_c \approx 0.5054. \quad (19.77)$$

In Monte-Carlo simulations of this model one obtains, on the other hand,⁴

$$\beta_c \approx 0.45. \quad (19.78)$$

Thus, in three dimensions, we can use the large- N result (19.76) practically for all $N \geq 2$.

For $D > 2$, where β_c has a finite positive value, the solution for $\beta > \beta_c$ requires special consideration. The situation is similar to what we encountered earlier in the free Bose liquid. One observes the formation of a condensate consisting of Goldstone bosons of zero momentum. For its theoretical description, we enclose the system

⁴See pages 390 and 391 in the textbook [3].

in a finite box of volume V and replace the integral over $\mathbf{k}$ by the corresponding momentum sum

$$\int \frac{d^D k a^D}{(2\pi)^D} \rightarrow \frac{a^D}{V} \sum_{\mathbf{k}}. \quad (19.79)$$

Since the integrand in (19.67) is singular at $\mathbf{k} = 0$, this mode has to be treated separately. We split the right-hand side of the gap equation (19.68) for $\beta > \beta_c$ as follows

$$1 = N \frac{a^D}{V} \left\{ \frac{1}{\beta \lambda a^2} + \frac{1}{\beta} \sum_{\mathbf{k} \neq 0} \frac{1}{\sum_{i=1}^D [2 - 2 \cos(k_i a)] + \lambda a^2} \right\}. \quad (19.80)$$

This equation can now be solved for $\beta > \beta_c$. For $\beta \gg \beta_c$, the very small prefactor a^D/V guarantees a solution with a very small λa^2 , that is of the order of $a^D/V\beta = a^D/L^D\beta$, where L is the linear size of the system. This follows from the observation that the first nonzero contribution in the sum is of the order

$$\frac{1}{(2\pi a/L)^2 + \lambda a^2} \approx \frac{1}{(2\pi a/L)^2 + a^D/L^D}. \quad (19.81)$$

For $D > 2$ and large L one has $a^D/L^D \ll a^2/L^2$, such that the second term in the denominator can be ignored, and the first term in (19.94) is much larger than the second term. For $\beta > \beta_c$, the gap equation in a large volume shows that

$$1 \approx N \frac{a^D}{V \beta \lambda a^2}. \quad (19.82)$$

What happens if β is only slightly larger than β_c ? Since $D > 2$, the sum on the right-hand side can again be replaced by an integral and we find the gap equation, valid for very large V , but arbitrary $\beta > \beta_c$:

$$1 = \frac{a^D}{V} \frac{1}{\beta} \frac{1}{\lambda a^2} + \frac{N}{\beta} v_0(0) = \frac{a^D}{V} \frac{N}{\beta} \frac{N}{\lambda a^2} + \frac{\beta_c}{\beta}. \quad (19.83)$$

Hence the square-mass λ of directional fluctuations is found to be

$$\lambda = \frac{1}{N} \frac{a^D}{V} \frac{1}{a^2} \frac{1}{\beta - \beta_c}. \quad (19.84)$$

This is positive and infinitely small for a large volume V . As a function of temperature $t = 1/\beta$, this looks very similar to the plot in (19.3).

Let us look in detail at the difference between the treatment of the gap equation on the lattice and that of the dimensionally regularized gap equation in the continuum field theory. This will allow us to understand the reason for the negative sign

of t in the ordered phase in the continuum model. To be specific, we assume $D = 3$. The integral appearing in the gap equation is, in dimensional regularization,

$$\begin{aligned} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{k^2 + m^2} &= S_D \frac{1}{2} \Gamma\left(\frac{D}{2}\right) \Gamma\left(1 - \frac{D}{2}\right) m^{D-2} \Big|_{D=3} \\ &= S_3 \frac{1}{2} \Gamma\left(\frac{3}{2}\right) \Gamma\left(-\frac{1}{2}\right) m \\ &= -\frac{1}{4\pi} m. \end{aligned} \quad (19.85)$$

The corresponding three-dimensional lattice expression is

$$\frac{1}{a^3} \int_{-\pi/a}^{\pi/a} \frac{d^3 k a^3}{(2\pi)^3} \frac{1}{a^{-2} \sum_i [2 - 2 \cos(k_i a)] + m^2} = \frac{1}{a} v_{m^2}^3(0) \quad (19.86)$$

where, for small m^2 ,

$$\frac{1}{a} v_0(0) \equiv \frac{1}{4\pi} m + \mathcal{O}(m). \quad (19.87)$$

In the lattice gap equation (19.68), the first term on the right-hand side of (19.94) goes to infinity in the continuum limit $a \rightarrow 0$. In the analytic continuation (19.67), on the other hand, it is absent. It is this term which, in the lattice model, is responsible for the fact that β is positive in both phases, with a positive $\beta_c > 0$ separating the two phases. In contrast to this, the two phases in the continuum theory exist for *opposite* signs of the bare quantity β . This curious situation, caused entirely by the mathematics of analytic regularization, is removed after renormalizing the theory. Along the renormalized $1/t_R$ -axis, the situation is again analogous to the more physical one in the lattice model, where β needs no renormalization.

19.7 Background Field Treatment of Cold Phase

There is another more elegant way of dealing with the low temperature phase. It does not require the delicate treatment of the $\mathbf{k} = 0$ -mode, and yields a consistent gap equation for all temperatures without the intermediate consideration of a finite volume. It follows from minimizing the effective action of the model, if that is calculated after expanding n^a around a background field. Let us denote this background field by $N^a(\mathbf{x})$, and the fluctuations around it by $\delta n^a(\mathbf{x}) = n^a(\mathbf{x}) - N^a(\mathbf{x})$. Then the one-loop effective action becomes

$$\begin{aligned} \Gamma[N^a] &= \frac{N}{2t} \int d^D x \left\{ (\nabla N_a)^2 + \lambda(\mathbf{x}) N_a^2(\mathbf{x}) \right\} + \frac{N}{2} \text{Tr} \log \left[-\nabla^2 - \lambda(\mathbf{x}) \right] \\ &+ \frac{N}{2t} \int d^D x \lambda. \end{aligned} \quad (19.88)$$

This has to be evaluated at the minimum with respect to $N^a(x)$ and the maximum with respect to λ . In the limit $N \rightarrow \infty$, the one-loop effective action $(1/N) \Gamma[N^a]$ is the exact one.

The new gap equation reads

$$-\frac{N_a^2}{t} + \frac{1}{t} = \int \frac{d^D k}{(2\pi)^D} \frac{1}{\mathbf{k}^2 + \bar{\lambda}}, \quad (19.89)$$

and the background field N_a satisfies the equation of motion

$$\left[-\nabla^2 + \bar{\lambda}(\mathbf{x}) \right] N_a(\mathbf{x}) = 0. \quad (19.90)$$

This equation shows that $\sqrt{\bar{\lambda}}^{-1}$ determines the correlation length of the N_a field. The ground state is obtained for a constant N_a field, which satisfies

$$\bar{\lambda} N_a = 0. \quad (19.91)$$

This has two solutions, $N_a = 0$ or $\bar{\lambda} = 0$. In the first case, the gap equation reduces to the previous one, which in dimensional regularization had a solution only for $t > 0$. In the other phase with $t > 0$, the gap equation turns into an equation for the size of N_a

$$-\frac{N_a^2}{t} + \frac{1}{t} = \int \frac{d^D k}{(2\pi)^D} \frac{1}{\mathbf{k}^2}. \quad (19.92)$$

The direction of N_a is arbitrary and will be chosen by the system statistically. This shows that for $t > 0$, the ground state displays a spontaneous breakdown of $O(N)$ -symmetry. It displays a spontaneous magnetization.

Comparison with Eq. (19.47) shows that the gap equation (19.92) coincides precisely with the previous gap equation on the lattice (19.94) for the low temperature phase, with N_a^2/t playing the role of $1/L^D \bar{\lambda}$. Given the previous solution for $\bar{\lambda}$, we can therefore identify, for $t > 0$,

$$N_a^2 = \frac{t}{\bar{\lambda}} \frac{1}{L^D}. \quad (19.93)$$

The quantity N_a^2 can be considered as an order parameter of the low temperature phase. It specifies the magnetization $M \equiv \sqrt{N_a^2}$.

In the framework of dimensional regularization, the integral on the right-hand side of the gap equation vanishes and the order parameter for $t_R < t_R^c$ has the value

$$N_a^2 = 1. \quad (19.94)$$

The background vector has the unit length of the original fluctuating field $n_a(\mathbf{x})$. The fact that N_a is of unit length for all $t > 0$ or $t_R < t_R^c$, is once more an artifact of dimensional regularization. On a lattice, the magnetization M goes to zero smoothly, with a power law in $\beta - \beta_c$:

$$M \propto (\beta - \beta_c)^\beta. \quad (19.95)$$

The power is conventionally denoted by β , which should, when it appears in this context, not be confused with the inverse temperature β . On a lattice, the gap equation (19.92) reads, for $\beta > \beta_c$,

$$1 - N_a^2 = \frac{N}{\beta} \int_{-\pi/a}^{\pi/a} \frac{d^D k a^D}{(2\pi)^D} \frac{1}{\sum_{i=1}^D [2 - 2 \cos(k_i a)]}, \quad (19.96)$$

such that

$$1 - N_a^2 = \frac{N v_0^D(\mathbf{0})}{\beta}. \quad (19.97)$$

From this we extract the power behavior

$$M = \sqrt{N_a^2} = \left(1 - \frac{\beta_c}{\beta}\right)^{1/2}, \quad (19.98)$$

showing that the critical exponent β has the value $1/2$.

19.8 Quantum Statistics at Nonzero Temperature

Let us also study quantum fluctuations in the nonlinear σ -model. For this we assume that one of the spatial coordinates $(x_1, \dots, x_D)$, for instance x_D , is an imaginary time variable τ restricted to the interval $\tau \in (0, \hbar\beta)$ with $\beta = 1/k_B T$. If the fields are periodic in τ with period $\hbar\beta$, we may think of this model as a nonlinear σ -model on an infinitely long spatial strip with periodic boundary conditions, whose width along the x_D -axis is β . In this context, we shall write the $D-1$ -dimensional purely spatial vectors as bold letters, whereas the D -dimensional spacetime vectors are denoted by light letters.

Since temperature enters the theory now via the period $\hbar\beta = 1/k_B T$, we shall return to the original notation g for the coupling constant, as in the partition function (19.2) [which had been traded for the reduced temperature t in (19.22) and (19.19)].

In the limit $N \rightarrow \infty$, we can study the effects of temperature exactly. The partition function is (19.26), and the gap equation has the same form as in (19.27), except that the momentum integral $\int dp_D/2\pi$ is replaced by a sum $T \sum_{p_D=\omega_m}$ over the Matsubara frequencies

$$\omega_m = 2\pi T m, \quad m = 0, \pm 1, \pm 2, \dots, \quad (19.99)$$

guaranteeing the periodicity of the fields on the interval $x_D \in (0, \beta)$. The gap equation (19.27) at finite temperature is therefore

$$\frac{1}{g} = (-\partial^2 + \lambda)^{-1} = \int \frac{d^{D-1}p}{(2\pi)^{D-1}} T \sum_m \frac{1}{\omega_m^2 + \mathbf{p}^2 + \lambda}. \quad (19.100)$$

We have gone to natural units with $\hbar = 1$, $k_B = 1$. This equation can be renormalized with the same renormalized coupling constant $g_R(\mu)$ as in the infinite system. We add and subtract, on the right-hand side, the $T = 0$ -limit of the right-hand side and obtain

$$\frac{1}{g} - \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 + \lambda} = \int \frac{d^{D-1} p}{(2\pi)^{D-1}} \left(T \sum_m \frac{1}{\omega_m^2 + \mathbf{p}^2 + \lambda} - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega^2 + \mathbf{p}^2 + \lambda} \right). \quad (19.101)$$

The left-hand side is the zero-temperature gap equation (19.27).

19.8.1 Two-Dimensional Model

For the subsequent discussion we focus attention on the two-dimensional case. Then the zero-temperature gap equation can be renormalized in $D = 2 + \epsilon$ dimensions using Eq. (19.32). This brings the left-hand side in (19.101) to the form

$$\frac{1}{g} + S_D \frac{1}{\epsilon} \mu^\epsilon + S_D \frac{\mu^\epsilon}{\epsilon} \left[\left(\frac{\lambda}{\mu^2} \right)^{\epsilon/2} - 1 \right] \approx \frac{1}{g_R(\mu)} + \frac{1}{2} S_2 \log \frac{\lambda}{\mu^2}. \quad (19.102)$$

The sum over m on the right-hand side of Eq. (19.177) can be performed using the sum formula

$$T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega^2} = \frac{1}{2\Omega} \coth \frac{\Omega}{2T}, \quad (19.103)$$

with $\Omega \equiv \sqrt{\mathbf{p}^2 + \lambda}$. In the limit $T \rightarrow 0$, this becomes

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega^2 + \Omega^2} = \frac{1}{2\Omega}. \quad (19.104)$$

Subtracting (19.104) from (19.103), and using (19.102), we obtain the temperature-dependent gap equation in two dimensions

$$\frac{1}{g_R(\mu)} + \frac{1}{4\pi} \log \frac{\lambda}{\mu^2} = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{1}{2\Omega} \left(\coth \frac{\Omega}{2T} - 1 \right). \quad (19.105)$$

Eliminating the arbitrary mass scale μ in favor of the solution $\lambda = \bar{\lambda}$ of this equation for $T = 0$, which is

$$\bar{\lambda} = \mu^2 e^{4\pi/g_R(\mu^2)}, \quad (19.106)$$

then Eq. (19.105) can be rewritten in a renormalization group invariant way:

$$\frac{1}{4\pi} \log \frac{\lambda}{\bar{\lambda}} = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{1}{2\Omega} \left(\coth \frac{\Omega}{2T} - 1 \right). \quad (19.107)$$

The right-hand side is a function of the dimensionless variable λ_T

$$\lambda_T \equiv \lambda / (2\pi T)^2 \quad (19.108)$$

and will be denoted by

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{1}{2\Omega} \left(\coth \frac{\Omega}{2T} - 1 \right) \equiv \frac{1}{2\pi} S_1(\lambda_T). \quad (19.109)$$

In terms of this function, the gap equation reads simply [compare with the forthcoming fermionic gap function (23.225)]

$$\log \frac{\lambda}{\lambda} = 2S_1(\lambda_T). \quad (19.110)$$

The functions $S_1(\lambda_T)$ can also be rewritten as follows

$$S_1(\lambda_T) = \int_0^{\infty} \frac{dp}{\Omega} \left[\coth \left(\frac{\Omega}{2T} \right) - 1 \right] = -2 \int_0^{\infty} \frac{dp}{\Omega} \left(1 - e^{\Omega/T} \right)^{-1}. \quad (19.111)$$

There exists no critical temperature T_c where λ vanishes.

The gap equation (19.110) is fast convergent only at low temperature. For high temperatures, it is better to keep the original sum over ω_m in (19.103). Inserting this sum into (19.111), and performing the integral over p gives

$$\begin{aligned} S_1(\lambda_T) &= \pi \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \frac{1}{\sqrt{\omega_m^2 + \lambda}} \\ &= \frac{1}{2} \left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} dm \right) \frac{1}{\sqrt{m^2 + \lambda_T}}. \end{aligned} \quad (19.112)$$

Treating the $m = 0$ term in the sum separately, the right-hand side can be rearranged as follows:

$$S_1(\lambda_T) = \frac{1}{2\sqrt{\lambda_T}} + \sum_{m=1}^{\infty} \left(\frac{1}{\sqrt{m^2 + \lambda_T}} - \frac{1}{m} \right) + \sum_1^{\infty} \frac{1}{m} - \int_0^{\infty} dm \frac{1}{\sqrt{m^2 + \lambda_T^2}}. \quad (19.113)$$

The last two terms diverge. The two divergences cancel each other. To see this we truncate the sum and the integral at some finite large integer value $m = M$. Then the two terms have the limits

$$\sum_{m=1}^M \frac{1}{m} \rightarrow \log M + \gamma + \mathcal{O}\left(\frac{1}{M}\right), \quad (19.114)$$

and

$$\arcsin \frac{M}{\sqrt{\lambda_T}} \rightarrow \log \frac{2M}{\sqrt{\lambda_T}} + \mathcal{O}\left(\frac{1}{M}\right), \quad (19.115)$$

respectively. Combining them, we obtain the alternative expression for $S_1(\lambda_T)$:

$$S_1(\lambda_T) = \tilde{S}_1(\lambda_T) + \frac{1}{2\sqrt{\lambda_T}} + \frac{1}{2} \log \frac{\lambda_T e^{2\gamma}}{4}, \quad (19.116)$$

where $\tilde{S}_1(\lambda_T)$ denotes the convergent sum:

$$\tilde{S}_1(\lambda_T) \equiv \sum_{m=1}^{\infty} \left(\frac{1}{\sqrt{m^2 + \lambda_T}} - \frac{1}{m} \right). \quad (19.117)$$

Inserting this into (19.116), we arrive at the desired alternative form for the gap equation which converges fast at high temperatures:

$$\log \frac{T}{\bar{T}} = \tilde{S}_1(\lambda_T) + \frac{1}{2\sqrt{\lambda_T}}, \quad (19.118)$$

where $\bar{T} \equiv \sqrt{\lambda} e^\gamma / 4\pi$.

It is straight-forward to calculate $\tilde{S}_1(\lambda_T)$ as a function of λ_T , and find from this $T(\lambda_T)$ as well as $\lambda = \lambda_T 4\pi^2 T$. Plotting $\lambda(T)$ we see that λ starts out with $\bar{\lambda}$ at $T = 0$, and grows rapidly to infinity.

The gap equation is obtained by extremizing the effective potential as a function of λ . The effective potential is given by

$$\frac{1}{N} v(\lambda) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} T \sum_m \log(\omega_m^2 + p^2 + \lambda) - \frac{\lambda}{2g}. \quad (19.119)$$

We split this again into the zero-temperature equation

$$\begin{aligned} \frac{1}{N} v_0(\lambda) &= \frac{1}{2} \int \frac{d^2 p}{(2\pi)^2} \log(p^2 + \lambda) - \frac{\lambda}{2g} \\ &= -\frac{\lambda}{8\pi} \left(\log \frac{\lambda}{\bar{\lambda}} - 1 \right), \end{aligned} \quad (19.120)$$

and a finite temperature correction

$$\begin{aligned} \frac{1}{N} \Delta_T v(\lambda) &= T \int_{-\infty}^{\infty} \frac{dp}{2\pi} \log(1 - e^{-\Omega/T}) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \left(T \sum_m - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2 + \lambda). \end{aligned} \quad (19.121)$$

The right-hand side depends only on λ_T , and will be denoted by $(\lambda/2\pi) S_0(\lambda_T)$, i.e.,

$$\frac{1}{N} \Delta_T v(\lambda) = \frac{\lambda}{2\pi} S_0(\lambda_T). \quad (19.122)$$

The integral over p in (19.120) can be performed after analytic regularization. For $D = 2$, this amounts to the sequence of steps

$$\begin{aligned} \int \frac{dp}{2\pi} \log(\omega_m^2 + p^2 + \lambda) &= - \int_0^\infty \frac{d\tau}{\tau} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp[-\tau(\omega_m^2 + p^2 + \lambda)] \\ &= - \int_0^\infty \frac{d\tau}{2\sqrt{\pi}\tau^{3/2}} \exp[-\tau(\omega_m^2 + \lambda)] \\ &= - \frac{\Gamma(-1/2)}{2\sqrt{\pi}} \sqrt{\omega_m^2 + \lambda}. \end{aligned} \quad (19.123)$$

Hence

$$\begin{aligned} S_0(\lambda_T) &= \frac{\pi}{\lambda} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \sqrt{\omega_m^2 + \lambda} \\ &= \frac{1}{2\lambda_T} \left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} dm \right) \sqrt{m^2 + \lambda_T}. \end{aligned} \quad (19.124)$$

Note that $S_0(\lambda_T)$ has the derivative

$$\frac{d}{d\lambda_T} \lambda_T S_0(\lambda_T) = \frac{1}{2} S_1(\lambda_T), \quad (19.125)$$

so that a differentiation of the potential

$$\frac{1}{N} v(\lambda) = -\frac{\lambda}{8\pi} \left(\log \frac{\lambda}{\lambda} - 1 \right) + \frac{\lambda}{2\pi} S_0(\lambda_T) \quad (19.126)$$

leads properly to the gap equation (19.110).

At high temperatures, it is useful to do the same manipulations with $S_0(\lambda_T)$ as with $S_1(\lambda_T)$, rewriting it as follows

$$S_0(\lambda_T) = \tilde{S}_0(\lambda_T) + \frac{1}{2\sqrt{\lambda_T}} + \frac{1}{4} \left(\log \frac{\lambda_T e^{2\gamma}}{4} - 1 \right), \quad (19.127)$$

where

$$\begin{aligned} \tilde{S}_0(\lambda_T) &= \frac{2\pi}{\lambda} T \sum_{m=1}^{\infty} \left(\sqrt{\omega_m^2 + \lambda} - \omega_m - \frac{\lambda}{2\omega_m} \right) \\ &= \frac{1}{\lambda_T} \sum_{m=1}^{\infty} \left(\sqrt{m^2 + \lambda_T} - m - \frac{\lambda_T}{2m} \right). \end{aligned} \quad (19.128)$$

Then the total potential becomes

$$\frac{1}{N} v(\lambda) = -\frac{\lambda}{4\pi} \log \frac{T}{\bar{T}} + \frac{\lambda}{4\pi\sqrt{\lambda_T}} + \frac{\lambda}{2\pi} \tilde{S}_0(\lambda_T). \quad (19.129)$$

In the close neighborhood of two dimensions, we set $D = 2 + \epsilon > 2$, and split the zero-temperature potential $v_0(\lambda)$ conveniently as follows:

$$\frac{1}{N} v_0(\lambda) = -\frac{\lambda}{2g} - \frac{\lambda}{2} c_\epsilon \frac{1}{1 + \epsilon/2} \lambda^{\epsilon/2} = -\frac{\lambda}{2g} - \frac{\lambda \mu^\epsilon}{2} c_\epsilon - \frac{\lambda}{2} c_\epsilon \left[\frac{1}{1 + \epsilon/2} \lambda^{\epsilon/2} - \mu^\epsilon \right], \quad (19.130)$$

with c_ϵ of Eq. (19.37) with the small- ϵ behavior (19.38).

The finite-temperature correction can be written as follows:

$$\frac{1}{N} \Delta_T v_T(\lambda_T) = -\frac{\lambda^{D/2}}{2\pi} a_D S_0(\lambda_T), \quad (19.131)$$

with

$$S_0(\lambda_T) = a_D^{-1} \frac{2\pi}{\lambda^{D/2}} \frac{1}{2} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2 + \lambda). \quad (19.132)$$

Here the constant a_D is chosen so that $S_0(\lambda_T)$ has a convenient form for all D :

$$a_D = -\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \frac{1}{(4\pi)^{(D-1)/2}}. \quad (19.133)$$

Special values are $a_2 = 1$ and $a_4 = -1/6\pi$ in $D = 2$ and $D = 4$ dimensions. By rewriting $\log a$ as the analytically regularized integral $-\int_0^\infty (d\tau/\tau) e^{-\tau a}$, Eq. (19.132) becomes

$$\begin{aligned} S_0(\lambda_T) &= -a_D^{-1} \frac{\pi}{\lambda^{D/2}} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \\ &\times \int_0^\infty \frac{d\tau}{\tau} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \exp(-\tau p^2) \exp[-\tau(\omega_m^2 + \lambda)]. \end{aligned} \quad (19.134)$$

The integral over p can now be performed, with the result

$$\int \frac{d^{D-1}p}{(2\pi)^{D-1}} \exp(-\tau p^2) = \frac{1}{(4\pi\tau)^{(D-1)/2}}. \quad (19.135)$$

Using here the integral formula

$$\int_0^\infty \frac{d\tau}{\tau} \tau^{-(D-1)/2} e^{-\tau E} = \Gamma\left(\frac{1-D}{2}\right) E^{(D-1)/2}, \quad (19.136)$$

we find

$$\begin{aligned} S_0(\lambda_T) &= \frac{2\pi}{\lambda^{D/2}} \frac{1}{2} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) (\omega_m^2 + \lambda)^{(D-1)/2} \\ &= \frac{1}{2\lambda_T^{D/2}} \left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} dm \right) (m^2 + \lambda_T)^{(D-1)/2}. \end{aligned} \quad (19.137)$$

For $D = 2$, this reduces to the previous sum (19.124).

In going from (19.132) to (19.137), we have of course rederived formula (11.134) in the form

$$\int \frac{d^{D-1}q}{(2\pi)^{D-1}} \log(\omega_m^2 + q^2) = \frac{1}{(4\pi)^{(D-1)/2}} \Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \sqrt{\omega_m^2}^{D-1}. \quad (19.138)$$

19.8.2 Four-Dimensional Model

For $D = 4$, we obtain

$$\begin{aligned} S_0(\lambda_T) &= \frac{\pi}{\lambda^2} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \sqrt{\omega_m^2 + \lambda}^3 \\ &= \frac{1}{2\lambda_T^2} \left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} dm \right) \sqrt{m^2 + \lambda_T}^3. \end{aligned} \quad (19.139)$$

By analogy with the two-dimensional expression (19.127), this can be processed further to a convergent sum

$$\tilde{S}_0(\lambda_T) = \frac{1}{\lambda_T^2} \sum_{m=1}^{\infty} \left\{ \sqrt{m^2 + \lambda_T}^3 - m^3 - \frac{3}{2} \lambda_T m - \frac{3}{8} \frac{\lambda_T^2}{m} \right\}. \quad (19.140)$$

19.8.3 Temperature Behavior in Any Dimension

In any dimension D , the expression $a^D S_0(\lambda_D)$ in the temperature correction (19.131) is derived as follows: First we perform the integral over ω_m in (19.137), and rewrite $a^D S_0(\lambda_T)$ as

$$a^D S_0(\lambda_T) = a_D \frac{1}{\lambda_T^{D/2}} \left[\lambda_T^{(D-1)/2} + 2 \sum_{m=1}^{\infty} (m^2 + \lambda_T)^{(D-1)/2} \right] + \pi c_\epsilon \frac{2}{D}, \quad (19.141)$$

the last term coming from the integral over ω_m in (19.137) [recall (19.37)]. Then we expand the second term in powers of λ_T as

$$a^D S_0(\lambda_T) = a_D \frac{1}{\lambda_T^{D/2}} \left[\lambda_T^{(D-1)/2} + 2 \sum_{m=1}^{\infty} \sum_{k=0}^{\infty} \binom{(D-1)/2}{k} m^{D-1-2k} \lambda_T^k \right] + \pi c_\epsilon \frac{2}{D}. \quad (19.142)$$

Performing the sum over m in the curly brackets gives

$$\left[\lambda_T^{(D-1)/2} + 2 \sum_{k=0}^{\infty} \binom{(D-1)/2}{k} \zeta(2k+1-D) \lambda_T^k \right]. \quad (19.143)$$

For an even dimension $D = \bar{D}$, the term with $k = \bar{D}/2$ has a singularity for D close to 2, 4, ... This singularity cancels a corresponding one in c_ϵ .

Let D be close to the even dimension $\bar{D}$, say $D = \bar{D} + \epsilon$. Then there are two singular terms in $a_D S_0(\lambda_T)$:

$$\begin{aligned} a_D S_0(\lambda_T) \Big|_{\text{sg}} &= -\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \frac{1}{\sqrt{4\pi}^{D-1}} \frac{1}{\lambda_T^{D/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{D}{2}\right)}{\Gamma\left(\frac{\bar{D}}{2} + 1\right) \Gamma\left(\frac{1}{2} + \frac{\epsilon}{2}\right)} \zeta(1-\epsilon) \lambda_T^{\bar{D}/2} \\ &\quad - \frac{1}{2\sqrt{4\pi}^{D-2}} \Gamma\left(1 - \frac{\bar{D}}{2} - \frac{\epsilon}{2}\right) \frac{1}{\bar{D} + \epsilon}. \end{aligned} \quad (19.144)$$

Expanding $\zeta(1-\epsilon) = -(1-\epsilon\gamma)/\epsilon + \dots$, the $1/\epsilon$ -singularity in the first term is given by

$$\frac{1}{\sqrt{4\pi}^{\bar{D}-1}} \Gamma\left(\frac{1}{2} - \frac{\bar{D}}{2}\right) \frac{\Gamma\left(\frac{1}{2} + \frac{\bar{D}}{2}\right)}{\Gamma\left(\frac{\bar{D}}{2} + 1\right) \Gamma\left(\frac{1}{2}\right)} \frac{1}{\epsilon} = \frac{1}{\sqrt{4\pi}^{\bar{D}-1}} \frac{(-)^{\bar{D}/2}}{\Gamma\left(\frac{\bar{D}}{2}\right) \frac{\bar{D}}{2} \epsilon}. \quad (19.145)$$

In the second term, we write

$$\Gamma\left(\frac{1}{2} - \frac{\bar{D}}{2} - \frac{\epsilon}{2}\right) = (-)^{\bar{D}/2} \frac{\Gamma(1 + \epsilon/2)}{\Gamma(\bar{D}/2 + \epsilon/2)} \frac{2}{\epsilon} \Gamma(1 - \epsilon/2) = \frac{(-1)^{\bar{D}/2} \pi}{\Gamma\left(\frac{\bar{D}}{2} + \frac{\epsilon}{2}\right) \sin \frac{\pi\epsilon}{2}}, \quad (19.146)$$

and see that the $1/\epsilon$ -singularities cancel each other. The finite- ϵ independent contribution is obtained by expanding

$$\Gamma(k + \epsilon) = \Gamma(k)[1 + \epsilon\psi(k)], \quad (19.147)$$

such that the first $1/\epsilon$ -singularity is accompanied by

$$\left\{1 + \frac{\epsilon}{2} \left[-\log \lambda_T - \psi\left(\frac{1}{2} - \frac{\bar{D}}{2}\right) + \psi\left(\frac{1}{2} + \frac{\bar{D}}{2}\right) - \psi\left(\frac{1}{2}\right) - 2\gamma - \log 4\pi \right] \right\}. \quad (19.148)$$

The second singularity has a residue

$$\left\{1 + \frac{\epsilon}{2} \left[-\log 4\pi - \frac{2}{\bar{D}} - \psi\left(\frac{\bar{D}}{2}\right) \right] \right\}. \quad (19.149)$$

Since

$$\psi\left(\frac{1}{2} + \frac{\bar{D}}{2}\right) - \psi\left(\frac{1}{2} - \frac{\bar{D}}{2}\right) = \pi \cot \frac{\pi \bar{D}}{2} = 0,$$

the difference is

$$-\frac{\epsilon}{2} \left(\log \frac{\lambda_T e^{2\gamma}}{4} - \sum_{k=1}^{\bar{D}/2} \frac{1}{k} \right). \quad (19.150)$$

Thus, altogether, we obtain for an even number of dimension $D = 2, 4, 6, \dots$ the finite sums

$$S_0(\lambda_T) = \frac{1}{2\lambda_T^{D/2}} \left[\lambda_T^{(D-1)/2} + 2 \sum_{k=0, \neq D/2}^{\infty} \binom{(D-1)/2}{k} \zeta(2k+1-D) \lambda_T^k \right] + S_0^L(\lambda_T), \quad (19.151)$$

where

$$S_0^L(\lambda_T) \equiv -\frac{a_D^{-1}(-)^{D/2}}{4\Gamma\left(1 + \frac{D}{2}\right)} \frac{1}{\sqrt{4\pi^{D-2}}} \left[\log \left(\frac{\lambda_T}{4e^{-2\gamma}} \right) - \sum_{k=1}^{D/2} \frac{1}{k} \right]. \quad (19.152)$$

It is now easy to split (19.151) into

$$S_0(\lambda_T) = \tilde{S}_0(\lambda_T) + \frac{1}{2\sqrt{\lambda_T}} + \tilde{S}_0(\lambda_T) + \tilde{\tilde{S}}_0(\lambda_T) + S_0^L(\lambda_T) \quad (19.153)$$

with the convergent sum

$$\tilde{S}_0(\lambda_T) = \frac{1}{\lambda_T^{D/2}} \sum_{k=D/2+1}^{\infty} \binom{(D-1)/2}{k} \zeta(2k+1-D) \lambda_T^k, \quad (19.154)$$

and the finite sum

$$\tilde{\tilde{S}}_0(\lambda_T) = \frac{1}{\lambda_T^{D/2}} \sum_{k=0}^{D/2-1} \binom{(D-1)/2}{k} \zeta(2k+1-D) \lambda_T^k. \quad (19.155)$$

Inserting the divergent representation $\sum_{m=1}^{\infty} m^{-z}$ for the ζ -function at negative z , this is formally equal to the divergent sum

$$\tilde{\tilde{S}}_0(\lambda_T) = \frac{1}{\lambda_T^{D/2}} \sum_{m=0}^{\infty} \left(m^{D-1} + \frac{D-1}{2} \lambda_T m^{D-3} + \dots \right), \quad (19.156)$$

where the last omitted term in parentheses is proportional to $\lambda_T^{D/2-1}/m$. The convergent sum (19.154) is obviously equal to a convergent power series expansion of the convergent infinite series

$$\tilde{S}_0(\lambda_T) = \frac{1}{2\lambda_T^{D/2}} \sum_{m=1}^{\infty} \left(\sqrt{m^2 + \lambda_T}^{D-1} - m^{D-1} - \frac{D-1}{2} \lambda_T m^{D-3} + \dots \right), \quad (19.157)$$

where as many powers of λ_T are subtracted as needed for convergence. These are the generalizations of the two- and four-dimensional expressions (19.128) and (19.140), respectively. The expression (19.153) written in this way converges fast for high temperatures.

Let us now derive an expression which converges fast at low temperature T . For this it is most convenient to use the D -dimensional generalization of Eq. (19.121):

$$\begin{aligned} \frac{1}{N} \Delta_T v(\lambda) &= \frac{1}{2} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \left(T \sum_m - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2 + \lambda) \\ &= T \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \log(1 - e^{-\Omega/T}), \end{aligned} \quad (19.158)$$

and expand the logarithm in powers of $e^{-\Omega/T}$. This gives

$$\begin{aligned} \frac{\lambda^{D/2}}{2\pi} a_D S_0(\lambda_T) &= -T \sum_{\tilde{m}=1}^{\infty} \frac{1}{\tilde{m}} \int \frac{dp^{D-1}}{(2\pi)^{D-1}} e^{-\tilde{m}\sqrt{p^2+\lambda}/T} \\ &= -\frac{1}{2\pi} S_{D-1} \lambda^{D/2} \frac{1}{\sqrt{\lambda_T}} \sum_{\tilde{m}=1}^{\infty} \frac{1}{\tilde{m}} \int_0^{\infty} ds s^{D-2} e^{-\tilde{m}\sqrt{\lambda}\sqrt{s^2+1}/T}. \end{aligned} \quad (19.159)$$

We now use the integral formula

$$K_{\nu}(z) = \left(\frac{z}{2}\right)^{\nu} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\nu + \frac{1}{2}\right)} \int_0^{\infty} ds s^{2\nu} (s^2 + 1)^{-1/2} e^{-z\sqrt{s^2+1}}, \quad (19.160)$$

and see that

$$S_0(\lambda_T) = 2\pi \frac{2^{D/2}}{\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \Gamma\left(\frac{1}{2}\right)} \sum_{\tilde{m}=1}^{\infty} \frac{1}{(2\pi\tilde{m}\sqrt{\lambda_T})^{D/2}} K_{D/2}\left(2\pi\tilde{m}\sqrt{\lambda_T}\right). \quad (19.161)$$

The same expression will be found once more in an exactly solvable fermionic model in Eq. (23.277), except for a fermionic alternating sign $(-)^{\tilde{m}-1}$.

For $D = 2$, the sum (19.161) reduces to

$$S_0(\lambda_T) = -2 \sum_{\tilde{m}=1}^{\infty} \frac{1}{2\pi\tilde{m}\sqrt{\lambda_T}} K_1\left(2\pi\sqrt{\lambda_T}\tilde{m}\right). \quad (19.162)$$

We can take the limit of large T , using $K_1(z) \xrightarrow{z \rightarrow 0} 1/z$, and find

$$S_0(\lambda_T) \xrightarrow{T \rightarrow \infty} -\frac{1}{2\pi^2\lambda_T} \sum_{\tilde{m}=1}^{\infty} \frac{1}{\tilde{m}^2} = -\frac{1}{2\pi^2\lambda_T} \zeta(2) = -\frac{1}{12\lambda_T}. \quad (19.163)$$

This yields the free energy of black-body radiation in two dimensions

$$\frac{1}{N} \Delta_T v(\lambda) \xrightarrow{T \rightarrow \infty} -T^2 \frac{\pi}{6}. \quad (19.164)$$

The same result could have been obtained from the divergent expression (19.119) using the generalized Euler-Maclaurin formula based on analytic continuation as in the formal calculation of the *Casimir effect* in Eq. (7.727):

$$\begin{aligned} \frac{1}{N} \Delta_T v(\lambda) &= \frac{1}{2} \int \frac{dp}{2\pi} T \left[\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right] \log(\omega_m^2 + p^2) \\ &= \frac{1}{2} T \sum_{m=-\infty}^{\infty} \sqrt{\omega_m^2} = 2\pi T^2 \zeta(-1) = -T^2 \frac{\pi}{6}. \end{aligned} \quad (19.165)$$

In the second step we have used the integral formula (11.134) in the form

$$\int \frac{d^{D-1}q}{(2\pi)^{D-1}} \log(\omega_m^2 + q^2) = \frac{1}{(4\pi)^{(D-1)/2}} \Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \sqrt{\omega_m^2}^{D-1}. \quad (19.166)$$

In four dimensions, we have

$$S_0(\lambda_T) = 6 \sum_{\tilde{m}=1}^{\infty} \frac{1}{(2\pi\tilde{m}\sqrt{\lambda_T})^2} K_2\left(2\pi\tilde{m}\sqrt{\lambda_T}\right) \quad (19.167)$$

which becomes for large T [using $K_2(z) \xrightarrow{z \rightarrow 0} 2/z^2$]

$$S_0(\lambda_T) \xrightarrow{T \rightarrow \infty} 12 \sum_{\tilde{m}=1}^{\infty} \frac{1}{(2\pi\tilde{m}\sqrt{\lambda_T})^4} = \frac{12T^4}{\lambda^2} \zeta(4) = \frac{12}{\lambda^2} T^4 \frac{\pi^4}{90}. \quad (19.168)$$

The potential

$$\frac{1}{N}\Delta_T v = \frac{\lambda^2}{2\pi}S_0 = -\frac{\lambda^2}{12\pi^2}S_2 = -T^4\frac{\pi^2}{90} \quad (19.169)$$

is the analog of the free energy density f of black-body radiation. It is related to the internal energy density u by $f = -\frac{1}{3}u$.

Recall the analog of the *Stefan-Boltzmann law* for the free energy density f of hot (or massless) bosons. In this limit, f has a pure power behavior of T^n , and the associated entropy density $s = -\partial f/\partial T$ is related to f by a factor $-4/T$. For the internal energy density $u \equiv E/V = f + TS$ and for the specific heat at constant volume $c_V = \partial u/\partial T|_V$, the factors are $1 - n$ and $(1 - n)n/T$, respectively.

The original Stefan-Boltzmann law for black body radiation is obtained from this by accounting for the two polarization degrees of freedom with an extra factor 2 so that

$$\Delta_T v = f = -\frac{1}{3}u = -2\frac{\pi^2 T^4}{90}. \quad (19.170)$$

In physical units, this becomes

$$f = -2\frac{2}{3}\frac{\sigma}{c}T^4, \quad (19.171)$$

where σ is the *Stefan-Boltzmann constant*

$$\sigma = \frac{\pi^2 k_B^4}{60\hbar^3 c^2} \approx 5.67 \times 10^{-5} \frac{\text{g}}{\text{sec}^\circ \text{K}^4}. \quad (19.172)$$

The same result could, of course, have been obtained directly from (19.132), which would have led to the four-dimensional version of Eq. (19.165). Using (19.166) for $D = 3$ we obtain

$$\begin{aligned} \frac{1}{N}\Delta_T v(\lambda) &= \frac{1}{2} \int \frac{d^3 p}{(2\pi)^3} T \left[\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right] \log(\omega_m^2 + p^2) \\ &= \frac{1}{2} T \sum_{m=-\infty}^{\infty} \frac{1}{(4\pi)^{3/2}} \frac{2}{3} \Gamma(-1/2) \sqrt{\omega_m^2}^3 = -\frac{4}{3\pi} T^4 \zeta(-3) = -T^4 \frac{\pi^2}{90}. \end{aligned} \quad (19.173)$$

In the last step we have used Eq. (7.728).

At arbitrary D , we use the small- z behavior

$$K_\nu(z) \approx \frac{1}{2} \left(\frac{2}{z} \right)^\nu \Gamma(\nu)$$

in (19.161) to find

$$\begin{aligned} S_0(\lambda_T) &\xrightarrow{T \rightarrow 0} -a_D^{-1} 2\pi^{1-D/2} \Gamma\left(\frac{D}{2}\right) \frac{1}{(2\pi\sqrt{\lambda_T})^D} \zeta(D) \\ &= -\frac{2\pi}{\lambda^{D/2} a_D} \frac{1}{\pi^{D/2}} \Gamma\left(\frac{D}{2}\right) T^D \zeta(D). \end{aligned} \quad (19.174)$$

Dropping the prefactor $2\pi/\lambda^{D/2}a_D$ gives the finite-temperature contribution $\Delta_T v(\lambda)/N$ to the free energy density in D dimensions:

$$\Delta_T v(\lambda)/N \xrightarrow{T \rightarrow \infty} -\frac{1}{\pi^{D/2}} \Gamma\left(\frac{D}{2}\right) T^D \zeta(D). \quad (19.175)$$

The same result could, of course, have been obtained directly from (19.132), using

$$\sum_{m=-\infty}^{\infty} \omega_m^{D-1} = (2\pi T)^{D-1} 2\zeta(1-D), \quad (19.176)$$

and the well-known identity for Riemann's ζ -functions⁵

$$\Gamma\left(\frac{1}{2} - \frac{z}{2}\right) \zeta(1-z) = \pi^{1/2-z} \Gamma\left(\frac{z}{2}\right) \zeta(z). \quad (19.177)$$

19.9 Criteria for the Onset of Fluctuations in Ginzburg-Landau Theories

The understanding of the nonlinear σ -model permits us to improve our understanding of the phase transition in ϕ^4 -theories with $O(N)$ -symmetry discussed in Chapter 25. We shall base the discussion on the euclidean version of the Lagrangian (16.1), which is then called *Ginzburg-Landau* Hamiltonian [5]:

$$\mathcal{H}(\phi_a, \partial\phi_a) = \frac{1}{2} (\partial\phi_a)^2 + \frac{m^2}{2} \phi_a^2 + \frac{g}{4} (\phi_a^2)^2. \quad (19.178)$$

In the associated partition function

$$Z = \int \mathcal{D}\phi_a e^{-\int d^D x \mathcal{H}/k_B T}, \quad (19.179)$$

a phase transition takes place at a temperature T_c which lies always *below* the mean field temperature T_c^{MF} , where the mass term in (19.178) changes its sign. It is possible to give a rough estimate of the shift $\Delta T \equiv T_c^{\text{MF}} - T_c$ which is caused by fluctuations.

After an obvious renormalization of field and mass, the Ginzburg-Landau energy density in D dimensions may be written as

$$\mathcal{H}(\phi_a, \partial\phi_a) = \frac{1}{2a^D} \left\{ \alpha^2 a^2 [\partial\phi_a(x)]^2 + \tau \phi_a^2(x) + \frac{g}{2} [\phi_a^2(x)]^2 \right\}. \quad (19.180)$$

From here on we use natural units with $k_B T_c^{\text{MF}} = 1$. The fields have zero engineering dimensions, a denotes some microscopic length scale of the system, usually the size of atoms or molecules, and g is some interaction strength. The parameter α

⁵See, for instance, I.S. Gradshteyn and I.M. Ryznik, op. cit., Academic Press, New York, 1980, formula 9.635.4.

specifies the zero-temperature coherence length of the system in units of a as being $\xi_0 = \alpha a / \sqrt{2}$. This can vary greatly from system to system. In superconductors, for example, α can lie anywhere between a few thousand and less than ten in high-temperature superconductors.

We shall here be concerned only with the destruction of the ordered state which lies *below* the critical temperature where $\tau < 0$. There the fields fluctuate around an ordered ground state with a constant field expectation $\langle \phi_a \rangle \equiv \Phi_a \equiv \langle \phi \rangle N_a \equiv \Phi N_a$. The size of the field $\phi(x)$ fluctuates around Φ which depends on τ as $\Phi = \sqrt{\Phi_a^2} = \sqrt{-\tau/g}$. At that field, the energy density is minimal, and has the value $\mathcal{H}_0 = \mathcal{H}(\Phi_a, 0) = -\tau^2/4ga^D$. The directional unit vector N_a breaks spontaneously the $O(N)$ -symmetry. The temperature-dependent coherence length $\xi = \alpha a / \sqrt{2|\tau|}$ describes the range of the size fluctuations of the order field.

19.9.1 Ginzburg's Criterion

The magnitude of the fluctuations is estimated by assuming the field to live in patches on a simple cubic lattice of spacing $\xi_l = l\xi$, choosing eventually a spacing parameter between $l = 1$ and 2 to ensure the independence of the patches. In the low-temperature ordered phase with $\tau < 0$, the small fluctuations $\delta\phi(x) = \phi(x) - \Phi$ of the size of the order field $\phi(x)$ around the minimum of (19.180) have a Hamiltonian

$$\mathcal{H}_{sz}(\phi_a, \partial\phi_a) \equiv \frac{1}{2a^D} \left\{ \alpha^2 a^2 [\partial\phi(x)]^2 + 2|\tau| \delta\phi^2(x) \right\}. \quad (19.181)$$

Their size is therefore given by

$$\langle [\phi(x) - \Phi]^2 \rangle = \int \frac{d^D k}{(2\pi)^D} \frac{a^D}{\alpha^2 a^2 k^2 + 2|\tau|} = \frac{a^{D-2}}{\xi_l^{D-2}} \frac{1}{\alpha^2} \int \frac{d^D q}{(2\pi)^D} \frac{1}{q^2 + l^2}, \quad (19.182)$$

where q is the dimensionless reduced momentum $\xi_l k$. Inserting ξ_l , the right-hand side can be rewritten as

$$\frac{l^{2-D}}{\alpha^D} (2|\tau|)^{D/2-1} \int \frac{d^D q}{(2\pi)^D} \frac{1}{q^2 + l^2}. \quad (19.183)$$

The relative size of the fluctuations can therefore be written as

$$\frac{\langle [\phi(x) - \Phi]^2 \rangle}{\Phi^2} = 2l^{2-D} (2|\tau|)^{D/2-2} g \alpha^{-D} v_l^D(0), \quad (19.184)$$

where $v_l^D(0)$ is the lattice Yukawa potential of reduced mass l of Eq. (19.67). Its size is calculated most easily with the help of the integral formula (19.72). Mean-field behavior breaks down if (19.184) is of the order unity, which for $D < 4$ happens at the reduced Ginzburg temperature

$$|\tau_G| \approx [l^{2-D} K v_l^D(0)]^{2/(4-D)}, \quad (19.185)$$

where

$$K \equiv 2^{D/2-1} g / \alpha^D, \quad (19.186)$$

i.e., at a Ginzburg temperature $T_G \equiv T_c^{\text{MF}}(1 - |\tau_G|)$. In his original paper [6], Ginzburg estimated $l \approx 1$ and $v_1^D(0)$ in three dimensions by an integral carried up to $|p| = \pi$:

$$v_1^D(0) \approx \int \frac{d^3p}{(2\pi)^3} \frac{1}{p^2 + 1} \approx \frac{1}{2\pi^2} \int_0^\pi dp p^2 \frac{1}{p^2 + 1} \approx \frac{1}{4\pi}. \quad (19.187)$$

This led him to the estimate

$$|\tau_G| \approx \frac{1}{8\pi^2} \frac{g^2}{\alpha^3}. \quad (19.188)$$

In old-fashioned type-II superconductors, $|\tau_G|$ can be as small as 10^{-8} [7], which explains why conventional superconductors are well described by mean-field theory. In modern high- T_c superconductors, on the other hand, Ginzburg's estimate leads to $|\tau_G| \approx 0.01$ [8], such that critical exponents should become observable.

Ginzburg's estimate $l \approx 1$ for a rough determination of the critical temperature interval is based on the assumption that the order field $\Phi(\mathbf{x})$ is properly defined only up to a length scale of the order of the coherence length. In an ordinary superconductor, this is indeed the case. There the order field describes the Cooper pairs of electrons whose wave function extends over a coherence length, such that the cutoff in all momentum integrals would be of this order. In modern superconductors, where the phase transition occurs at higher critical temperature being of the order of 100 K, however, the Cooper pairs could have a much smaller diameter than the coherence length [9]. In this case, l would be considerably smaller than unity. If the Cooper pairs are bound very strongly, another effect appears: The phase transition is caused by quantum fluctuations. In this limit, the Cooper pairs form an almost free gas of almost point-like bosons which undergo Bose-Einstein condensation of the type described in Subsection 2.15.3. The relevant length scale is then the de Broglie wavelength of thermal motion

$$\lambda = \frac{2\pi\hbar}{\sqrt{2Mk_B T}}, \quad (19.189)$$

where M is the mass of the Cooper pairs.

For $D > 4$, the right-hand side in (19.184) decreases when approaching the critical point, so only mean-field behavior is observed. If $D = 4 - \varepsilon$ lies only slightly below four, the right-hand side of (19.184) behaves like $|\tau|^{-\varepsilon/2}$, implying a good mean-field description as long as $|\tau|$ is sufficiently small.

19.9.2 Azimuthal Correction to Ginzburg's Criterion

If a ϕ^4 -theory has only a single real field, Ginzburg's criterion gives a rough estimate of the temperature at which fluctuations become important. In an $O(N)$ -symmetric system with Nambu-Goldstone modes, however, it grossly underestimates the temperature shift ΔT of the transition. A better estimate is based on the observation

that the kinetic term defines a second, completely independent, energy scale of the system. To identify it, we split the fields according to size and direction in $O(N)$ field space as $\phi_a = \phi n_a$, $n_a^2 = 1$. The directions n_a describe the long-range fluctuations of the Goldstone modes. Sufficiently far from the critical regime, we may neglect the gradient term of the size $\phi(x)$, and approximate the energy density by

$$\mathcal{H}(\phi, \partial n_a) = \frac{1}{2a^D} \left\{ \alpha^2 a^2 \phi^2(x) [\partial n_a(x)]^2 + \tau \phi^2(x) + \frac{g}{2} \phi^4(x) \right\}.$$

The fluctuations of the Goldstone modes are controlled by the gradient term whose magnitude depends on the size Φ of ϕ at the minimum of the potential. The gradient energy density is

$$\mathcal{H}_{n_a}(\partial n_a) = \frac{\beta}{2\xi_l^{D-2}} [\partial n_a(x)]^2, \quad (19.190)$$

with

$$\beta = \beta(\Phi) = \alpha^2 \left(\frac{\xi_l}{a} \right)^{D-2} \Phi^2 = \frac{\alpha^D l^{D-2}}{2(2|\tau|)^{D/2-2} g} = \frac{1}{K} \frac{l^{D-2}}{|\tau|^{D/2-2}}. \quad (19.191)$$

This is the second energy scale. It measures how much energy is spent when reversing the direction vector n_a over the distance ξ_l . It is the continuous version of the *stiffness* of the directional field defined for a lattice model in Eq. (19.64).

From the discussion of the spherical model in Section 19.6 we know that directional fluctuations disorder a system if the bending stiffness drops below a certain critical value β_{cr} . For the $O(N)$ -symmetry with large N , this critical value was found on a cubic lattice in three, four, and large dimensions D , respectively, to have the values [see Table 19.1 and the hopping expansion (19.74)]

$$\beta_{\text{cr}} = N v_0^D(0) \approx N 0.2527, \quad N 0.1549, \quad N/2D. \quad (19.192)$$

We have remarked below Eq. (19.76) that, although these values were derived only for large N , Monte Carlo simulations show that they can be trusted already for $D = 3$ and $N = 2$ with an error of only 10%.

The simulations are done by putting the Heisenberg model on a lattice of unit spacing, so that the energy density for $N = 2$ takes the XY-model form

$$\mathcal{H}_{XY}(\partial n_a) \approx \beta \sum_{\mu=1, \dots, D} [1 - \cos \nabla_\mu \gamma(x)], \quad (19.193)$$

where ∇_i denotes the lattice gradient in the i th coordinate direction, and $\gamma \equiv \arctan n_2/n_1$. Since the quality of the approximation increases with N and D , we can trust Eq. (19.192) within 10% for *all* N and $D \geq 3$. This accuracy will be sufficient for the criterion to be derived here.

The critical stiffness can, incidentally, be also estimated by calculating its re-normalized version from a sum of an infinite number of terms in a perturbation expansion. Expanding the cos-function in the energy (19.193) into a Taylor series,

and calculating the harmonic expectation values of quartic, sextic, etc. terms, we find, in a self-consistent approximation of the Hartree-Fock-Bogoliubov type, that the stiffness has a renormalized value $\beta_R = \beta e^{-1/2D\beta_R}$ [12]. This softens with increasing temperature $1/\beta$, until β reaches a critical value $\beta_{cr} = e/2D$, where β_R drops to zero. In $D = 3$ dimensions, this happens at $\beta_{cr} = 0.4530 \dots$, a value which is in excellent agreement with the Monte Carlo number $\beta_{cr}^{MC} \approx 0.45$. The prediction of such sharp drop is true only in two dimensions, as shown by Kosterlitz and Thouless [11]. For $D > 2$ it is an artefact of the approximations, and the exact stiffness goes to zero like $|T_c - T|^{(D-2)\nu}$, with a critical exponent $\nu \approx 1/2 + (4 - D)/10 + \dots$.

The estimate for the critical stiffness (19.192) leads now directly to the announced criterion: The phase fluctuations disorder the system if the stiffness β in Eq. (19.190) drops below the critical value (19.192), which happens at a reduced temperature

$$|\tau_K| \approx [Nl^{2-D} K v_0^D(0)]^{2/(4-D)}, \quad D < 4, \quad N \geq 2. \quad (19.194)$$

Thus we obtain the important result that

$$|\tau_K| \approx [N v_0^D(0)/v_2^D(0)]^{2/(4-D)} |\tau_G|, \quad D < 4, \quad N \geq 2. \quad (19.195)$$

This implies that, for all systems with $N \geq 2$, directional fluctuations destroy the order *before* size fluctuations become large. They cause a phase transition below the Ginzburg temperature, at $T_K \equiv T_c^{MF}(1 - |\tau_K|)$. For $D = 3$, and $l = (1, 3/2, 2)$, the relation becomes $|\tau_K| \approx N^2 |\tau_G| \times (2.20, 3.48, 5.56)$. Thus, if the critical regime is approached in a ϕ^4 -theory with a well-formed mean-field regime, the transition is *always* initiated by directional fluctuations. In particular, the estimates for the critical regime of the high- $|T_c|$ superconductors [8] will receive a factor ≈ 9 .

The dominance of directional fluctuations is, of course, most prominent in the limit of large N , and it is therefore not surprising that the critical exponents of the ϕ^4 -theory and the Heisenberg model have the same $1/N$ -expansions in any dimension $D > 2$, this being a pleasant demonstration of the universality of critical phenomena.

By adding the energy density of directional fluctuations with the field-dependent stiffness $\beta = \beta(\phi) = \alpha^D \phi^2 l^{D-2} / (2|\tau|)^{D/2-1}$ to the field energy density $\mathcal{H}(\phi, \partial n_a)$, we can study, as in Ref. [13], the combined energy density in the disordered phase where the symmetry is restored but the average Φ of the size of the order field ϕ is nonzero.

The directional fluctuations play a crucial role in pion physics, as pointed out in Ref. [13] and discussed in detail in Section 23.10.

19.9.3 Experimental Consequences

How do we determine experimentally the fluctuation parameter K to estimate $|\tau_G|$ and $|\tau_K|$? In magnetic systems, one measures the susceptibility tensor $\chi_{AB}(k) \equiv \int d^D x e^{ikx} \langle \phi_a(x) \phi_b(0) \rangle$ at wave vector k , and decomposes it into parallel and perpendicular parts as $\chi_{AB}(k) = (\Phi_a \Phi_b / \Phi^2) \chi_{\parallel}(k) + (\delta_{AB} - \Phi_a \Phi_b / \Phi^2) \chi_{\perp}(k)$. The mean-field behavior of these quantities is $\chi_{\parallel}(k) \approx a^D / (\alpha^2 a^2 k^2 + 2|\tau|)$ and $\chi_{\perp}(k) \approx a^D / \alpha^2 a^2 k^2$. Combining these at $k = 0$ with the mean-field behavior of the spontaneous magnetization $\Phi = \sqrt{|\tau|/g}$, and with the temperature-dependent coherence length ξ , we see

that the size of K can immediately be estimated from a plot, versus $t \equiv T/T_c - 1$, of either of the dimensionless experimental quantities

$$K_{\text{exp}} \approx |t|^{2-D/2} \frac{k^2}{\xi^{D-2}} \frac{\chi_{\perp}(k)}{k_B T \Phi^2} \Big|_{k \rightarrow 0}, \quad (19.196)$$

or

$$K_{\text{exp}} \approx |t|^{2-D/2} \frac{1}{\xi^D} \frac{\chi_{\parallel}(0)}{k_B T \Phi^2}, \quad (19.197)$$

these being written down in physical units. Note that t measures the temperature distance from the experimental T_c , in contrast to $\tau \equiv T/T_c^{\text{MF}} - 1$. In the mean-field regime, where $t \approx \tau$, K_{exp} is constant and can be inserted into Eq. (19.194) to find the temperature T_K where directional fluctuations destroy the order.

In superfluid helium we may plot, in analogy to the transverse susceptibility expression for K_{exp} , the quantity $K_{\text{exp}} \approx |t|^{2-D/2} M^2 k_B T / \xi^{D-2} \hbar^2 \rho_s$, where M is the atomic mass and ρ_s the superfluid mass density, which at the mean-field level is defined by writing the gradient energy (19.190) as $(\rho_s/2k_B T)(\hbar^2/M^2)[\partial n_a(x)]^2$. In the critical regime, the three expressions for K_{exp} go universally to zero like $|t|^{2-D/2}$, since $\xi \propto |t|^{-\nu}$, $\chi_{\parallel}(0) \approx |t|^{(\eta-2)\nu}$, $k^2 \chi_{\perp}(k)|_{k \rightarrow 0} \approx |t|^{\eta\nu}$, $\Phi^2 \approx |t|^{\nu(D-2+\eta)}$, $\rho_s \approx |t|^{(D-2)\nu}$, with $\eta \approx [(N+2)/2(N+8)^2](4-D)^2 + \dots$.

Experimentally, the superfluid density of helium for $D = 3$ shows no mean-field behavior à la Ginzburg-Landau down to $T \approx T_c/4$, such that the above formulas cannot properly be applied. Let us nevertheless estimate orders of magnitude of a would-be mean-field behavior: $\rho_s/\rho \approx 2|\tau|$ [14], where $\rho = M/a^3$ is the total mass density, with $a \approx 3.59 \text{ \AA}$ [15]. Then the factor $k_B T_c$ at $T_c = 2.18 \text{ K}$ can be expressed as $k_B T_c \approx 2.35 \hbar^2 / M a^3$ [15]. With $\xi_0 \approx 2 \text{ \AA}$, we obtain an estimate $K \approx 1.2 a / \xi_0 \approx 2$. Inserting this into Eq. (19.194) and the relation (19.195), we obtain, for $l = 1$ and 2,

$$|\tau_K| \approx 1, \quad |\tau_G| \approx 0.12 \quad \text{and} \quad |\tau_K| \approx 0.255, \quad |\tau_G| \approx 0.03, \quad (19.198)$$

respectively. The large size of $|\tau_K|$ reflects the bad quality of a mean-field description. The larger l gives the more physical estimate.

Notes and References

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It was beautiful and simple, as truly great swindles are.
O. HENRY (1862–1910)

20

The Renormalization Group

In the previous chapter we discussed some solvable models which illustrate an important aspect of the renormalization procedure: When defining renormalized quantities in a massless theory, we cannot avoid introducing some mass parameter μ . Its value is a matter of choice. If the Lagrangian density contains the mass m of a physical particle, the role of μ can be played by m itself. But this is not always the most convenient choice. Often we want to study the limit $m \rightarrow 0$ of a theory. Then it is preferable to renormalize also a massive theory with the help of an auxiliary mass μ . As long as $m \neq 0$, this amounts to an overparametrization of the theory. It is a useful technical trick to derive the characteristic behavior of experimental observables for an important set of physical phenomena. These are the *critical phenomena* which occur as a function of temperature T in many-body systems as temperature tends towards a so-called critical temperature T_c , where the system undergoes a *second-order phase transition*. At T_c , fluctuations acquire an infinitely long range which implies that the mass m of the relevant fields goes to zero. The mass parameter vanishes near T_c like

$$m^2 = \mu_0^2 \left(\frac{T}{T_c} - 1 \right). \quad (20.1)$$

Suppose that we want to study the temperature behavior of a field theory in the neighborhood of $m^2 = 0$, and that we have chosen the mass m itself as the mass scale μ of renormalization. Then we are able to calculate renormalized Green functions as long as $m^2 \neq 0$. At the limiting point $m^2 = 0$, we have to change the renormalization procedure and introduce some non-zero mass scale μ . Obviously, such a procedure is not well adapted to study the limit $m \rightarrow 0$. A unified renormalization of massive and massless theories with a single arbitrary mass scale μ is preferable. Certainly, all physical quantities must be independent of the mass parameter μ when expressed in terms of the observable quantities.

20.1 Example for Redundancy in Parametrizing the Renormalized Theory

As an example, recall the situation in the $O(N)$ -symmetric self-interacting four-fermion theory. In the limit $N \rightarrow \infty$, the effective potential reads at zero input fermion mass [recall b_ε from Eq. (23.20)]:

$$\frac{1}{N}v(\Sigma) = \frac{1}{2} \left(\frac{\Sigma^2}{g_0} - b_\varepsilon \Sigma^{2+\varepsilon} \right) = \frac{\mu^\varepsilon}{2} \left[\frac{\Sigma^2}{g_0 \mu^\varepsilon} - b_\varepsilon \left(\frac{\Sigma}{\mu} \right)^{2+\varepsilon} \mu^2 \right]. \quad (20.2)$$

This expression is trivially independent of the arbitrary mass parameter μ . The necessity of introducing the mass parameter μ arises only if we want to go to the limit of two dimensions, with $\varepsilon = D-2 \rightarrow 0$. Then we want to define the theory with the help of a finite renormalized coupling constant, and this cannot be done without some mass parameter μ . The renormalized coupling constant will necessarily depend on μ , as long as the bare coupling constant g_0 is held fixed. The μ -dependence is given by

$$\frac{1}{g(\mu, \varepsilon)} = \frac{1}{g_0 \mu^\varepsilon} - b_\varepsilon. \quad (20.3)$$

To emphasize the μ -dependence at fixed g_0 , as well as the dependence on ε , we have added these arguments to the renormalized coupling g .

In a more general renormalizable theory, all renormalized quantities are functions of μ and ε . We shall make these dependences explicit by writing

$$m = m(m_0, g_0, \mu, \varepsilon) \quad (20.4)$$

$$g = g(m_0, g_0, \mu, \varepsilon). \quad (20.5)$$

The fields are renormalized by a factor

$$\phi = \phi_0 Z_\phi^{-\frac{1}{2}}(m_0, g_0, \mu, \varepsilon). \quad (20.6)$$

If we vary the mass parameter μ at fixed bare quantities, the Green functions remain the same. The renormalized quantities m, g change with μ . This implies that they are not directly observable in experiments. Experimental quantities such as particle masses and scattering amplitudes cannot depend on the dummy mass parameter μ . At $\varepsilon \neq 0$, these depend only on the initial *bare* quantities. The main observable of the $O(N)$ -symmetric four-fermion theory with zero initial mass is the fermion mass M_f arising from a spontaneous symmetry breakdown. It is given by the value of Σ' at the minimum of the potential v :

$$M_f = \left(\frac{2/D}{g_0 b_\varepsilon} \right)^{1/\varepsilon}. \quad (20.7)$$

In the limit $\varepsilon \rightarrow 0$, the finite physical mass M_f must be reproduced by theory. Since b_ε diverges, the bare coupling has to become infinitesimally small.

The mass scale μ is needed to describe the situation in the limit $\varepsilon \rightarrow 0$ in terms of finite quantities. To do this, we express (20.7) in terms of the renormalized coupling constant g , which is defined by the relation

$$\frac{1}{g(\mu, \varepsilon)} \equiv \frac{1}{g_0 \mu^\varepsilon} - b_\varepsilon, \quad (20.8)$$

we obtain the equation for M_f

$$\frac{M_f}{\mu} = \left(\frac{2/D}{g_0 \mu^\varepsilon b_\varepsilon} \right)^{1/\varepsilon} = \left[\frac{2}{D} \left(1 + \frac{1}{b_\varepsilon g(\mu, \varepsilon)} \right) \right]^{1/\varepsilon}. \quad (20.9)$$

Here we can easily take the limit $\varepsilon \rightarrow 0$, where the right-hand side becomes

$$\begin{aligned} \frac{M_f}{\mu} &= \exp \left\{ \frac{1}{\varepsilon} \log \left[\frac{2}{D} \left(1 + \frac{1}{b_\varepsilon g(\mu, \varepsilon)} \right) \right] \right\} \\ &= \exp \left\{ \frac{1}{\varepsilon} \log \left[\left(1 - \frac{\varepsilon}{2} \right) \left(1 + \frac{1}{b_\varepsilon g(\mu, \varepsilon)} \right) \right] \right\} \\ &\approx \exp \left\{ \frac{1}{\varepsilon} \left(-\frac{\varepsilon}{2} + \frac{1}{b_\varepsilon g(\mu, \varepsilon)} - \frac{\varepsilon}{b_\varepsilon g(\mu, \varepsilon)} \right) \right\} \\ &\xrightarrow{\varepsilon \rightarrow 0} \exp \left\{ -\left(\frac{1}{2} + \frac{\pi}{g(\mu)} \right) \right\}, \end{aligned} \quad (20.10)$$

where we have used the abbreviation

$$g(\mu) \equiv g(\mu, 0). \quad (20.11)$$

This equation shows very clearly how the renormalization process leads to an over-parametrization of the theory by the parameter μ . The physical mass M_f is fixed, and the equation specifies in which way the renormalized coupling $g(\mu)$ depends on μ to guarantee a certain mass M_f (see Fig. 20.1 for an illustration). Such a relation between μ and $g(\mu)$ is typical for a large variety of theories, as we shall see in the sequel.

In general, the μ -dependence of the renormalized observables is governed by a partial differential equation called the *Callan-Symanzik equation*. This equation allows to find curves in the two-parameter space of renormalized coupling and mass parameters g and m , along which a field theory has identical observables. They are called *renormalization group trajectories*, and the movement along them, if μ is changed, is referred to as a *renormalization flow*.

Since the theory is renormalizable, the relations between observable quantities must all be finite. The model potential (20.2) illustrates this fact. Inverting relation (20.7), we express the bare coupling constant g_0 in terms of the fermion mass M_f . After inserting the result into (20.2), we obtain

$$\frac{1}{N} v(\Sigma) = \frac{M_f^\varepsilon}{2} \Sigma^2 \left[\frac{D}{2} - b_\varepsilon \left(\frac{\Sigma}{M_f} \right)^\varepsilon \right]. \quad (20.12)$$

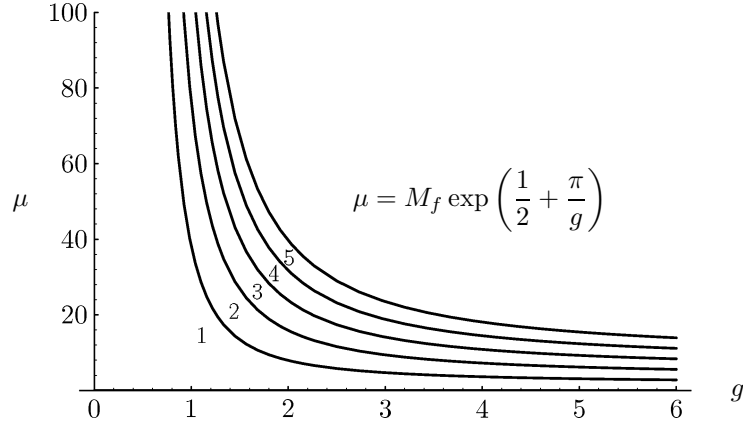


FIGURE 20.1 Curves in the (μ, g) -plane corresponding to the same physical fermion mass $M_f = 1, \dots, 5$, and thus to identical physical observables. These curves are the renormalization group trajectories of the $O(N)$ -symmetric four-fermion model in the limit $N \rightarrow \infty$.

This is a finite relation for all values of ε , in particular for $\varepsilon \rightarrow 0$, where it has the limit

$$\frac{1}{N}v(\Sigma) = \frac{\Sigma^2}{2\pi} \left[\log \left(\frac{\Sigma}{M_f} \right) - \frac{1}{2} \right]. \quad (20.13)$$

Note that, by expressing $v(\Sigma)$ in terms of the physical observable M_f rather than the finite quantity $g(\mu)$, we have arrived at an expression which is finite *and* independent of μ . This $v(\Sigma)$ will be called a *renormalization group invariant* version of the effective potential.

We shall see that an understanding of the renormalization group will permit us to find an economic way of expressing all renormalized quantities in such a μ -independent way. Mathematically speaking, the determination of physical observables, which do not depend on the renormalization scheme, will amount to a search for invariants under the renormalization group.

To develop the general theory we shall focus our attention again on the ϕ^4 -theory in $D = 4 - \varepsilon$ dimensions, renormalized via an ε -expansion.

20.2 Renormalization Scheme

In Chapter 11 we have learned how to obtain order by order in perturbation theory, all finite vertex functions $\Gamma^{(n)}(p, g, m, \mu)$ of the ϕ^4 -theory in four spacetime dimensions. Besides the physical parameters g and m , it was convenient to carry along an auxiliary mass parameter μ . The finiteness of the Feynman graphs was achieved by adding to the renormalized Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 - \frac{g\mu^\varepsilon}{4!}\phi^4 \quad (20.14)$$

a corresponding set of counterterms which are divergent in the limit $\varepsilon \rightarrow 0$

$$\mathcal{L}_c = \frac{1}{2}c^\phi(\partial\phi)^2 - \frac{m^2}{2}c^m\phi^2 - \frac{g\mu^\varepsilon}{4!}c^g\phi^4. \quad (20.15)$$

We have replaced the original renormalized coupling constant g by $g\mu^\varepsilon$, where g is now dimensionless. As we have seen before in Chapter 11, this has the advantage of turning all counterterms into functions of the new dimensionless renormalized coupling constant g [recall (11.264)]. The counterterms were calculated at every order in perturbation theory from the primitively divergent diagrams in the limit $\varepsilon \rightarrow 0$. Renormalizability of the theory implies that no other divergent counterterms are necessary than those which can be written in the same form as the original Lagrangian in Eq. (20.15). Then all divergencies can be absorbed in a multiplicative redefinition of field, mass, and coupling constant. The total Lagrangian $\mathcal{L} + \mathcal{L}_c$ is

$$\mathcal{L}_0 = \mathcal{L} + \mathcal{L}_c = \frac{1}{2}(\partial\phi_0)^2 - \frac{m_0^2}{2}\phi_0^2 - \frac{g_0}{4!}\phi_0^4, \quad (20.16)$$

and this may be identified with the initial bare Lagrangian, in which the bare field, mass, and coupling constant are related to the finite renormalized ones by

$$\begin{aligned} \phi_0 &\equiv Z_\phi^{1/2}\phi, \\ m_0^2 Z_\phi &\equiv m^2 \bar{Z}_{m^2}, \\ g_0 Z_\phi^2 &\equiv g\mu^\varepsilon \bar{Z}_g, \end{aligned} \quad (20.17)$$

with the renormalization constants

$$\begin{aligned} Z_\phi &\equiv 1 + c^\phi(g, \varepsilon), \\ \bar{Z}_{m^2} &\equiv 1 + c^m(g, \varepsilon), \\ \bar{Z}_g &\equiv 1 + c^g(g, \varepsilon). \end{aligned} \quad (20.18)$$

The bare Green functions

$$G_0^{(n)}(x_1, \dots, x_n; g_0, m_0, \varepsilon) = \langle 0 | T \phi_0(x_1) \dots \phi_0(x_n) | 0 \rangle, \quad (20.19)$$

when calculated in $4 - \varepsilon$ dimensions, are finite objects as long as $\varepsilon \neq 0$. When multiplied by the renormalization constants $Z_\phi^{n/2}$, they turn into the renormalized Green functions which remain finite in the limit $\varepsilon \rightarrow 0$:

$$G^{(n)}(x_1, \dots, x_n; g, m, \mu) \equiv Z_\phi^{n/2}(g, \varepsilon) G_0^{(n)}(x_1, \dots, x_n; g_0, m_0, \varepsilon). \quad (20.20)$$

Correspondingly, the bare vertex functions

$$\begin{aligned} \Gamma_0^{(n)}(x_1, \dots, x_n; g_0, m_0, \mu) &\equiv -i \int dx'_1 \dots dx'_n \\ &\times G_0^{-1}(x_1, x'_1; g_0, m_0, \varepsilon) \dots G_0^{-1}(x_n, x'_n; g_0, m_0, \varepsilon) G_0^{(n)}(x'_1, \dots, x'_n; g_0, m_0, \varepsilon) \end{aligned} \quad (20.21)$$

become finite after being renormalized by the inverse factors $Z_\phi^{-n/2}(g, \varepsilon)$ of (20.20):

$$\Gamma^{(n)}(x_1, \dots, x_n; g, m, \mu) = Z_\phi^{-n/2} \Gamma_0^{(n)}(x_1, \dots, x_n; g_0, m_0, \varepsilon). \quad (20.22)$$

As discussed in Chapter 11, there are different possible methods of fixing the counterterms. The most common choice is based on the normalization conditions

$$\frac{\partial}{\partial p^2} \Gamma^{(2)}|_{p^2=-\mu^2} = 1, \quad (20.23)$$

$$\Gamma^{(2)}|_{p^2=-\mu^2} = m^2, \quad (20.24)$$

$$\Gamma^{(4)}|_{\text{symm point}} = \mu^\varepsilon, \quad (20.25)$$

where the symmetry point is defined by

$$p_i p_j = -\frac{\mu^2}{4}(4\delta_{ij} - 1); \quad i, j = 1, \dots, 4. \quad (20.26)$$

The *minimal subtraction scheme* due to 't Hooft requires, instead, the cancellation of all $1/\varepsilon, 1/\varepsilon^2, 1/\varepsilon^3, \dots$ -pole terms in the vertex functions. This has the pleasant property that the resulting counterterms depend only on the coupling constants and not on the mass m .

In both schemes, the arbitrary mass parameter μ can be avoided by setting it equal to m when the fields are massive. It is unavoidable, however, if the theory contains no mass term.

20.3 The Renormalization Group Equation

As discussed above, physical observables should be independent on the choice of μ , and this fundamental property will now be formulated quantitatively. Suppose we calculate perturbatively the bare n -point vertex function at a fixed bare coupling g_0 and mass m_0 with the bare vertices in $4 - \varepsilon$ dimensions:

$$\Gamma_0^{(n)}(p_1, \dots, p_n; g_0, m_0, \varepsilon). \quad (20.27)$$

The result is trivially independent of the choice of the mass parameter μ which was introduced only to define the finite renormalized coupling strength $g = g(\mu)$ and mass $m = m(\mu)$. We therefore have the obvious relation

$$\mu \frac{\partial}{\partial \mu} \Gamma_0^{(n)}(p_1, \dots, p_n; g_0, m_0, \varepsilon) = 0. \quad (20.28)$$

This obvious relation turns into a nontrivial one for the renormalized vertex functions

$$\Gamma^{(n)}(p_1, \dots, p_n; g, m, \mu) \equiv Z_\phi^{-n/2}(g_0, m_0, \varepsilon) \Gamma_0^{(n)}(p_1, \dots, p_n; g_0, m_0, \varepsilon). \quad (20.29)$$

If the bare parameters g_0, m_0, ε are kept fixed, the μ dependence in $\Gamma^{(n)}$ can come from the renormalized quantities g and m whose values depend on the choice of μ ,

which is emphasized by writing them as $g(\mu)$ and $m(\mu)$. By applying (20.28) to (20.29), we see, from the chain rule of differentiation, that

$$\begin{aligned} & \left(\mu \partial_\mu + \mu \partial_\mu g|_{g_0, m_0, \varepsilon} - n \mu \partial_\mu \log Z_\phi^{1/2}|_{g_0, m_0, \varepsilon} + \mu \partial_\mu \log m^2|_{g_0, m_0, \varepsilon} m^2 \partial_{m^2} \right) \\ & \quad \times \Gamma^{(n)}(p_1, \dots, p_n; g, m, \mu) = 0, \end{aligned} \quad (20.30)$$

where we have written ∂_μ for $\partial/\partial\mu$, to save space. The coefficient functions of this differential equation can be expressed as finite functions of g, m , and μ . One defines

$$\beta = \mu \partial_\mu g|_{g_0, m_0, \varepsilon}, \quad (20.31)$$

$$\gamma = \mu \partial_\mu \log Z_\phi^{1/2}|_{g_0, m_0, \varepsilon}, \quad (20.32)$$

$$\gamma_m = \mu \partial_\mu \log m^2|_{g_0, m_0, \varepsilon}, \quad (20.33)$$

and reexpresses these as functions of g, m , and μ . With these, Eq.(20.30) takes the following form:

$$(\mu \partial_\mu + \beta \partial_g - n \gamma + \gamma_m m^2 \partial_{m^2}) \Gamma^{(n)}(p_1, \dots, p_n; g, m, \mu) = 0. \quad (20.34)$$

This is the celebrated *renormalization group equation* (RGE). If we did not use the minimal subtraction scheme but some cutoff Λ in momentum space, then the parameter ε in Eqs.(20.27)–(20.33) would be replaced by the cutoff Λ . The RGE is the quantitative formulation of the change of the vertex functions $\Gamma^{(n)}(p_1, \dots, p_n; g, m, \mu)$ under a change of the auxiliary mass scale μ in the μ -dependent renormalized quantities $g = g(\mu)$ and $m = m(\mu)$.

20.4 Calculation of Coefficient Functions from Counter Terms

The solution of a partial differential equation like (20.34) is, in general, awkward, since β, γ, γ_m may depend on g, m and μ . It is an important special property of 't Hooft's renormalization scheme, that the counterterms c^g , c^{m^2} , and c^ϕ happen to be independent of the masses m . At fixed $\varepsilon = 4 - D$, they depend only on the coupling constant g . This makes their calculation simple and, moreover, produces coefficient functions β, γ, γ_m in the RGE (20.34) which depend only on g and ε . Suppressing the ε -argument, we shall therefore write $\beta(g), \gamma(g), \gamma_m(g)$.

Consider first $\gamma(g)$. Since Z_ϕ depends only on g we certainly have

$$\gamma(g) = \mu \partial_\mu g|_{g_0, m_0, \varepsilon} \cdot \frac{d}{dg} \log Z_\phi^{1/2}(g).$$

With the help of (20.31), this can be rewritten as

$$\gamma(g) = \beta(g) \frac{d}{dg} \log Z_\phi^{1/2}(g). \quad (20.35)$$

Similarly, using the renormalization equation $m^{-2} = m_0^{-2} \bar{Z}_m(g) Z_\phi^{-1}(g)$, we see that

$$\gamma_m(g) = -\beta(g) \left(\frac{d}{dg} \log \bar{Z}_m - \frac{d}{dg} \log Z_\phi \right) \quad (20.36)$$

or

$$\gamma_m(g) - 2\gamma(g) \equiv \bar{\gamma}_m(g) = -\beta(g) \frac{d}{dg} \log \bar{Z}_m(g). \quad (20.37)$$

Finally, we use

$$g_0 = g \mu^\varepsilon \bar{Z}_g(g) Z_\phi^{-2}(g) \quad (20.38)$$

to find

$$\begin{aligned} \beta(g) &= \frac{-\mu \partial_\mu g_0|_g}{\partial_g g_0|_\mu} = -\varepsilon \left[\frac{d}{dg} \log(g \bar{Z}_g Z_\phi^{-2}) \right]^{-1} \\ &= -\frac{\varepsilon g}{1 + g[\log(g \bar{Z}_g)]' - 2g[\log(\bar{Z}_\phi)]'}, \end{aligned} \quad (20.39)$$

or, using (20.35),

$$\beta(g) = \frac{-\varepsilon + 4\gamma(g)}{\log[g \bar{Z}_g(g)]'}. \quad (20.40)$$

All three functions depend only on g .

The formulas can be brought to a more practical shape by making use of the explicit $1/\varepsilon$ -expansion structure of the counterterms as functions of g . Then we may rewrite Eqs. (20.35), (20.37), (20.40) as follows:

$$\gamma(g) \left(1 + \sum_{\nu=1}^{\infty} c_\nu^\phi(g) \varepsilon^{-\nu} \right) = \frac{1}{2} \beta(g) \sum_{\nu=1}^{\infty} c_\nu^\phi(g)' \varepsilon^{-\nu}, \quad (20.41)$$

$$[-\gamma_m(g) + 2\gamma(g)] \left(1 + \sum_{\nu=1}^{\infty} c_\nu^m(g) \varepsilon^{-\nu} \right) = \beta(g) \sum_{\nu=1}^{\infty} c_\nu^m(g)' \varepsilon^{-\nu}, \quad (20.42)$$

$$\beta(g) \left(\sum_{\nu=1}^{\infty} [g c_\nu^g(g)]' \varepsilon^{-\nu} \right) = [-\varepsilon + 4\gamma(g)] g \left(1 + \sum_{\nu=1}^{\infty} c_\nu^g(g) \varepsilon^{-\nu} \right). \quad (20.43)$$

For a renormalizable theory, the functions $\beta(g)$, $\gamma(g)$, $\gamma_m(g)$ have to remain finite in the limit $\varepsilon \rightarrow 0$. Thus we can expand these quantities in a power series of ε with powers $\varepsilon^0, \varepsilon^1, \varepsilon^2, \dots$. By inserting (20.41) into (20.43) we see that $\beta(g)$ can at most contain the following powers of ε :

$$\beta(g) = \beta_0(g) + \varepsilon \beta_1(g). \quad (20.44)$$

When inserting this into (20.41), (20.42), we find $\gamma(g)$ and $\gamma_m(g)$ to be independent of ε . Equating the regular parts of the three equations yields

$$\begin{aligned}\beta_0 + \varepsilon\beta_1 + \beta_1(c_1^g + gc_1^{g'}) &= (-\varepsilon + 4\gamma)g - gc_1^g, \\ \gamma &= \frac{1}{2}\beta_1 c_1^{\phi'}, \\ \bar{\gamma}_m &\equiv \gamma_m - 2\gamma = -\beta_1 c_1^{m'}.\end{aligned}\quad (20.45)$$

These are satisfied if

$$\begin{aligned}\beta_1(g) &= -g, \\ \beta_0(g) &= g^2 c_1^g(g)' + 4\gamma g.\end{aligned}\quad (20.46)$$

Thus, amazingly, the three functions $\beta(g)$, $\gamma(g)$, and $\gamma_m(g)$ can be expressed in terms of g -derivatives of the three residues $c_1^g(g)$, $c_1^\phi(g)$, and $c_1^m(g)$ of the simple $1/\varepsilon$ -poles in the counterterms:

$$\begin{aligned}\beta(g) &= -\varepsilon g + g^2 c_1^g(g)' + 4\gamma g, \\ \gamma(g) &= -\frac{g}{2} c_1^\phi(g)', \\ \bar{\gamma}_m(g) &= \gamma_m(g) - 2\gamma(g) = g c_1^m(g)'. \end{aligned}\quad (20.47)$$

The finiteness of $\beta(g)$, $\gamma(g)$, $\gamma_m(g)$ at $\varepsilon = 0$ forces all higher residues in Eqs. (20.41)–(20.43) to disappear. This implies an infinite set of consistency relations among the expansion coefficients which are useful for checking the final results:

$$\beta_0(gc_\nu^g)' - g(gc_{\nu+1}^g)' = 4\gamma gc_\nu^g g - c_{\nu+1}^g, \quad (20.48)$$

$$\gamma c_\nu^\phi = \beta_0 c_\nu^{\phi'} - g c_{\nu+1}^{\phi'}, \quad (20.49)$$

$$(\gamma_m - 2\gamma)c_\nu^m = -\beta_0 c_\nu^{m'} + g c_{\nu+1}^{m'}. \quad (20.50)$$

Let us now turn to the actual calculation of $\beta(g)$, $\gamma(g)$, $\gamma_m(g)$ in the $O(N)$ -symmetric ϕ^4 -theory. The renormalization constants were given in Section 11.8. Replacing gS_D by g , for brevity (so that it becomes equal to our former λ), we obtain [recall Eqs. (11.258)]

$$\begin{aligned}\bar{Z}_g &= 1 + c^g = 1 + g\frac{3}{2}T_I\frac{1}{\varepsilon} + g^2\left\{\frac{15}{4}T_{I^2}\frac{1}{\varepsilon^2} - 3T_{I_4}\left(\frac{1}{2\varepsilon^2} + \frac{1}{4\varepsilon}\right)\right\}, \\ Z_\phi &= 1 + c^\phi = 1 - g^2\frac{1}{48}T_{D_3}\frac{1}{\varepsilon}, \\ \bar{Z}_m &= 1 + c^m = 1 + g\frac{1}{2}T_{D_1}\frac{1}{\varepsilon} + \frac{g^2}{4}\left\{3T_{D_1D_2}\frac{1}{\varepsilon^2} - T_{D_3}\left(\frac{1}{\varepsilon^2} + \frac{1}{2\varepsilon}\right)\right\}.\end{aligned}\quad (20.51)$$

The $1/\varepsilon$ -pole terms are

$$\begin{aligned}c_1^g &= g\frac{3}{2}T_I - g^2\frac{3}{4}T_{I_4}, \\ c_1^\phi &= -g^2\frac{1}{48}T_{D_3}, \\ c_1^{m^2} &= g\frac{1}{2}T_{D_1} - g^2\frac{1}{8}T_{D_3}.\end{aligned}\quad (20.52)$$

Inserting these into (20.47), we find

$$\begin{aligned}\beta(g) - 4\gamma(g)g &= -\varepsilon g + \frac{3}{2}g^2T_I - \frac{3}{2}g^3T_{I_4}, \\ \gamma(g) &= g^2\frac{1}{48}T_{D_3}, \\ \gamma_m(g) - 2\gamma(g) &= \frac{g}{2}T_{D_1} - \frac{g^2}{4}T_{D_3}.\end{aligned}\tag{20.53}$$

The reduced matrix elements $T_I, \dots, T_{I_4}$ were given in (11.243)–(11.253). For $N = 1$, all T 's are equal to unity.

Explicitly, we can solve (20.53) for $\beta(g), \gamma(g), \gamma_m(g)$ with the functions

$$\begin{aligned}\beta(g) &= -\varepsilon g + g^2\frac{3}{2}T_I - g^3\left(\frac{3}{2}T_{I_4} - \frac{1}{12}T_{D_3}\right) \\ &= -\varepsilon g + \frac{N+8}{6}g^2 - \frac{3N+14}{12}g^3,\end{aligned}\tag{20.54}$$

$$\gamma(g) = g^2\frac{1}{48}T_{D_3} = g^2\frac{1}{48}\frac{N+2}{3},\tag{20.55}$$

$$\gamma_m(g) = g\frac{1}{2}T_{D_1} - g^2\frac{5}{24}T_{D_3} = \left(g\frac{1}{2} - g^2\frac{5}{24}\right)\frac{N+2}{3}.\tag{20.56}$$

With the help of Eqs. (20.48)–(20.50) we check these results for consistency, up to terms of the order of g^2 .

It is instructive to observe the cancellation of $1/\varepsilon^n$ -singularities in Eqs. (20.35)–(20.40) somewhat more explicitly. Take for instance $\gamma(g)$ of Eq. (20.35), and the five-loop result for the β -function to be stated in (20.189) for $N = 1$:

$$\begin{aligned}\beta(g) &= -\varepsilon g + \frac{3}{2}g^2 - \frac{17}{12}g^3 + \left[\frac{145}{64} + \frac{3\zeta(3)}{2}\right]g^4 \\ &+ \left[-\frac{3499}{768} + \frac{\pi^4}{80} - \frac{39\zeta(3)}{8} - \frac{15\zeta(5)}{2}\right]g^5 + \\ &+ \left[\frac{764621}{73728} - \frac{1189\pi^4}{23040} - \frac{5\pi^6}{448} + \frac{7965\zeta(3)}{512} + \frac{45\zeta(3)^2}{32} + \frac{987\zeta(5)}{32} + \frac{1323\zeta(7)}{32}\right]g^6.\end{aligned}\tag{20.57}$$

The logarithmic derivative of the renormalization constant has the five-loop expansion:

$$\begin{aligned}[\log Z_\phi(g)]' &= -\frac{1}{24\varepsilon}g - \left(\frac{1}{16\varepsilon^2} - \frac{1}{64\varepsilon}\right)g^2 + \left(-\frac{3}{32\varepsilon^3} + \frac{95}{1152\varepsilon^2} - \frac{65}{1536\varepsilon}\right)g^3 \\ &+ \left[-\frac{9}{64\varepsilon^4} + \frac{163}{768\varepsilon^3} - \frac{553}{3072\varepsilon^2} + \frac{3709}{36864\varepsilon} + \frac{\pi^4}{2880\varepsilon} - \frac{\zeta(3)}{16\varepsilon^2} - 3\frac{\zeta(3)}{256\varepsilon}\right]g^4 \\ &+ \left[-\frac{13}{3072\varepsilon^4} + \frac{179}{55296\varepsilon^3} - \frac{23}{16384\varepsilon^2}\right]g^5.\end{aligned}\tag{20.58}$$

When forming the product $\beta(g) \cdot [\log Z_\phi(g)]'$ to get $\gamma(g)$ via (20.35), the only ε -term in $\beta(g)$ reduces the highest $1/\varepsilon^n$ singularities in the g^n -term of $[\log Z_\phi(g)]'$ by one

power of $1/\varepsilon$. For $n \geq 2$ the resulting terms are still singular, but they are canceled by the product of the finite g^2 -term in $\beta(g)$ and the singular terms associated with the lower power g^{n-1} in $[\log Z_\phi(g)]'$, and so on.

20.5 Solution of Renormalization Group Equations for Vertex Functions

The subtraction of divergencies via the ε -expansion rendered coefficient functions β, γ, γ_m which depend only on the renormalized coupling constant $g(\mu)$. This makes it easy to solve the renormalization group equation (20.34). Suppose we have calculated the renormalized vertex functions for some initial mass scale μ with a renormalized coupling $g = g(\mu)$ and mass $m = m(\mu)$. Then the coupling $g(\mu') = g(\sigma\mu)$ at an arbitrary mass scale $\mu' = \sigma\mu$, which we shall denote for brevity by $\equiv g_\sigma$, is given by

$$\sigma \frac{d}{d\sigma} g_\sigma = \beta(g_\sigma). \quad (20.59)$$

Equation (20.59) can be rewritten as

$$\frac{d \ln \sigma}{dg_\sigma} = \frac{1}{\beta(g_\sigma)}. \quad (20.60)$$

This is solved with the initial condition

$$g_1 = g. \quad (20.61)$$

The result is

$$\ln \sigma = \int_g^{g_\sigma} \frac{dg'}{\beta(g')}. \quad (20.62)$$

Similarly we have, for the μ -dependence of the renormalized mass $m(\mu)$, the equation

$$m^{-2}(\mu) \mu \frac{d}{d\mu} m^2(\mu) = \gamma_m(g_\sigma), \quad (20.63)$$

which can be rewritten with the notation $m_\sigma \equiv m(\sigma\mu) = m(\mu')$ as

$$\frac{d \ln m_\sigma^2}{d \ln \sigma} = \gamma_m(g_\sigma). \quad (20.64)$$

This is solved with the initial condition

$$m_1 = m \quad (20.65)$$

by

$$\ln \frac{m_\sigma^2}{m^2} = \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma_m(g_{\sigma'}). \quad (20.66)$$

Using the functions g_σ and m_σ , the renormalization group equation for the vertex functions, which is initially a partial differential equation, can be rephrased as an ordinary differential equation:

$$\left[\sigma \frac{d}{d\sigma} - n\gamma(g_\sigma) \right] \Gamma^{(n)}(p_i; g_\sigma, m_\sigma, \sigma\mu) = 0. \quad (20.67)$$

For brevity, we have written p_i collectively for $p_1, \dots, p_n$. Equation (20.67) is immediately integrated as follows

$$\Gamma^{(n)}(p_i; g_\sigma, m_\sigma, \sigma\mu) = \exp \left[n \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'}) \right] \Gamma^{(n)}(p_i; g, m, \mu), \quad (20.68)$$

which shows the full σ -dependence of the renormalized vertex functions.

This equation can now be used to study the critical behavior of $\Gamma^{(n)}(p_i; g, m, \mu)$, i.e., the behavior of $\Gamma^{(n)}$ as the renormalized mass m goes to zero at a fixed mass scale μ . For this purpose it is useful to take advantage of the dimensional structure of the vertex functions. In D dimensions, a field has a (mass) dimension $d_\phi = D/2 - 1$. A Green function containing n fields has the dimension $d_\phi = n(D/2 - 1)$. When performing $n - 1$ Fourier transforms of the fields to momentum space by spatial integrals $\int d^D x e^{ipx}$, the dimension becomes $nd_\phi - (n - 1)D$. The Fourier transformed two-point function $G^{(2)}(p)$ has the dimension -2 for all D . The vertex function $\Gamma^{(n)}$ is obtained by multiplying the Fourier transformed Green function $G^{(n)}$ by n factors $G^{(2)}(p)^{-1}$. The total mass dimension of $\Gamma^{(n)}$ is therefore $D - nd_\phi = D - n(D/2 - 1)$. Then, since the dimensions of p_i , g , m , μ are 1, 0, 1, 1, respectively, the vertex function $\Gamma^{(n)}$ must satisfy the trivial identity valid for any scale parameter σ ,

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma^{D - \frac{n}{2}(D-2)} \Gamma^{(n)}(p_i/\sigma; g, m/\sigma, \mu/\sigma). \quad (20.69)$$

Inserting on the right-hand side the left-hand side of (20.68), we obtain

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma^{D - n(D/2 - 1)} \exp \left[-n \int_1^\sigma d\sigma' \frac{\gamma(g_{\sigma'})}{\sigma'} \right] \Gamma^{(n)}(p_i/\sigma, g_\sigma, m_\sigma/\sigma, \mu). \quad (20.70)$$

We now choose $\sigma = \sigma_m$ so that the rescaled mass m_σ/σ is equal to the mass parameter μ :

$$m_\sigma/\sigma|_{\sigma=\sigma_m} = \mu. \quad (20.71)$$

Then (20.70) becomes

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma_m^{D - n(D/2 - 1)} \exp \left[-n \int_1^{\sigma_m} d\sigma' \frac{\gamma(g_{\sigma'})}{\sigma'} \right] \Gamma^{(n)}(p_i/\sigma_m, g_{\sigma_m}, \mu, \mu). \quad (20.72)$$

This equation relates the renormalized vertex functions $\Gamma^{(n)}(p_i, g, m, \mu)$ of an arbitrary mass to those of a fixed mass equal to the mass parameter μ at rescaled

momenta p_i/σ and a running coupling constant g_σ . Apart from a trivial overall rescaling factor $\sigma_m^{D-n(D/2-1)}$ due to the naive dimension, there is also a nontrivial exponential function.

Explicitly, the parameter σ_m in (20.71) is found by using Eq. (20.66) to calculate the ratio

$$\begin{aligned} \frac{m^2}{\mu^2} &= \frac{m_\sigma^2}{\mu^2} \exp \left\{ \int_0^{\sigma_m} \frac{d\sigma'}{\sigma'} [-\gamma_m(g_{\sigma'})] \right\} \\ &= \frac{m_\sigma^2}{\sigma^2 \mu^2} \exp \left\{ \int_0^{\sigma_m} \frac{d\sigma'}{\sigma'} [2 - \gamma_m(g_{\sigma'})] \right\} \\ &= \exp \left\{ \int_0^{\sigma_m} \frac{d\sigma'}{\sigma'} [2 - \gamma_m(g_{\sigma'})] \right\}. \end{aligned} \quad (20.73)$$

Our goal is to study the behavior of the vertex functions on the left-hand side of (20.72) in the critical region where $m \rightarrow 0$. On the right-hand side, the mass dependence resides in the rescaling parameter σ_m .

In many-body systems undergoing a second-order phase transition, the mass m approaches zero proportional to $T - T_c$. Equation (20.73) specifies how the auxiliary scale parameter σ_m , which rules the scaling relation (20.72), behaves for $T \rightarrow T_c$.

Near the critical point $T = T_c$, experimental correlation functions show a simple scaling behavior. Such a behavior can be found from Eqs. (20.72) and (20.73) if, in the limit $m \rightarrow 0$, the coupling constant g runs into a *fixed point* g^* , which is the constant limiting value of g_σ where it becomes independent of σ :

$$\left[\frac{dg_\sigma}{d\sigma} \right]_{g=g^*} = 0. \quad (20.74)$$

Assuming that $\gamma_m^* \equiv \gamma_m(g^*) < 2$, which is true in the present field theory, the integrand in Eq. (20.73) is singular at $\sigma = 0$, and the asymptotic behavior of σ_m for $m \rightarrow 0$ can immediately be found:

$$\frac{m^2}{\mu^2} \stackrel{m \rightarrow 0}{\approx} \exp \left\{ \int_0^{\sigma_m} \frac{d\sigma'}{\sigma'} [2 - \gamma_m(g^*)] \right\} = \sigma_m^{2-\gamma_m^*}. \quad (20.75)$$

We see that σ_m goes to zero for $m \rightarrow 0$ with the power law

$$\sigma_m \approx \left(\frac{m^2}{\mu^2} \right)^{1/(2-\gamma_m^*)}. \quad (20.76)$$

In applications to second-order phase transitions we shall identify m^2/μ^2 with the relative distance from the critical temperature

$$\frac{m^2}{\mu^2} \equiv \tau \equiv \frac{T - T_c}{T_c}, \quad (20.77)$$

and write (20.76) as

$$\sigma_m \approx \tau^{1/(2-\gamma_m^*)}. \quad (20.78)$$

In this limit, the exponential prefactor in (20.72) has the power behavior

$$\exp \left[-n \int_1^{\sigma_m} \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'}) \right] \stackrel{\sigma_m \approx 0}{\approx} \tau^{n\gamma^*/(2-\gamma_m^*)}, \quad (20.79)$$

where $\gamma^* \equiv \gamma(g^*)$. The n -point vertex function behaves therefore like

$$\Gamma^{(n)}(p_i; g, m, \mu) \stackrel{m \approx 0}{\approx} \sigma_m^{D-n(D/2-1)-n\gamma^*} \Gamma^{(n)}(p_i/\sigma_m; g^*, \mu, \mu). \quad (20.80)$$

For the two-point vertex function this implies a momentum dependence

$$\Gamma(p; g, m, \mu) \stackrel{m \approx 0}{\approx} p^{2-2\gamma^*} \tilde{f}(p/\sigma_m), \quad (20.81)$$

with some function $\tilde{f}(\kappa)$. When going over to the two-point function in x -space

$$G(\mathbf{x}; g, m, \mu) = \int \frac{d^D p}{(2\pi)^D} e^{i\mathbf{p}\mathbf{x}} \frac{1}{\Gamma(p; g, m, \mu)}, \quad (20.82)$$

this amounts to an x -dependence

$$G(\mathbf{x}; g, m, \mu) \stackrel{m \approx 0}{\approx} \frac{1}{r^{D-2+2\gamma^*}} \tilde{g}(\mathbf{x}/\sigma_m) = \frac{1}{r^{D-2+2\gamma^*}} \tilde{g}(\mathbf{x}(m^2/\mu^2)^{1/(2-\gamma_m^*)}). \quad (20.83)$$

This is of a general form discovered by Kadanoff for connected correlation functions:

$$G_c^{(2)}(r) = \frac{f(r/t^{-\nu})}{r^{D-2+\eta}}. \quad (20.84)$$

With the identification (20.77), we see that the critical exponent ν in (20.84) is given by

$$\nu = \frac{1}{2 - \gamma_m^*}. \quad (20.85)$$

For $T \rightarrow T_c$, the length scale $\xi(t)$ diverges like

$$\xi(t) = \xi_0 |t|^{-\nu}. \quad (20.86)$$

By comparing the power behavior at the critical point in (20.83) with that in (20.84), we identify the critical exponent η as

$$\eta = 2\gamma^* : \quad (20.87)$$

20.6 Renormalization Group for Effective Action and Effective Potential

The same methods can be applied to find the one parameter set of identical theories for the full effective action $\Gamma[\Phi]$ for different values of the mass parameter μ . Consider the power series expansion of the effective action in terms of vertex functions

$$\Gamma[\Phi; g, m, \mu] = \sum_{n=0}^{\infty} \frac{1}{n!} \int \frac{d^D p_1}{(2\pi)^D} \cdots \frac{d^D p_n}{(2\pi)^D} \Phi(p_1) \cdots \Phi(p_n) \Gamma^{(n)}(p_1, \dots, p_n; g, m, \mu) \quad (20.88)$$

and apply the RGE (20.34) to every coefficient. This effectively replaces the factor n in front of $\gamma(g)$ as follows

$$n \rightarrow \int \frac{d^D p}{(2\pi)^D} \Phi(p) \frac{\delta}{\delta \Phi(p)}. \quad (20.89)$$

Hence we find immediately the RGE

$$\left[\mu \partial_\mu + \beta(g) \partial_g - \gamma(g) \int \frac{d^D p}{(2\pi)^D} \Phi(p) \frac{\delta}{\delta \Phi(p)} + \gamma_m(g) m^2 \partial_m \right] \Gamma[\Phi; g, m, \mu] = 0. \quad (20.90)$$

A corresponding result holds for the effective potential

$$v(\Phi) = -L^{-D} \Gamma[\Phi; g, m, \mu] |_{\Phi(x)=\text{const}=\Phi}, \quad (20.91)$$

where L is the size of the D -dimensional box under consideration. The effective potential satisfies the differential equation

$$\left[\mu \partial_\mu + \beta(g) \partial_g - \gamma(g) \Phi \frac{\partial}{\partial \Phi} + \gamma_m(g) m^2 \partial_m \right] v(\Phi; g, m, \mu) = 0. \quad (20.92)$$

Because of its relevance to physical applications we shall first solve only this latter equation along the lines of Eqs.(20.62)–(20.67). We introduce an additional running field strength Φ_σ satisfying the differential equation

$$\frac{1}{\Phi_\sigma} \sigma \frac{d}{d\sigma} \Phi_\sigma = -\gamma(g(\sigma)), \quad (20.93)$$

with the initial condition

$$\Phi_1 = \Phi. \quad (20.94)$$

This is solved by

$$\frac{\Phi_\sigma}{\Phi} = \exp \left[- \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g'_\sigma) \right]. \quad (20.95)$$

Using Φ_σ , we have the following identity along the renormalization trajectory

$$v(\Phi_\sigma; g_\sigma, m_\sigma, \sigma\mu) \equiv v(\Phi; g, m, \mu). \quad (20.96)$$

Note that there is no prefactor here, in contrast to (20.72). All m -dependence is contained in m_σ and $\Phi(\sigma)$ via (20.95). In the limit $\sigma \rightarrow 0$, the field behaves like

$$\frac{\Phi_\sigma}{\Phi} \approx \sigma^{-\gamma^*}. \quad (20.97)$$

Since $\Gamma[\Phi]$ is dimensionless and $v(\Phi)$ is related to $\Gamma[\Phi]$ by (20.91), the dimensional transformation corresponding to (20.69) becomes simply

$$v(\Phi; g, m, \mu) = \sigma^D v(\Phi/\sigma^{D/2-1}; g, m/\sigma, \mu/\sigma) \quad (20.98)$$

Combining this with (20.96), we find

$$v(\Phi; g, m, \mu) = \sigma^D v(\Phi_\sigma / \sigma^{D/2-1}, g, m_\sigma / \sigma, \mu). \quad (20.99)$$

At the mass-dependent value σ_m of Eq. (20.71), we obtain the analog of (20.72) for the effective potential

$$v(\Phi; g, m, \mu) = \sigma_m^D v(\Phi_{\sigma_m} / \sigma_m^{D/2-1}; g_{\sigma_m}, \mu, \mu). \quad (20.100)$$

In the critical regime, where $\sigma \rightarrow 0$, Eq. (20.95) becomes

$$\frac{\Phi_{\sigma_m}}{\Phi} \approx \sigma_m^{-\gamma^*}, \quad (20.101)$$

and the effective potential has the power behavior

$$v(\Phi; g, m, \mu) \stackrel{m \approx 0}{\approx} \sigma_m^D v(\Phi / \sigma_m^{\gamma^* + D/2-1}; g^*, \mu, \mu). \quad (20.102)$$

For applications to systems below T_c it is most convenient to consider, instead of $\Gamma[\Phi; g, m, \mu]$, the vertex functions in the presence of an external magnetic field. They are obtained by expanding $\Gamma[\Phi; g, m, \mu]$ functionally around $\Phi(x) \equiv \Phi_0$:

$$\Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, m, \mu) \equiv \frac{\delta^n}{\delta \Phi(x_1) \dots \delta \Phi(x_n)} \Gamma[\Phi; g, m, \mu] \Big|_{\Phi \equiv \Phi_0}. \quad (20.103)$$

This gives

$$\Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, g, m, \mu) = \sum_{n'=0}^{\infty} \frac{\Phi_0^{n+n'}}{n'!} \Gamma^{(n+n')}(p_1, \dots, p_n, 0, \dots, 0; g, m, \mu), \quad (20.104)$$

where the zeros after $p_1, \dots, p_n$ indicate that there are n' more momenta $p_{n+1}, \dots, p_{n+n'}$ which have been set equal to zero since each constant field Φ_0 has a momentum dependence $\delta^{(D)}(p)\Phi_0$. Thus the renormalization group equation for the vertex function at a non-zero field, $\Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, \mu)$, can be obtained from those at vanishing field $\Gamma^{(n+n')}(p_1, \dots, p_n, p_{n+1}, \dots, p_{n+n'}; \mu)$, in which the last n' momenta are set equal to zero, i.e., from

$$\left[\mu \partial_\mu + \beta(g) \partial_g - (n + n') \gamma(g) + \gamma_m(g) m^2 \partial_m \right] \Gamma^{(n+n')}(p_1, \dots, p_n, 0, \dots, 0; g, m, \mu) = 0. \quad (20.105)$$

Inserting these equations into (20.104), we obtain the RGE

$$\left[\mu \partial_\mu + \beta(g) \partial_g - \gamma(g) \left(\Phi_0 \frac{\partial}{\partial \Phi_0} \right) + \gamma_m(g) m^2 \partial_m \right] \Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, g, m, \mu) = 0. \quad (20.106)$$

When treated as above, this leads to the scaling relation

$$\Gamma^{(n)}(p_i; \Phi_0, g, m, \mu) = e^{-n \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'})} \Gamma^{(n)}(p_i; \Phi_{0\sigma}, g_\sigma, m_\sigma, \mu\sigma). \quad (20.107)$$

Together with the trivial scaling relation

$$\Gamma^{(n)}(p_i; \Phi_0, g, m, \mu) = \sigma^{D-n(D/2-1)} \Gamma^{(n)}(p_i/\sigma; \Phi_0/\sigma^{D/2-1}, g, m/\sigma, \mu/\sigma), \quad (20.108)$$

we find

$$\begin{aligned} \Gamma^{(n)}(p_i; \Phi_0, g, m, \mu) &= \sigma^{D-n(D/2-1)} e^{-n \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'})} \\ &\times \Gamma^{(n)}(p_i/\sigma; \Phi_{0\sigma}/\sigma^{D/2-1}, g_\sigma, m_\sigma/\sigma, \mu), \end{aligned} \quad (20.109)$$

which becomes at $\sigma = \sigma_m$ of Eq. (20.71):

$$\begin{aligned} \Gamma^{(n)}(p_i; \Phi_0, g, m, \mu) &= \sigma_m^{D-n(D/2-1)} e^{-n \int_1^{\sigma_m} \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'})} \\ &\times \Gamma^{(n)}(p_i/\sigma_m; \Phi_{0\sigma_m}/\sigma_m^{D/2-1}, g_{\sigma_m}, \mu, \mu), \end{aligned} \quad (20.110)$$

and thus, near the critical point,

$$\Gamma^{(n)}(p_i; \Phi_0, g, m, \mu) = \sigma_m^{D-n(\gamma^*+D/2-1)} \Gamma^{(n)}(p_i/\sigma_m; \Phi_0/\sigma_m^{\gamma^*+D/2-1}, g^*, \mu, \mu). \quad (20.111)$$

20.7 Approach to Scaling

In Eq. (20.83) we have extracted Kadanoff's scaling law (20.84) from the scaling relation (20.80) for the two-point vertex function. From this we read off the critical exponents $\nu = 1/(2 - \gamma_m^*)$ for the temperature behavior of the coherence length, and the exponent $\eta = 2\gamma^*$ for the critical power behavior of the Green function.

There exists a further important critical exponent which governs the approach to the scaling law (20.83). In order to find this we expand the right-hand side of Eq. (20.72) around g^* and write

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma_m^{D-n(D/2-1)} \exp \left[-n \int_1^{\sigma_m} d\sigma' \frac{\gamma(g_{\sigma'})}{\sigma'} \right] \quad (20.112)$$

$$\times \Gamma^{(n)}(p_i/\sigma_m, g^*, \mu, \mu) \times C^{(n)}(p_i/\sigma_m; g_{\sigma_m}, \mu, \mu). \quad (20.113)$$

Using Eq. (20.7), we obtain the correction factor

$$C^{(n)}(p_i; \sigma_m, g^*, \mu, \mu) = 1 + (g_{\sigma_m} - g^*) \psi^{(n)}(p_i/\sigma_m; g^*, \mu, \mu) + \dots, \quad (20.114)$$

where $\psi^{(n)}$ is the dimensionless function

$$\psi^{(n)}(p_i/\sigma_m; g^*, \mu, \mu) = \frac{\partial}{\partial g} \log \Gamma^{(n)}(p_i/\sigma_m; g^*, \mu, \mu). \quad (20.115)$$

The way in which $g(\sigma)$ tends to g^* when approaching the critical point can readily be deduced from Eq. (20.62). Let ω be the slope of the β -function at g^* :

$$\omega \equiv \left. \frac{d\beta(g)}{dg} \right|_{g=g^*}. \quad (20.116)$$

Then we can expand $\beta(g)$ near g^*

$$\beta(g) = \omega(g - g^*) + \mathcal{O}((g - g^*)^2), \quad (20.117)$$

and deduce from (20.62) the behavior

$$\log \sigma \approx \frac{1}{\omega} \log(g_\sigma - g^*) + \dots, \quad (20.118)$$

implying for small m the approach to g^* :

$$g_{\sigma_m} - g^* \approx \sigma_m^\omega + \dots. \quad (20.119)$$

Inserting this into the correction factor (20.114), we see that

$$C^{(n)}(p_i; \sigma_m, g^*, \mu, \mu) = 1 + \sigma_m^\omega \psi^{(n)}(p_i/\sigma_m; g^*, \mu, \mu) + \dots. \quad (20.120)$$

In the scaling limit $\sigma_m \rightarrow 0$, a finite correction to scaling is observed if $\psi^{(n)}$ is homogenous in the variables p_i/σ_m of degree ω . For the two-point vertex function one may have

$$C^{(2)}(p_i; \sigma_m, g, 1, 1) \stackrel{m \approx 0}{\approx} 1 + \text{const} \times (g - g^*) \sigma_m^\omega (p/\mu \sigma_m)^{-\omega} + \dots. \quad (20.121)$$

Then

$$\Gamma^{(2)}(p; g, m, \mu) = \sigma_m^2 \exp \left[-2 \int_1^{\sigma_m} \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'}) \right] \Gamma^{(2)}(p/\sigma_m, g^*, \mu, \mu) C^{(2)}(p; \sigma_m; g_{\sigma_m}, \mu, \mu) \quad (20.122)$$

behaves for $t \approx 0$ like

$$\Gamma^{(2)}(p; g, m, \mu) \stackrel{m \approx 0}{\approx} p^{2-\eta} f(p/\mu t^\nu) \left[1 + (g - g^*) \times \text{const} \times \left(\frac{p}{\mu} \right)^{-\omega} + \dots \right]. \quad (20.123)$$

Thus the approach to scaling is controlled by the slope ω of the beta function at the fixed point g^* . From the above discussion it is obvious that, for an infrared-stable fixed point, the slope ω is positive.

At this point one may wonder about the universality of this result. In principle, other corrections to scaling might arise if higher powers of the field are included in the energy functional, for example ϕ^6 or $\phi^2(\partial\phi)^2$. Those terms are found to be irrelevant by dimensional considerations and by studying the renormalization group equations in the presence of such terms. The scaling behavior and the approach to it remain unchanged.

20.8 Explicit Solution of RGE Close to $D=4$ Dimensions

Up to the two-loop level, the β -function was found in (20.54) to have, in $D = 4 - \varepsilon$ dimensions, the simple form

$$\beta(g) = -\varepsilon g + bg^2 \quad (20.124)$$

with $b = (N + 8)/6$. This function starts out with negative slope and has a zero at

$$g^* = \varepsilon/b. \quad (20.125)$$

If ε is small enough, this statement is reliable even if we know $\beta(g)$ only to order g^2 in perturbation theory. Inserting (20.124) into equation (20.62), we may calculate $g(\sigma)$ explicitly with $\sigma \equiv \mu_1/\mu$. Rewriting $g(\mu\sigma)$ briefly as $g(\sigma)$, we see that

$$\log \sigma = \int_g^{g(\sigma)} \frac{dg}{-\varepsilon g + bg^2}. \quad (20.126)$$

Here we realize the important consequence of a zero g^* in the β -function: If g is sufficiently close to g^* then, in the limit $\sigma \rightarrow 0$, the value $g(\sigma)$ always runs into g^* , no matter whether $g = g(1)$ lies slightly above or below g^* . The point g^* is called a *fixed point* of the renormalization group equation. Since g^* is reached in the limit $\sigma \rightarrow 0$, one speaks of an *infrared-stable* fixed point. The flow of $\gamma(\sigma)$ when sending $\sigma \rightarrow 0$ is illustrated in Fig. (20.2) by an arrow.

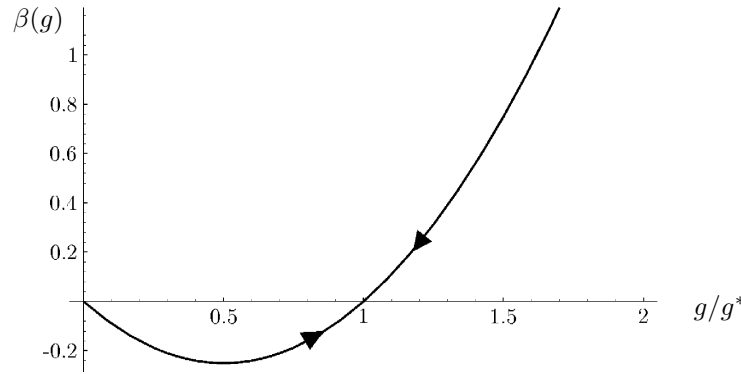


FIGURE 20.2 Flow of the coupling constant $g(\sigma)$ as the scale parameter σ approaches zero (infrared limit). For the opposite direction (ultraviolet limit), the arrows are reversed.

Using the variable $1/g$ instead of g , Eq. (20.126) becomes

$$\log \sigma = \frac{1}{\varepsilon} \int_{1/g}^{1/g(\sigma)} \frac{dx}{1/g^* - x}. \quad (20.127)$$

This can be integrated directly to

$$\sigma = \frac{|1/g^* - 1/g(\sigma)|^{1/\varepsilon}}{|1/g^* - 1/g|^{1/\varepsilon}}, \quad (20.128)$$

so that

$$g(\sigma) = \frac{g^*}{1 + \sigma^\varepsilon (g^*/g - 1)}. \quad (20.129)$$

In general, the β -function may behave in many different ways for larger g . In particular, there may be more zeros to the right of g^* . We can see from Eq. (20.126) that, for negative $\beta(g)$, the coupling constant $g(\sigma)$ will always runs towards zero from the right. The opposite statement holds for positive $\beta(g)$.

In general, the initial coupling $g(\mu) \approx g$ can flow only into a zero lying in its *range of attraction*. In the present case this is guaranteed, for small ε , if the initial g is sufficiently small. In the limit $\sigma \rightarrow \infty$, we see from Eq. (20.129) that g_σ tends to zero which is the other trivial zero of the beta function. This happens for any zero with a positive slope of $\beta(g)$. The limit $\sigma \rightarrow \infty$ corresponds to $m^2 \rightarrow \infty$, and for this reason such zeros are called *ultraviolet stable*. In this limit, the coupling constant goes to zero $g(\sigma) \rightarrow 0$, and so do the renormalization group functions $\gamma(g(\sigma)) \rightarrow 0$ and $\gamma_m(g(\sigma)) \rightarrow 0$. Then scaling relation (20.76) ensures that $\sigma_m = m/\mu$, and the correlation functions behave like

$$\Gamma^{(n)}(p_i; g, m, \mu) \stackrel{m \approx 0}{\approx} \left(\frac{m}{\mu}\right)^{D-n(D/2-1)} \Gamma^{(n)}(p_i/(m/\mu); 0, \mu, \mu). \quad (20.130)$$

This is the behavior of a free-field theory where the fields fluctuate in a trivial purely Gaussian way. The zero in $\beta(g)$ at $g = 0$ is therefore called the *trivial* or *Gaussian fixed point*. In ϕ^4 -theory, the Gaussian fixed point is ultraviolet-stable (UV-stable). Since the theory tends in the limit $m \rightarrow \infty$ against a free theory, one also says that it is ultraviolet-free. Note that this is true only in less than 4 dimensions. In $D = 4$ dimensions where $\varepsilon = 0$, the beta function has only one fixed point, the trivial Gaussian fixed point at the origin. The theory is UV unstable and IR trivial.

It is interesting to observe in which way the renormalization group equation (20.126) sums up an infinite number of diagrams of the perturbation expansion. At the one-loop level, the perturbative relation (20.38) between bare and renormalized coupling constant reads, according to (20.51) [and using $g^* = \varepsilon/b$ from (20.125)]:

$$g_0 = g\mu^\varepsilon \left[1 + g \frac{N+8}{9\varepsilon} + \mathcal{O}(g^2) \right] = g\mu^\varepsilon \left[1 + \frac{g}{g^*} + \mathcal{O}(g^2) \right]. \quad (20.131)$$

This may be rewritten as

$$\frac{1}{g_0\mu^{-\varepsilon}} = \frac{1}{g} - \frac{1}{g^*} + \mathcal{O}(g). \quad (20.132)$$

The solution (20.129), on the other hand, can be brought to the form

$$\frac{1}{g(\sigma)} - \frac{1}{g^*} = \sigma^\varepsilon \left(\frac{1}{g} - \frac{1}{g^*} \right). \quad (20.133)$$

This solution may be compared with the perturbative one in the limit of large σ where g_σ is small. In this limit we identify

$$\frac{1}{g_0(\mu\sigma)^{-\varepsilon}} = \frac{1}{g(\sigma)} - \frac{1}{g^*}. \quad (20.134)$$

With this, Eq. (20.133) reads

$$\frac{1}{g_0\mu^{-\varepsilon}} = \frac{1}{g_\mu} - \frac{1}{g^*}. \quad (20.135)$$

The renormalized coupling constant g on the right-hand side depends on the scale μ and should be denoted more clearly as g_μ . It differs from the perturbative expansion (20.132) by omitting the *higher order correction terms* collected in $\mathcal{O}(g)$. The renormalization group equation has resummed the first-order result (20.132) to (20.135). By taking the inverse of (20.135), we find the geometric series

$$g_0\mu^{-\varepsilon} = g \left[1 + \left(\frac{g}{g^*} \right)^2 + \left(\frac{g}{g^*} \right)^3 + \mathcal{O}(g^4) \right]. \quad (20.136)$$

The first correction is due to a single loop, the second is due to two loops, etc. Thus the geometric series represents a loop expansion of the bare in powers of the renormalized coupling constant.

A relation of the type (20.135) was encountered before in the context of exactly solvable $O(N)$ -symmetric ϕ^4 -theories. Indeed, that relation being exact must also be an exact solution of the renormalization group equation. The difference between that and the present equation is a factor 3 which is due to the fact that, for $N \rightarrow \infty$, only one of the three Wick contractions contributes [recall the discussion after Eq. (18.57)].

The critical coupling g^* , where $\beta(g)$ vanishes, can be calculated for the $O(N)$ -symmetric ϕ^4 -theory in $4 - \varepsilon$ dimensions as a power series expansion in ε starting from Eq. (20.54) [recalling the reduced matrix elements T_{D_1} etc. calculated in Eqs. (11.243)–(11.253)]:

$$\begin{aligned} g^* &= \frac{2}{3T_I}\varepsilon + \left(\frac{3}{2}T_{I_4} - \frac{1}{12}T_{D_3} \right) \left(\frac{2}{3T_I} \right)^3 \varepsilon^2 + \dots \\ &= \frac{6}{N+8} \left[\varepsilon + 3 \frac{3N+14}{(N+8)^2} \varepsilon^2 + \dots \right]. \end{aligned} \quad (20.137)$$

Inserting this into (20.55) and (20.56) we find the ε expansions for γ^*, γ_m^* up to this order:

$$\gamma^* \equiv \gamma(g^*) = \frac{1}{108} \frac{T_{D_3}}{T_I^2} \varepsilon^2 = \frac{1}{4} \frac{N+2}{(N+8)^2} \varepsilon^2 \equiv \frac{\eta}{2}, \quad (20.138)$$

$$\begin{aligned} \gamma_m^* - 2\gamma^* &\equiv \bar{\gamma}_m(g^*) \\ &= \frac{1}{3} \frac{T_{D_1}}{T_I} \varepsilon + \left[\frac{4}{27} \left(\frac{3}{2}T_{I_4} - \frac{1}{12}T_{D_3} \right) \frac{T_{D_1}}{T_I} - \frac{1}{9}T_{D_3} \right] \frac{\varepsilon^2}{T_I^2} \\ &= \frac{N+2}{N+8} \varepsilon \left[1 + 6 \frac{N+3}{(N+8)^2} \varepsilon \right] = 2 - \nu^{-1} - \eta, \end{aligned} \quad (20.139)$$

so that

$$\gamma_m^* = \frac{N+2}{N+8} \varepsilon \left[1 + \frac{13N+44}{2(N+8)^2} \varepsilon \right] = 2 - \nu^{-1}. \quad (20.140)$$

The last equation yields the ε -expansion for the critical exponent ν :

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)} \varepsilon + \frac{(N+2)(N+3)(N+20)}{8(N+8)^3} + \dots \quad (20.141)$$

For $\omega = d\beta/dg|_{g=g^*}$ we obtain from (20.54) and (20.137)

$$\omega = \varepsilon + \left(\frac{1}{3} T_{D_3} - 6T_{I_4} \right) \left(\frac{\varepsilon}{3T_I} \right)^2 = \varepsilon - 3 \frac{3N+14}{(N+8)^2} \varepsilon^2 + \dots \quad (20.142)$$

20.9 Further Critical Relations

We shall now derive some more consequences of the above general scaling relations (20.72), (20.100), (20.111). To have some specific physical system in mind, we may think of $\phi(x)$ as being a field with $N = 3$ components that describes the local fluctuating magnetization vector in some magnetic system. At the mean-field level we see that, if the square mass m^2 is larger than zero, the field expectation value $\Phi = \langle \phi \rangle$ vanishes. This corresponds to being above the transition temperature for magnetic ordering.

For $m^2 < 0$, on the other hand, the size Φ takes the non-zero value $\sqrt{6m^2/g}$. This corresponds to the spontaneous magnetization of a ferromagnet. Certainly, in a proper magnetic system, the magnetization can take any spatial direction, while in the model with a real ϕ -field, it allows only two opposite directions. It should, however, be noted that experimentally it is often possible to find special magnetic systems in which the lattice anisotropy inhibits strongly the rotational degrees of freedom and favors only two directions of magnetization. Such systems are referred to as *Ising-like*. The following discussions will apply to these if we identify Φ with the Ising like magnetization in the z -direction $M = \Phi$.

A linear coupling to an external current j leads to an effective action

$$\Gamma[\Phi; g, m^2, \mu] + \int d^D x \Phi j \equiv \Gamma[\mathbf{M}, g, m^2, \mu] + \int d^D x M H, \quad (20.143)$$

which represents typically a coupling of the magnetization to an external magnetic field. The mass square is identified with the relative temperature distance from critical value T_c as in Eq. (20.1). From what we have learned in Section (20.6), we conclude that the values of the renormalization group functions at the fixed point $g = g^*$ govern the leading behavior of all vertex functions close to the critical temperature. They determine the critical exponents ν, η , and the third exponent ω , taken from the derivative of the β -function at g^* [recall (20.116)], which governs the approach to the critical behavior as T moves near T_c .

Let us derive the scaling relations of several important thermodynamic quantities and correlation functions.

Scaling Relations above T_c

Consider at first the regime $T \geq T_c$ with a vanishing external field H .

Specific Heat Consider the specific heat as a function of temperature. The ground state energy above T_c is given by the effective potential at zero average field $v(\Phi = 0)$ which, according to (20.102) and (20.78), has the scaling behavior

$$v(\Phi = 0) \stackrel{m \approx 0}{\approx} \sigma_m^D \times \text{const.} \approx \tau^{D/(2-\gamma_m^*)} = \tau^{D\nu}. \quad (20.144)$$

Forming twice the derivative with respect to τ we find, for the specific heat at constant volume:

$$C \stackrel{t \approx 0}{\approx} \tau^{D/(2-\gamma_m^*)-2} = \tau^{D\nu-2}, \quad \tau > 0. \quad (20.145)$$

This behavior has been observed experimentally and the critical exponent has been named α :

$$C \stackrel{t \approx 0}{\approx} t^{-\alpha}; \quad t > 0. \quad (20.146)$$

Thus we can identify

$$\alpha = 2 - D/(2 - \gamma_m^*) = 2 - D\nu. \quad (20.147)$$

Susceptibility Suppose now that the system at $T > T_c$ is brought into an external field $j \neq 0$ which we shall call “magnetic field” setting $j = H$ with the notation indicating the applications to magnetism. The equilibrium value of the internal “magnetic field” is no longer zero but $M_H \equiv \Phi_j$. It is determined by the equation of state

$$j = \left. \frac{\partial v(\Phi)}{\partial \Phi} \right|_{\Phi_j} = v'(\Phi_j). \quad (20.148)$$

From (20.102) we see that

$$j \stackrel{\tau \approx 0}{\approx} \sigma_m^{D-\gamma^*-(D/2-1)} v'(\Phi/\sigma_m^{\gamma^*+D/2-1}; g^*, \mu, \mu), \quad \tau > 0. \quad (20.149)$$

The *susceptibility* is obtained by an additional differentiation

$$\chi^{-1} \equiv \left. \frac{\partial^2 v}{\partial \Phi^2} \right|_{\Phi=\Phi_j} \stackrel{\tau \approx 0}{\approx} \sigma_m^{D-(D-2)} \sigma_m^{-2\gamma^*} v''(\Phi/\sigma_m^{\gamma^*+D/2-1}; g^*, \mu, \mu), \quad \tau > 0. \quad (20.150)$$

For $\tau > 0$ and zero external field j one has $\Phi = 0$, thus finding

$$\chi^{-1} \propto \sigma_m^{2-2\gamma^*} = \tau^{2(1-\gamma^*)/(2-\gamma_m^*)}. \quad (20.151)$$

Experimentally, this power of τ defines the critical exponent γ :

$$\chi^{-1} \stackrel{\tau \approx 0}{\approx} \tau^\gamma, \quad \tau > 0. \quad (20.152)$$

Hence we can identify

$$\gamma = 2 \frac{1 - \gamma^*}{2 - \gamma^*} = \nu(2 - \eta). \quad (20.153)$$

Critical Magnetization At the critical point, the proportionality of H and M is destroyed by quantum fluctuations. Experimentally one observes

$$H \rightarrow M^\delta; \quad t = 0. \quad (20.154)$$

Equation (20.149) shows that if the effective potential is supposed to be finite at the critical point where $\sigma_m = 0$, the derivative v' must behave like some power

$$v' \stackrel{t \approx 0}{\approx} \text{const.} \times \left(\Phi / \sigma^{\gamma^* + D/2 - 1} \right)^\delta, \quad t > 0. \quad (20.155)$$

Then, since $j \propto \sigma_m^{D - \gamma^* - (D/2 - 1)} v'$, the power δ which makes j finite for $\sigma_m \rightarrow 0$ must satisfy

$$D - \gamma^* - (D/2 - 1) + [\gamma^* + (D/2 - 1)] \delta = 0. \quad (20.156)$$

From this we obtain

$$\delta = \frac{D + 2 - 2\gamma^*}{D - 2 + 2\gamma^*} = \frac{D + 2 - \eta}{D - 2 + \eta}. \quad (20.157)$$

Scaling Relations below T_c

Let us now turn to scaling results *below* T_c . Since all individual vertex functions in the expansion of the effective action (20.88) can be calculated for $m^2 < 0$ just as well as for $m^2 > 0$, the main difference lies in $v(\Phi)$ not having a minimum at $\Phi = 0$ but at $\Phi = \Phi_0 \neq 0$ for vanishing external fields. In addition, the scaling variable σ_m is not fixed by the condition (20.71), but by a similar relation with an opposite sign

$$m_\sigma^2 / \sigma^2|_{\sigma=\sigma_m} = -\mu^2, \quad (20.158)$$

so that we obtain via (20.73) the relation

$$-\frac{m^2}{\mu^2} \stackrel{m \approx 0}{\approx} \exp \left\{ \int_0^{\sigma_m} \frac{d\sigma'}{\sigma'} [2 - \gamma_m(g^*)] \right\} = \sigma_m^{2 - \gamma_m^*}, \quad (20.159)$$

rather than (20.75), leading to

$$\sigma_m \approx (-\tau)^{1/(2 - \gamma_m^*)} \quad (20.160)$$

instead of (20.78).

Spontaneous Magnetization Consider first the behavior of the spontaneous magnetization $M_0 \equiv \Phi_0$ as the temperature approaches T_c from below. The equilibrium value of Φ is determined by the minimum of the effective potential $v(\Phi)$. According to the general scaling form (20.102), the minimum must be situated at a fixed

$$\Phi_0 / \sigma_m^{\gamma^* + D/2 - 1} = \text{const.} \quad (20.161)$$

Hence Φ_0 depends on m^2 and thus on the reduced temperature t as follows:

$$M_0 \equiv \Phi_0 \propto \sigma_m^{\gamma^*+D/2-1} = (-\tau)^{(\gamma^*+D/2-1)/(2-\gamma_m^*)}. \quad (20.162)$$

Thus we derive the experimentally observable relation

$$M_0 \equiv \Phi_0 \propto (-\tau)^\beta \quad (20.163)$$

with the critical exponent [not to be confused with the β -function (20.31)]

$$\beta = \frac{\gamma^* + D/2 - 1}{2 - \gamma_m^*} = \frac{\nu}{2}(D - 2 + \eta). \quad (20.164)$$

Coherence Length Consider now the temperature dependent coherence length below T_c . From (20.111) we read off that the two-point function satisfies

$$\Gamma^{(2)}(p; \Phi_0, g, m^2, \mu) \stackrel{\tau \approx 0}{\approx} \sigma_m^{2-2\gamma^*} \Gamma^{(2)}\left(p/\sigma_m; \Phi_0/\sigma_m^{\gamma^*+D/2-1}, g^*, \mu, \mu\right), \quad \tau > 0. \quad (20.165)$$

As in the previous case $T > T_c$, this is a function of

$$p/\sigma_m = \xi(\tau)p, \quad (20.166)$$

with the same temperature behavior as in (20.86). The same critical exponent governs the divergence of the coherence length below and above T_c .

This above-below symmetry is found for the critical indices α and γ of specific heat and susceptibility. When deriving the scaling behavior for $\tau < 0$, we have to keep track of the change of the average field Φ_0 as a function of temperature.

Specific Heat The exponent of the specific heat, α' , follows now from the potential

$$v(\Phi_0) \stackrel{t \approx 0}{\approx} \sigma_m^D v\left(\Phi_0/\sigma_m^{\gamma^*+D/2-1}, g^*, \mu, \mu\right), \quad \tau > 0. \quad (20.167)$$

Since the temperature change of Φ_0 takes place at a constant combination (20.161), the presence of $\Phi_0 \neq 0$ can be ignored and we obtain the same result as in (20.144), implying a temperature behavior

$$v(\Phi_0) \propto \sigma_m^D \sim \tau^{D\nu}. \quad (20.168)$$

This agrees with the $T > T_c$ behavior (20.144), leading to the same critical exponent of the specific heat as in (20.147).

Susceptibility Suppose now that an external magnetic field is switched on. The equilibrium value Φ shifts by $\delta\Phi \equiv \Phi_j - \Phi_0$ from Φ_0 to Φ_j , which is determined by (20.148), (20.149). For $\delta\Phi$ we obtain the scaling relation

$$j \rightarrow \sigma_m^{D-(\gamma^*+D/2-1)} v'((\Phi_0 + \delta\Phi)/\sigma_m^{\gamma^*+D/2-1}, g^*, \mu, \mu). \quad (20.169)$$

Expanding this to first order in $\delta\Phi$ gives

$$\delta j \rightarrow \delta\Phi \sigma_m^{2-2\gamma^*} v''(\Phi_0/\sigma_m^{\gamma^*+D/2-1}, g^*, \mu, \mu). \quad (20.170)$$

Since Φ_0 changes with t according to (20.163), the last factor is independent of temperature, and the susceptibility $\chi(t)$ has the same functional form as in (20.150), exhibiting the same critical exponent γ as in (20.152).

Widom's Relation Finally it is worth noting that Eq. (20.149) corresponds exactly to the scaling relation proposed and investigated first by Widom (1965) for the free energy at a fixed magnetization M :

$$F(t, M) = \tau^{2-\alpha} \psi(\tau/M^{1/\beta}), \quad (20.171)$$

where ψ is some smooth function of its arguments.

Differentiating this with respect to M , we find the magnetic equation of state

$$H = \tau^{2-\alpha} M^{-1-1/\beta} \psi'(\tau/M^{1/\beta}). \quad (20.172)$$

This can be rewritten as

$$\frac{H}{M^\delta} = f\left(\frac{\tau}{M^{1/\beta}}\right) \quad (20.173)$$

with some function $f(x)$, as is easily proved by inserting on the left-hand side the scaling relation $\delta = -1 + (2 - \alpha)/\beta$. In terms of the variables of our field theory, the equation of state (20.173) may be rewritten as

$$j = \tau^{\delta\beta} \left(\frac{\tau}{\Phi^{1/\beta}}\right)^{-\delta\beta} f\left(\frac{\tau}{\Phi^{1/\beta}}\right) = \tau^{\delta\beta} g\left(\frac{\Phi}{\tau^\beta}\right), \quad (20.174)$$

where $g(x)$ is some other function. By comparing this with (20.149), we see that

$$\delta\beta = [D - \gamma^* - (D/2 - 1)] \frac{1}{2 - \gamma_m^*} = \frac{\nu}{2}(D + 2 - \eta). \quad (20.175)$$

20.10 Comparison of Scaling Relations with Experiments

For a comparison with experiment we may pick two critical parameters γ and γ_m^* and determine from these the values of η , ν . The remaining critical exponents can

then be found from the above-derived scaling relations which we list once more, for convenience:

$$\alpha = \alpha' = 2 - 2\beta - \gamma, \quad (20.176)$$

$$\gamma = \gamma' = \nu(2 - \eta) \quad (20.177)$$

$$\gamma = \nu(2 - \eta), \quad (20.178)$$

$$\alpha = 2 - \nu D, \quad (20.179)$$

$$\delta = (D + 2 - \eta)/(D - 2 + \eta). \quad (20.180)$$

These are called *hyperscaling relations*.

As an example take the magnetic system CrBr_3 where one measures

$$\beta \approx 0.368, \quad \delta \approx 4.3, \quad \gamma \approx 1.215.$$

Inserting these into the scaling relation

$$\beta = \gamma/(\delta - 1), \quad (20.181)$$

which follows (20.176) and (20.180), we see that it is satisfied excellently. Inserting δ into the relation

$$\eta = \frac{D + 2 - (D - 2)\delta}{\delta + 1}, \quad (20.182)$$

we find for $D = 3$

$$\eta \approx 0.132, \quad (20.183)$$

and from the relation $\nu = \gamma(2 - \eta)$,

$$\nu \approx 0.65. \quad (20.184)$$

Results with Various $O(N)$ -Symmetries

Let us compare these numbers with the results obtained from the ε -expansion in various $O(N)$ -symmetries. Using Eqs. (20.137)–(20.139) and the above formulas for the critical exponents in terms of γ^* , γ_m^* , we find the series:

$$\eta = \frac{N + 2}{2(N + 8)^2} \varepsilon^2 + \dots, \quad (20.185)$$

$$\nu = \frac{1}{2} + \frac{N + 2}{4(N + 8)} \varepsilon + \frac{(N + 2)(N^2 + 23N + 60)}{8(N + 8)^3} \varepsilon^2 + \dots. \quad (20.186)$$

These results are valid only for infinitesimal ε . For applications, one assumes that the ε -expansions can be used also in $D = 3$ dimensions, i.e., for $\varepsilon = 1$, where physics takes place. The justification of this rather ad hoc procedure lies in an approximate

numerical decrease of the ε and ε^2 terms in (20.137)–(20.139). Thus we find for $N = 1, 2, \infty$,

$$\begin{aligned}\nu &= \frac{1}{2} + \frac{1}{12}\varepsilon + \frac{7}{9 \cdot 9 \cdot 2}\varepsilon^2 + \dots = \frac{203}{9 \cdot 9 \cdot 4} + \dots \approx 0.627, & N = 1, \\ \nu &= \frac{1}{2} + \frac{1}{10}\varepsilon + \frac{11}{200}\varepsilon^2 + \dots = \frac{131}{200} + \dots \approx 0.655, & N = 2, \\ \nu &= \frac{1}{2} + \frac{1}{4}\varepsilon + \frac{1}{8}\varepsilon^2 + \dots = \frac{7}{8} + \dots \approx 0.875, & N = \infty.\end{aligned}\quad (20.187)$$

The other critical index is, in the three cases,

$$\begin{aligned}\eta &= \frac{1}{54}, & N = 1, \\ \eta &= \frac{1}{15}, & N = 2, \\ \eta &= \frac{1}{2}, & N = \infty.\end{aligned}\quad (20.188)$$

The ε -expansion for ν has decreasing contributions of higher orders. The value up to order ε^2 , $\nu \approx 0.627$, is in reasonable agreement with the experimental value $\nu \approx 0.65$. $\nu^{-1} - 2 = -\frac{1}{3}$, $\nu \sim 0.6$, and this is in good agreement with the experimental value (20.184). There is only one term to order ε , so that no convergence can be judged. The agreement with experiment is reasonable. The value to order ε^2 at $\varepsilon = 1$ is $\eta \approx 0.019$ which, via the scaling relation $\nu = \gamma/(2 - \eta)$, corresponds to $\nu \approx 0.61$, quite close to the experimental value 0.65.

It is not advisable to calculate to higher order than ε^2 , since the agreement to order ε^3 usually becomes worse. In fact, the series does not converge at all—it is merely an asymptotic series, and it is meaningless to carry the expansion any further. The rough agreement up to order ε at $\varepsilon = 1$ is all one can hope for.

20.11 Higher-Order Expansion

In the last twenty years, efficient mathematical methods have been developed to extract accurate results from divergent asymptotic series. In fact, there exists a simple mathematical procedure for converting divergent weak-coupling expansions into convergent strong-coupling expansions [1] (see also the quantum mechanical predecessor in [2]). It is therefore worthwhile to state presently known higher powers in ε .

After some tedious work [3], supported by algebraic computer programs, one finds the beta function, up to order ε^4 :

$$\begin{aligned}\beta(g) &= \frac{g^2}{6}[N + 8] - \frac{g^3}{6}[3N + 14] \\ &\quad + \frac{g^4}{432}[33N^2 + 922N + 2960 + \zeta(3) \cdot 96(5N + 22)] \\ &\quad - \frac{g^5}{7776}[-5N^3 + 6320N^2 + 80456N + 196648 \\ &\quad \quad + \zeta(3) \cdot 96(63N^2 + 764N + 2332) \\ &\quad \quad - \zeta(4) \cdot 288(5N + 22)(N + 8) \\ &\quad \quad + \zeta(5) \cdot 1920(2N^2 + 55N + 186)] \\ &\quad + \frac{g^6}{124416}[13N^4 + 12578N^3 + 808496N^2 + 6646336N + 13177344]\end{aligned}$$

$$\begin{aligned}
& + \zeta(3) \cdot 16(-9N^4 + 1248N^3 + 67640N^2 + 552280N + 1314336) \\
& + \zeta^2(3) \cdot 768(-6N^3 - 59N^2 + 446N + 3264) \\
& - \zeta(4) \cdot 288(63N^3 + 1388N^2 + 9532N + 21120) \\
& + \zeta(5) \cdot 256(305N^3 + 7466N^2 + 66986N + 165084) \\
& - \zeta(6)(N+8) \cdot 9600(2N^2 + 55N + 186) \\
& + \zeta(7) \cdot 112896(14N^2 + 189N + 526) \, , \tag{20.189}
\end{aligned}$$

and the critical indices

$$\begin{aligned}
\eta(\varepsilon) = & \frac{(N+2)\varepsilon^2}{2(N+8)^2} \left\{ 1 + \frac{\varepsilon}{4(N+8)^2} [-N^2 + 56N + 272] \right. \\
& - \frac{\varepsilon^2}{16(N+8)^4} [5N^4 + 230N^3 - 1124N^2 - 17920N - 46144 \\
& \quad + \zeta(3)(N+8) \cdot 384(5N + 22)] \\
& - \frac{\varepsilon^3}{64(N+8)^6} [13N^6 + 946N^5 + 27620N^4 + 121472N^3 \\
& \quad - 262528N^2 - 2912768N - 5655552 \\
& \quad - \zeta(3)(N+8) \cdot 16(N^5 + 10N^4 + 1220N^3 - 1136N^2 - 68672N - 171264) \\
& \quad + \zeta(4)(N+8)^3 \cdot 1152(5N + 22) \\
& \quad \left. - \zeta(5)(N+8)^2 \cdot 5120(2N^2 + 55N + 186)] \right\} \, , \tag{20.190}
\end{aligned}$$

and

$$\begin{aligned}
1/\nu(\varepsilon) = & 2 + \frac{(N+2)\varepsilon}{N+8} \left\{ -1 - \frac{\varepsilon}{2(N+8)^2} (13N + 44) \right. \\
& + \frac{\varepsilon^2}{8(N+8)^4} [3N^3 - 452N^2 - 2672N - 5312 \\
& \quad + \zeta(3)(N+8) \cdot 96(5N + 22)] \\
& + \frac{\varepsilon^3}{32(N+8)^6} [3N^5 + 398N^4 - 12900N^3 - 81552N^2 - 219968N - 357120 \\
& \quad + \zeta(3)(N+8) \cdot 16(3N^4 - 194N^3 + 148N^2 + 9472N + 19488) \\
& \quad + \zeta(4)(N+8)^3 \cdot 288(5N + 22) \\
& \quad \left. - \zeta(5)(N+8)^2 \cdot 1280(2N^2 + 55N + 186)] \right. \\
& + \frac{\varepsilon^4}{128(N+8)^8} [3N^7 - 1198N^6 - 27484N^5 - 1055344N^4 \\
& \quad - 5242112N^3 - 5256704N^2 + 6999040N - 626688 \\
& \quad - \zeta(3)(N+8) \cdot 16(13N^6 - 310N^5 + 19004N^4 + 102400N^3 \\
& \quad \quad - 381536N^2 - 2792576N - 4240640) \\
& \quad - \zeta^2(3)(N+8)^2 \cdot 1024(2N^4 + 18N^3 + 981N^2 + 6994N + 11688) \\
& \quad + \zeta(4)(N+8)^3 \cdot 48(3N^4 - 194N^3 + 148N^2 + 9472N + 19488) \\
& \quad + \zeta(5)(N+8)^2 \cdot 256(155N^4 + 3026N^3 + 989N^2 - 66018N - 130608) \\
& \quad - \zeta(6)(N+8)^4 \cdot 6400(2N^2 + 55N + 186) \\
& \quad \left. + \zeta(7)(N+8)^3 \cdot 56448(14N^2 + 189N + 526)] \right\} \, . \tag{20.191}
\end{aligned}$$

The higher orders in ε start growing rapidly for $\varepsilon = 4 - D = 1$, where physics takes place, due to the asymptotic nature of the ε -expansions.

20.12 Mean-Field Results for Critical Indices

In mean-field theory, fluctuations are neglected and the effective action is equal to the bare action with the quantum field ϕ replaced by the expectation value $\Phi = \langle \phi \rangle$:

$$\Gamma[\Phi] = \int d^D x \left[\frac{1}{2}(\partial\Phi)^2 - \frac{m^2}{2}\Phi^2 - \frac{g}{4}\Phi^4 + \Phi j \right]. \quad (20.192)$$

The mass is assumed to behave as

$$m^2 = \mu^2 \left(\frac{T}{T_c} - 1 \right) \equiv \mu^2 \tau, \quad (20.193)$$

and Φ and j are interpreted as magnetization M and magnetic field H , respectively. The two-point function is

$$\Gamma^{(2)}(p) = p^2 - m^2, \quad (20.194)$$

from which we read off, at $m^2 = 0$ or $T = T_c$, that the critical index η , which determines the power behavior of the correlation function, vanishes:

$$\eta = 0. \quad (20.195)$$

Above T_c , we rewrite $\Gamma^{(2)}$ in the rescaled form (20.69):

$$\Gamma^{(2)}(p; g, m, \mu) = \sigma^2 \left[(p/\sigma)^2 - m^2/\sigma^2 \right]. \quad (20.196)$$

Thus we identify $\sigma_m = m/\mu$, and the coherence length has the temperature behaviour

$$\xi(\tau) = \frac{1}{\mu\sigma_m} = \frac{1}{m} \sim \tau^{-1/2}. \quad (20.197)$$

This implies the critical index

$$\nu = \frac{1}{2}. \quad (20.198)$$

We now turn to the regime $T < T_c$. Then the effective potential has a nontrivial minimum at

$$\Phi_0 = \sqrt{-\frac{m^2}{g}} \propto (-\tau)^{1/2}. \quad (20.199)$$

The critical exponent β is therefore determined to be

$$\beta = \frac{1}{2}. \quad (20.200)$$

Inserting $\Phi = \Phi_0 + \delta\Phi$ into the effective action (20.192), we find the two-point function below T_c

$$\Gamma^{(2)} = \left. \frac{\delta^2 \Gamma}{\delta \Phi \delta \Phi} \right|_{\Phi=\Phi_0} = p^2 + 2m^2. \quad (20.201)$$

This shows that the coherence length is equal to

$$\xi(\tau) = \frac{1}{\sqrt{-2m^2}} \sim \tau^{-1/2}. \quad (20.202)$$

Hence the index ν' below T_c is the same as ν above T_c :

$$\nu' = \frac{1}{2}. \quad (20.203)$$

Consider now the specific heat. The equilibrium energy above T_c and below T is:

$$\begin{aligned} \nu &\equiv 0, & T &\geq T_c, \\ \nu &\equiv -\frac{m^4}{4g}, & T &< T_c, \end{aligned} \quad (20.204)$$

respectively. Differentiating this twice with respect to m^2 , we see that

$$C = \text{const}, \quad T < T_c, \quad (20.205)$$

which implies that

$$\alpha' = 0. \quad (20.206)$$

Note that the index α above T_c is undetermined at the mean-field level since $C \equiv 0$.

Let us now admit a nonzero magnetic field. Then for $T < T_c$, the equilibrium value of Φ_0 is given by

$$m^2\Phi_0 + g\Phi_0^3 = j. \quad (20.207)$$

For $T = T_c$, this has the solution

$$j = g\Phi_0^3, \quad (20.208)$$

so that we can read off [see (20.154)]

$$\delta = 3. \quad (20.209)$$

For $T > T_c$, we see that for small j

$$\Phi \approx \frac{1}{m^2}j, \quad (20.210)$$

so that the susceptibility is

$$\chi \approx (m^2)^{-1} \propto \tau^{-1}, \quad (20.211)$$

giving the critical index [see (20.152)]

$$\gamma = -1. \quad (20.212)$$

Below T_c , on the other hand, we insert $\Phi = \Phi_0 + \delta\Phi$ and find

$$(m^2 + 3g\Phi_0^2)\delta\Phi = j \quad (20.213)$$

or

$$\delta\Phi = -\frac{1}{2m^2}j \quad (20.214)$$

which amounts to

$$\chi = -\frac{1}{2m^2} \propto (-\tau)^{-1}. \quad (20.215)$$

Thus γ' is the same as γ :

$$\gamma' = \gamma = -1. \quad (20.216)$$

Note that χ measures the size of the fluctuations of the magnetization field $M(\mathbf{x})$ around the equilibrium value. It is determined by the curvature of the effective potential at the minimum. Above T_c this is m^2 , below T_c it is twice the opposite of m^2 (which is again positive).

The critical indices satisfy the general scaling relations (20.176)–(20.180). Indeed, with $\nu = \eta/2 = 0$, we see that the relations are

$$\alpha = \alpha' = 2 - \frac{D}{2}, \quad \delta = \frac{D+2}{D-2}, \quad \gamma = \gamma' = 1, \quad \beta = \frac{1}{2} \left(\frac{D}{2} - 1 \right). \quad (20.217)$$

For $D = 4$ they yield once more the above derived mean field exponent.

20.13 Effective Potential in the Critical Regime to Order ε

From (20.102), (20.76), (20.85), and (20.164), the effective potential has, for small mass values, the universal form

$$\begin{aligned} v(\Phi; g, m, \mu) &\xrightarrow{m \rightarrow 0} \mu^D \left(\frac{m^2}{\mu^2} \right)^{D\nu} w \left(\frac{\Phi/\mu^{(D-2)/2}}{(m^2/\mu^2)^{\nu(\gamma^* + D/2 - 1)}} \right) \\ &= \mu^D \tau^{D\nu} w \left(\frac{\Phi/\mu^{(D-2)/2}}{\tau^\beta} \right), \end{aligned} \quad (20.218)$$

where w is some dimensionless function. In the presence of an external magnetic field $H \equiv j$, this corresponds to an equation of state in the Widom form (20.174):

$$j = \frac{\partial v}{\partial \Phi} = \mu^{D/2+1} \tau^{D\nu-\beta} w' \left(\frac{\Phi/\mu^{(D-2)/2}}{\tau^\beta} \right) = \tau^{\delta\beta} g \left(\frac{\Phi}{\tau^\beta} \right). \quad (20.219)$$

We shall now demonstrate how the function w can be calculated at the one-loop level. The renormalization group analysis of the previous sections made statements only on the numerical values for the critical indices. Nothing was known on the specific shape of the effective action v and thus of the general Widom function $f(x)$. To lowest order in ε it is possible to calculate v from the one-loop effective potential.

Consider the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 - \frac{g_0}{4}\mu^\varepsilon\phi^4, \quad (20.220)$$

in which we have taken the factor μ^ε out of g_0 to make g_0 a dimensionless number in $D = 4 - \varepsilon$ dimensions. The one-loop correction to the effective action is calculated in the usual way. The partition function of the theory reads

$$Z = \int \mathcal{D}\phi e^{i\mathcal{A}[\phi]/\hbar} = \int \mathcal{D}\phi e^{(i/\hbar) \int d^D x \mathcal{L}(x)}. \quad (20.221)$$

Expanding around the classical solution

$$\phi(x) = \Phi + \delta\phi(x), \quad (20.222)$$

the exponent has the lowest terms

$$\int d^D x \mathcal{L}(\Phi) - \int d^D x \frac{1}{2} \delta\phi(x) \left(\partial^2 + m_0^2 + \frac{g_0}{2} \mu^\varepsilon \Phi^2 \right) \delta\phi(x) + \dots \quad (20.223)$$

Performing the path integral over the quadratic fluctuations gives

$$\begin{aligned} Z &\approx e^{(i/\hbar) \int d^D x \mathcal{L}(\Phi)} \det^{-1/2} \left(\partial^2 + m_0^2 + \frac{g_0}{2} \mu^\varepsilon \Phi^2 \right) \\ &= \exp \left\{ \frac{i}{\hbar} \left[\int d^D x \mathcal{L}(\Phi) + \frac{i}{2} \hbar \text{Tr} \log \left(\partial^2 + m_0^2 + \frac{g_0}{2} \mu^\varepsilon \Phi^2 \right) \right] \right\} \equiv e^{i\mathcal{A}_{1\text{ loop}}[\Phi]}. \end{aligned} \quad (20.224)$$

As shown before, one can replace Φ directly by the extremal value in the one-loop corrected action $\mathcal{A}_{1\text{ loop}}[\Phi]$, thus obtaining the correct effective action $\Gamma[\Phi]$ to order $\hbar$. The evaluation is easiest at a constant Φ field, where $\Gamma[\Phi]$ determines the effective potential as

$$v(\Phi) = -L^D \Gamma[\Phi]|_{\Phi=\text{const}},$$

with L^D being the volume of the system in D dimensions. Then the trace of the logarithm is simply the integral

$$\sum_{\mathbf{p}} \log \left(-p^2 + m_0^2 + \frac{g_0}{2} \mu^\varepsilon \Phi^2 \right) = L^D \int \frac{d^D p}{(2\pi)^D} \log \left(-p^2 + m_0^2 + \frac{g_0}{\varepsilon} \mu^\varepsilon \Phi^2 \right),$$

and the effective potential at the one-loop level reads

$$v(\Phi) = \frac{m_0^2}{2} \Phi^2 + \frac{g_0}{4!} \mu^\varepsilon \Phi^4 - \frac{i}{2} \hbar \int \frac{d^D p}{(2\pi)^D} \log \left(-p^2 + m_0^2 + \frac{g_0}{\varepsilon} \mu^\varepsilon \Phi^2 \right). \quad (20.225)$$

Performing a Wick rotation to euclidean momenta p_ε^μ with $p_E^2 = -p^2$, $d^D p \equiv i d^D p_E$, the third term becomes

$$\frac{1}{2} \int \frac{d^D p_E}{(2\pi)^D} \log \left(p_E^2 + m_0^2 + \frac{g_0}{2} \mu^\varepsilon \Phi^2 \right). \quad (20.226)$$

This integral was calculated in Eq. (11.134) for all dimensions D as

$$\int \frac{d^D p_E}{(2\pi)^D} \log(p_E^2 + m_0^2) = \mathcal{S}_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \frac{2}{D} (m_0^2)^{D/2}, \quad (20.227)$$

and brings the potential to the form

$$v = \frac{m^2}{2}\Phi^4 + \frac{g}{4!}\mu^\varepsilon\Phi^4 + \frac{1}{2}S_D\frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}\left(m_0 + \frac{g_0}{2}\mu^\varepsilon\Phi^2\right)^{D/2}. \quad (20.228)$$

It will be more convenient to consider directly the equation of state rather than v itself and derive

$$j = \frac{\partial v}{\partial \Phi} = m_0^2\Phi + \frac{g_0}{3!}\mu^\varepsilon\Phi^3 + \frac{1}{4}S_D\Gamma(2-\varepsilon/2)\Gamma(-1+\varepsilon/2)\hbar g_0\mu^\varepsilon\Phi\left(m_0^2 + \frac{g_0\mu^\varepsilon}{2}\Phi^2\right)^{1-\varepsilon/2}. \quad (20.229)$$

Close to $\varepsilon = 0$, the last term can be expanded as

$$-\frac{g_0\mu^\varepsilon}{2}S_D\Phi\left(\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon)\right)\left(m_0^2 + \frac{g_0\mu^\varepsilon}{2}\Phi^2\right)\mu^{-\varepsilon}\left[1 - \frac{\varepsilon}{2}\log\left(\frac{m_0^2}{\mu^2} + \frac{g_0\mu^\varepsilon}{2}\frac{\Phi^2}{\mu^2}\right) + \mathcal{O}(\varepsilon)\right]. \quad (20.230)$$

According to the minimal subtraction scheme in dimensional regularization we may simply drop the singular $1/\varepsilon$ -piece and arrive at the renormalized expression

$$j = \frac{\partial v}{\partial \Phi} = m^2\Phi + \frac{g}{3}\mu^\varepsilon\Phi^3 + \hbar\frac{S_D g}{4}\left(m^2 + \frac{g}{2}\mu^\varepsilon\Phi^2\right)\Phi\log\left(\frac{m^2}{\mu^2} + \frac{g}{2}\mu^\varepsilon\frac{\Phi^2}{\mu^2}\right). \quad (20.231)$$

The potential is

$$v = \frac{m^2}{2}\Phi^2 + \frac{g\mu^\varepsilon}{3!}\Phi^3 + \hbar\frac{S}{8}\mu^{-\varepsilon}\left(m^2 + \frac{g\mu^\varepsilon}{2}\Phi^2\right)^2\left[\log\left(\frac{m^2}{\mu^2} + \frac{g}{2}\mu^\varepsilon\frac{\Phi^2}{\mu^2}\right) - \frac{1}{2}\right]. \quad (20.232)$$

Let us now see how these expressions can be brought to the universal forms (20.218) and (20.219). Neglecting, for a moment, the logarithmic $\hbar$ -correction, we rewrite the first two terms in (20.231) as

$$\begin{aligned} j = \frac{\partial v}{\partial \Phi} &= \mu^{3+\varepsilon/2}\frac{\Phi}{\mu^{1+\varepsilon/2}}\left(\frac{m^2}{\mu^2}\right)\left[1 + \frac{g}{3!}\left(\frac{\Phi}{\mu^{1+\varepsilon/2}}/\sqrt{\frac{m^2}{\mu^2}}\right)^2\right] \\ &= \mu^{3+\varepsilon/2}\left(\frac{m^2}{\mu^2}\right)^{3/2}\left(\frac{\Phi}{\mu^{1+\varepsilon/2}}/\sqrt{\frac{m^2}{\mu^2}}\right)\left[1 + \frac{g}{3!}\left(\frac{\Phi}{\mu^{1+\varepsilon/2}}/\sqrt{\frac{m^2}{\mu^2}}\right)^2\right]. \end{aligned} \quad (20.233)$$

Comparing this with (20.219), we can identify the mean-field critical indices [as in (20.200), (20.209)]

$$\delta = 3, \quad \beta = \frac{1}{2}. \quad (20.234)$$

We shall now calculate the lowest-order corrections to these critical indices by considering two specific scaling relations. First, we consider the limit $\Phi \rightarrow 0$. For

$\tau > 0$, the derivative $\partial v / \partial \Phi$ has to carry a factor Φ . Then equation (20.219) shows that $\partial v / \partial \Phi$ should behave as a function of τ as follows:

$$j \propto \Phi \mu^2 \tau^{D\nu-2\beta} = \Phi \mu^2 \tau^{(\delta-1)\beta} = \Phi \mu^2 \tau^\gamma. \quad (20.235)$$

From (20.233) we see, on the other hand, that

$$j = \frac{\partial v}{\partial \Phi} = \Phi \mu^2 \frac{m^2}{\mu^2} \left(1 + \hbar \frac{S_D g}{4} \log \frac{m^2}{\mu^2} \right). \quad (20.236)$$

This is a first-order expansion in g of the power law

$$= \Phi \mu^2 \left(\frac{m^2}{\mu^2} \right)^{1+\hbar S_D g/4} + \mathcal{O}(g^2). \quad (20.237)$$

From this, we read off the one-loop corrected critical exponent which rules the divergence of the magnetic susceptibility near the critical point via $\xi \propto \tau^{-\gamma}$:

$$\gamma \equiv \nu(2 - \eta) = 1 + \frac{\hbar S_D g}{4} + \mathcal{O}(g^2). \quad (20.238)$$

For a second independent exponent we work directly at the critical point $m = 0$. By Widom's relation, $\partial v / \partial \Phi$ behaves like $(\Phi / \mu^{(D-2)/2})^\delta$. From (20.233) we find the power law

$$\begin{aligned} \frac{\partial v}{\partial \Phi} &= \frac{g}{3!} \mu^{3-\frac{5}{2}\varepsilon} \sqrt{\frac{2}{g}} \left(\sqrt{\frac{g}{2}} \frac{\Phi}{\mu^{1-\varepsilon/2}} \right)^3 \left[1 + \hbar \frac{S_D g}{2} \log \left(\sqrt{\frac{g}{2}} \frac{\Phi}{\mu^{1-\varepsilon/2}} \right) \right] \\ &= \frac{g}{3!} \mu^{3-\frac{5}{2}\varepsilon} \left(\frac{2}{g} \right)^{3/2} \left(\sqrt{\frac{g}{2}} \frac{\Phi}{\mu^{1-\varepsilon/2}} \right)^{3+\hbar 3 S_D g/2} + \mathcal{O}(g^2). \end{aligned} \quad (20.239)$$

We can therefore identify the critical index δ with which the critical magnetization responds to an external field (in the scaling law $H \propto M^\delta$)

$$\delta = 3 + \hbar \frac{3}{2} S_D g + \mathcal{O}(g^2). \quad (20.240)$$

Using (20.176)–(20.180), we can calculate the exponent

$$\beta = \frac{D\nu}{1 + \delta}, \quad (20.241)$$

which rules the way in which the spontaneous magnetization vanishes for $\tau \rightarrow -0$ [in the scaling law $M \propto (-\tau)^\beta$]. The ratio

$$\nu = \frac{\gamma}{D} \frac{\delta + 1}{\delta - 1} \quad (20.242)$$

is the exponent which governs the divergence of the coherence length by the power law $\xi \propto \tau^{-\nu}$.

Note that β satisfies the scaling relation

$$\beta = \frac{\gamma}{\delta - 1}, \quad (20.243)$$

as it should according to (20.181). Inserting (20.238) and (20.240), we find

$$\beta = (1 + \hbar S g/4)/(2 + \hbar \frac{3}{2} S_D g) = \frac{1}{2} - \hbar S g/4 + \mathcal{O}(g^2). \quad (20.244)$$

We can use these results to explicitly find the function $g(x)$ in the universal Widom expressions (20.219), (20.174) at the one-loop level. We define the dimensionless field variable

$$y = \sqrt{\frac{g}{2}} \frac{\Phi}{\mu^{1-\varepsilon/2}} \quad (20.245)$$

and the combined variable occurring in (20.239)

$$x \equiv \tau/y^{1/\beta}. \quad (20.246)$$

Then $\partial v/\partial \Phi$ in (20.239) is expressible in the form

$$\frac{\partial v}{\partial \Phi} = \Phi \mu^2 y^{\delta-1} f(x), \quad (20.247)$$

with a function $f(x)$ related to the potential v by

$$f\left(\sqrt{\frac{2}{g}}x\right) = x^{-\delta} v'(x). \quad (20.248)$$

By rewriting (20.233) in terms of y we find

$$\frac{\partial v}{\partial \Phi} = \Phi \mu^2 \left[(\tau + y^2/3) + \hbar \frac{S_D g}{4} (\tau + y^2) \log(\tau + y^2) \right]. \quad (20.249)$$

Upon identifying

$$x = \frac{\tau}{y^{1/\beta}} = \frac{\tau}{y^{2+\hbar S_D g}} \approx \frac{\tau}{y^2} \left(1 - \hbar S \frac{g}{2} \log y^2 \right), \quad (20.250)$$

this can obviously be brought to the form

$$\begin{aligned} \frac{\partial v}{\partial \Phi} = \Phi \mu^2 y^{\delta-1} & \left(1 - \hbar S \frac{3}{4} g \log y^2 \right) \left\{ \left[\frac{1}{3} + x \left(1 + \hbar S \frac{g}{2} \log y^2 \right) \right] \right. \\ & \left. + \hbar S g/4 \left[(1+x) \left(1 + \hbar S \frac{g}{2} \log y^2 \right) \right] \times \left[\log y^2 + \log(1+x) \left(1 + \hbar S \frac{g}{2} \log y^2 \right) \right] \right\}. \end{aligned} \quad (20.251)$$

Since we are working at the one-loop level, the g^2 corrections can be neglected and we remain with

$$\frac{\partial v}{\partial \Phi} = \Phi \mu^2 y^{\delta-1} \left[\left(\frac{1}{3} + x \right) + \hbar \frac{S_D g}{4} (1+x) \log(1+x) \right]. \quad (20.252)$$

To the same order in g , this may be approximated by

$$\frac{\partial v}{\partial \Phi} = \Phi \mu^2 y^{\delta-1} \left[-\frac{2}{3} + (1+x)^\gamma \right]. \quad (20.253)$$

We have identified the leading power of $1+x$ with γ since it determines the τ -behaviour of the susceptibility for $\Phi \rightarrow 0$, $x \rightarrow \infty$. The expression (20.253) is of the desired universal form (20.247).

Note that this form has been obtained at the one-loop level by working in exactly 4 dimensions and calculating the first correction to g . Nowhere have we needed the ε -expansion and the critical indices δ , γ etc. as functions of the running coupling constant $g(\mu)$. Continuation to $4-\varepsilon$ dimensions becomes only necessary as we are trying to approach the physical situation $D=3$. If we move only an infinitesimal piece ε away from $D=4$, the running coupling stabilizes at $\hbar S_D g = \frac{2}{3}\varepsilon$. This is extracted from the coupling constant renormalization

$$\frac{1}{g(\mu)} = \frac{\mu^\varepsilon}{g_0} - \frac{3S_D \hbar}{2\varepsilon} \quad (20.254)$$

by going to the infrared limit $\mu \rightarrow 0$. This is what finally determines the critical indices as functions of ε :

$$\begin{aligned} \delta &= 3 + \varepsilon, & \eta &= 0, \\ \beta &= \frac{1}{2} - \frac{\varepsilon}{6}, & \gamma &= 1 + \varepsilon/6, \\ \nu &= \frac{1}{2} + \frac{\varepsilon}{12}. \end{aligned} \quad (20.255)$$

If the function $f(x)$ in the universal form (20.247) is desired to higher orders in ε , the calculation becomes quite cumbersome already at the next order in ε .

20.14 O(N)-Symmetric Theory

For completeness, let us generalize the previous calculation to the full O(N)-symmetric case with the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial\phi_a)^2 - \frac{m_0^2}{2}\phi_0^2 - \frac{g_0\mu^\varepsilon}{4!}(\phi_a^2)^2. \quad (20.256)$$

Now the quadratic fluctuations are given by

$$\delta^2 \mathcal{A} = \int d^4x \frac{1}{2} \delta\phi_a \left[-\partial^2 - m_0^2 - \frac{g_0\mu^\varepsilon}{6}(\delta_{ab}\Phi^2 + 2\Phi_a\Phi_b) \right] \delta\phi_b, \quad (20.257)$$

so that the one-loop corrected effective action becomes

$$\begin{aligned} \Gamma[\Phi] &= \frac{1}{2}(\partial\Phi_a)^2 - \frac{m_0^2}{2}\Phi_a^2 - \frac{g_0\mu^\varepsilon}{4}(\Phi_a^2)^2 \\ &\quad - \frac{i}{2} \hbar \text{tr} \log \left[(-\partial^2 - m^2)\delta_{ab} - \frac{g_0\mu^\varepsilon}{6}(\delta_{ab}\Phi^2 + 2\Phi_a\Phi_b) \right], \end{aligned} \quad (20.258)$$

with an effective potential

$$v[\Phi] = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\varepsilon}{4!}(\Phi_a^2)^2 + \frac{1}{2}\text{tr} \int \frac{d^D p_E}{(2\pi)^D} \log \left[(p_E^2 + m^2)\delta_{ab} + \frac{g_0\mu^\varepsilon}{6}(\delta_{ab}\Phi^2 + 2\Phi_a\Phi_b) \right]. \quad (20.259)$$

The trace of the logarithm of the matrix is calculated as the sum of the logarithms of the eigenvalues which are. These are

$$p^2 + m_0^2 + \frac{g_0\mu^\varepsilon}{6N}\Phi^2 \quad (20.260)$$

for the $N - 1$ unit vectors orthogonal to Φ and

$$p^2 + m^2 + \frac{g_0\mu^\varepsilon}{2N}\Phi^2 \quad (20.261)$$

for the N th unit vector parallel to Φ_a : Hence

$$v(\Phi) = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\varepsilon}{4!N}(\Phi_a^2)^2 + \frac{\hbar}{2} \int \frac{d^D p_E}{(2\pi)^D} \left[(N+1) \log \left(p_E^2 + m_0^2 + \frac{g_0\mu^\varepsilon}{6N}\Phi^2 \right) + \log \left(p_E^2 + m_0^2 + \frac{g_0\mu^2}{2N}\Phi^2 \right) \right]. \quad (20.262)$$

Performing the momentum integral, this becomes

$$v(\Phi_a) = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\varepsilon}{4!N}(\Phi_a^2)^2 + \frac{\hbar}{2} S \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \frac{2}{D} \times \left[(N-1) \left(m_0^2 + \frac{g_0\mu^\varepsilon}{6N}\Phi^2 \right)^{D/2} + \left(m_0^2 + \frac{g_0\mu^\varepsilon}{2\omega}\Phi^2 \right)^{D/2} \right]. \quad (20.263)$$

The corresponding equation is

$$j_a = \frac{\partial v(\Phi_a)}{\partial \Phi_a} = \Phi_a \left\{ m_0^2 + \frac{g_0\mu^\varepsilon}{3!}\Phi_a^2 + \hbar \frac{g_0\mu^\varepsilon}{4N} S \Gamma(D/2) \Gamma(1 - D/2) \times \left[\frac{1}{3}(N-1) \left(m_0^2 + \frac{g_0\mu^\varepsilon}{6N}\Phi^2 \right) + \left(m_0^2 + \frac{g_0\mu^\varepsilon}{2N}\Phi^2 \right)^{1-\varepsilon/2} \right] \right\}. \quad (20.264)$$

Expanding this to lowest order in $\varepsilon = 4 - D$, we find after renormalization

$$v(\Phi) = \frac{m^2}{2}\Phi_a^2 + \frac{g\mu^\varepsilon}{4!}(\Phi_a^2)^2 + \hbar\mu^{-\varepsilon} \frac{S}{8} \left\{ (N-1) \left(m^2 + \frac{g\mu^\varepsilon}{6}\Phi^2 \right)^2 \log \left(m^2 + \frac{g\mu^\varepsilon}{6}\Phi^2 \right) + \left(m^2 + \frac{g}{2}\Phi^2 \right)^2 \log \left(m^2 + \frac{g\mu^\varepsilon}{2}\Phi^2 \right) \right\}, \quad (20.265)$$

with an equation of state

$$j_a = \frac{\partial v}{\partial \Phi_a} = \Phi_a \left\{ m^2 + \frac{g\mu^\varepsilon}{3!}\Phi_a^2 + \hbar \frac{g}{4} S \left[\frac{1}{3}(N-1) \left(m^2 + \frac{g\mu^\varepsilon}{6}\Phi_a^2 \right) \log \left(m^2 + \frac{g\mu^\varepsilon}{6}\Phi_a^2 \right) + \left(m_0^2 + \frac{g\mu^\varepsilon}{2}\Phi_a^2 \right) \log \left(m^2 + \frac{g\mu^\varepsilon}{2}\Phi_a^2 \right) \right] \right\}. \quad (20.266)$$

Again, we may identify the susceptibility by taking $\Phi_a \rightarrow 0$:

$$j_a = m^2 \left\{ 1 + \hbar \frac{g\mu^\varepsilon}{4D} \left[\frac{1}{3}(N-1) + 1 \right] \log m^2 \right\} \approx (m^2)^{1+\hbar \frac{g\mu^\varepsilon}{4} S \frac{N+2}{3} + \mathcal{O}(g^2)} \quad (20.267)$$

so that [compare (20.238)]

$$\gamma = 1 + \hbar \frac{g\mu^\varepsilon}{4} S_D \frac{N+2}{3}. \quad (20.268)$$

The critical exponent δ is found by comparing the $m^2 = 0$ -relation (20.247) [recall also (20.239)]

$$j_a \rightarrow \Phi_a \frac{g\mu^\varepsilon}{3!} \Phi_a^2 \left[1 + \left(\frac{N-1}{3} + 3 \right) \hbar \frac{g\mu^\varepsilon}{4} \log \Phi^2 \right] \quad (20.269)$$

with the defining relation

$$j_a \approx \Phi_a (\Phi_a^2)^{(\delta-1)/2}. \quad (20.270)$$

This gives

$$\frac{\delta-1}{2} = 1 + \hbar \frac{S_D g\mu^\varepsilon}{4} \left(\frac{N-1}{3} + 3 \right). \quad (20.271)$$

Using the same reduced variables as before, i.e.,

$$\begin{aligned} y &= \sqrt{\frac{g}{2}} \frac{\sqrt{\Phi_a^2}}{\mu^{1-\varepsilon/2}} \\ x &= \tau/y^{1/\beta}, \quad m^2 = \mu^2 \tau, \end{aligned} \quad (20.272)$$

the equation of state can be brought to the universal form

$$\begin{aligned} j_a = \frac{\partial v}{\partial \Phi_a} &= \Phi_a \mu^2 y^{\delta-1} \left\{ \left(\frac{1}{3} + x \right) \right. \\ &\quad \left. + \hbar S \frac{g}{4} \left[\frac{1}{3}(N-1) \left(1 + \frac{x}{3} \right) \log \left(1 + \frac{x}{3} \right) + (1+x) \log(1+x) \right] \right\}. \end{aligned} \quad (20.273)$$

Using once more γ from (20.268), this can be rewritten, by analogy with (20.253), as

$$j_a = \frac{\partial v}{\partial \Phi_a} = \Phi_a \mu^2 y^{\delta-1} \left\{ \frac{2}{3}(N-2) + \frac{3}{N+2}(1+x)^\gamma + \frac{N-1}{N+2} \left(1 + \frac{x}{3} \right)^\gamma \right\}. \quad (20.274)$$

At this level, the exponents δ and γ do not yet have their infrared fixed-point values. From (20.137) we know that the fixed-point lies at

$$g^* \equiv \hbar g S = \frac{6\varepsilon}{N+8}. \quad (20.275)$$

This allows us to express δ in terms of ε as

$$\delta = 3 + \varepsilon, \quad (20.276)$$

valid for any N . Actually, this would have followed directly from the general scaling relations (20.176)–(20.180) and the fact that the anomalous dimension η vanishes to order ε [see (20.138)].

Finally, comparing (20.268) with (20.275), we obtain

$$\gamma = 1 + \frac{1}{2} \frac{N+2}{N+8} \varepsilon. \quad (20.277)$$

Thus we can calculate the other critical indices as

$$\nu = \frac{\gamma}{2-\eta} = \frac{1}{2} + \frac{N+2}{4(N+8)} \varepsilon, \quad (20.278)$$

$$\beta = \gamma(\delta-1) = \frac{1}{2} - \frac{3}{2(N+8)} \varepsilon. \quad (20.279)$$

20.15 Direct Scaling Form in the Limit of Large N

In the limit $N \rightarrow \infty$, effective action and potential are known exactly and it is possible to retrieve the scaling properties most directly. Consider the potential in $D = 4 - \varepsilon$ dimensions as calculated in (8.4): (here we use $\frac{g_0}{N}$ as a coupling constant rather than g_0)

$$v(\Phi) = \frac{1}{2} \Delta \Phi_a^2 + \frac{m_0^2}{2g_0} - \frac{N}{4g_0} \Delta^2 + \frac{1}{2} NS \frac{1}{2} \Gamma(2 - \varepsilon/2) \Gamma(-1 + \varepsilon/2) \frac{2}{4 - \varepsilon} \Delta^{2-\varepsilon/2}, \quad (20.280)$$

where Δ is the function of Φ_a^2 :

$$\Phi_a^2 = \frac{N}{g_0} \Delta - \frac{Nm_0^2}{g_0} - NS \frac{1}{2} \Gamma(2 - \varepsilon/2) \Gamma(-1 + \varepsilon/2) \Delta^{1-\varepsilon/2}. \quad (20.281)$$

We see that m_0^2 and Φ_a^2 scale in the same way so that v is a function of Φ_a^2/m_0^2 and m_0^2 . If we let $m_0^2 \rightarrow 0$ with Φ_a^2/m_0^2 fixed, the last term in Eq. (20.281) dominates the first and we find the limit

$$\left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0} \right) m_0^2 \xrightarrow{m_0 \rightarrow 0} -NS \frac{1}{2} \Gamma(2 - \varepsilon/2) \Gamma(-1 + \varepsilon/2) \Delta^{1-\varepsilon/2}. \quad (20.282)$$

Similarly, in v the last term dominates the third so that we can write

$$\begin{aligned} v(\Phi) &\rightarrow \Delta \frac{m_0^2}{2} \left[\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0} \right] + \frac{1}{2} NS \frac{1}{2} \Gamma(2 - \varepsilon/2) \Gamma(-1 + \varepsilon/2) \frac{2}{4 - \varepsilon} \Delta^{2-\varepsilon/2} \\ &\rightarrow \Delta \frac{m_0^2}{2} \left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0} \right) \frac{2 - \varepsilon}{4 - \varepsilon} \rightarrow \text{const} \times \left[m_0^2 \left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0} \right) \right]^{1+1/(1-\varepsilon/2)}. \end{aligned} \quad (20.283)$$

Comparing this with Widom's parametrization

$$v(\Phi) \sim (\Phi_a^2)^{(\delta+1)/2} f \left(\frac{m_0^2}{(\Phi_a^2)^{1/\beta}} \right), \quad (20.284)$$

we see that

$$\beta = \frac{1}{2}, \quad (20.285)$$

and

$$\frac{\delta + 1}{2} = \frac{2 - \varepsilon/2}{1 - \varepsilon/2}, \quad (20.286)$$

or

$$\delta = \frac{6 - \varepsilon}{2 - \varepsilon} = \frac{D + 2}{D - 2}. \quad (20.287)$$

This agrees with the $N \rightarrow \infty$ limit of (20.276)–(20.279).

Note that we have done the calculations in terms of the unrenormalized quantities m_0^2 and g_0 . If we go over to the renormalized ones m and g , the changes affect only the terms which were dropped in the limit $m_0^2 \rightarrow 0$ [i.e. the third term in (20.277) and the first one in (20.278)]. The result remains therefore the same.

20.16 QED and Landau Ghosts

In QED, the lowest-order renormalization of the charge in $4 - \varepsilon$ dimensions can be expressed for the inverse of the coupling constant $g \equiv e^2/4\pi = \alpha$ in the same form as in Eq. (20.135):

$$\frac{1}{g_\mu} = \frac{1}{g_0^2 \mu^{-\varepsilon}} + \frac{1}{6\pi^2 \varepsilon}. \quad (20.288)$$

Rewriting this as

$$\frac{\mu^\varepsilon}{g_0} = \frac{1}{g_\mu} - \frac{1}{6\pi^2 \varepsilon}, \quad (20.289)$$

we can go to the limit of $D = 4$ dimensions by letting $\varepsilon \rightarrow 0$, where we obtain

$$\frac{1}{g_0} = \frac{1}{g_\mu} + \frac{1}{6\pi^2} \ln \frac{\mu}{\mu_0}. \quad (20.290)$$

For the scale-dependent electromagnetic coupling constant this amounts to the flow equation

$$\frac{1}{\alpha} = \frac{1}{\alpha_\mu} + \frac{1}{3\pi^2} \ln \frac{\mu^2}{\mu_0^2} \quad (20.291)$$

or

$$\alpha_\mu = \frac{e_\mu^2}{4\pi} = \frac{\alpha}{1 - \frac{\alpha}{3\pi^2} \ln \frac{\mu^2}{\mu_0^2}}. \quad (20.292)$$

If the mass scale increases, the electromagnetic coupling grows beyond bounds.

In general, the scale-dependence of the coupling constant solves the differential equation (20.126)

$$\log \mu = \int_{\alpha}^{\alpha(\mu)} \frac{d\alpha}{\beta(\alpha)}, \quad (20.293)$$

where $\beta(g)$ is the β -function defined by $\beta(\alpha) \equiv \mu \partial_{\mu} \alpha_{\mu}$ [recall (20.59)]. The β -function starts out linearly like $-\varepsilon\alpha$ for small α and runs through a zero at $\alpha = g^* = \varepsilon/b$, where $b = 1/6\pi^2$. For larger α it grows, possibly indefinitely. In Fig. 20.3 we display the partial sums of increasing order as calculated in Ref. [4]:

$$\frac{\beta(\alpha)}{\alpha} = -\varepsilon + \frac{2}{3}\frac{\alpha}{\pi} + \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^2 - \frac{121}{144}\left(\frac{\alpha}{\pi}\right)^3 + \left(-\frac{61}{1296} + \frac{2}{27}\pi^2 + \frac{1}{2}\zeta(3)\right)\left(\frac{\alpha}{\pi}\right)^4 + \dots \quad (20.294)$$

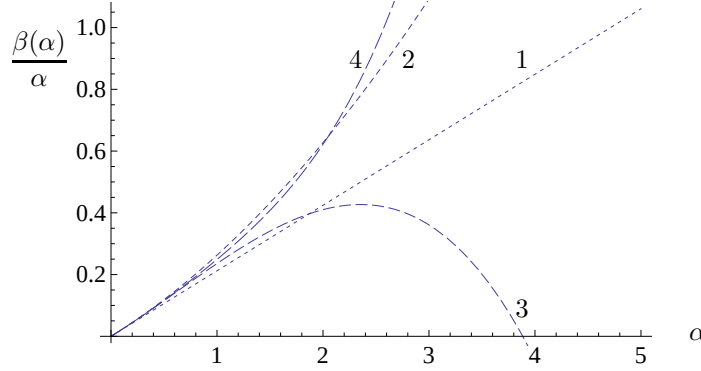


FIGURE 20.3 Flow of the coupling constant α_{μ} from left to right as the scale parameter μ increases (ultraviolet limit).

In the plots we have omitted the infinitesimal parameter ε .

When performing the integral (20.293) for the full $\beta(\alpha)$ -function in the denominator, a resummation of the divergent series is necessary since the power series for $\beta(\alpha)$ is an asymptotic expansion. Therefore a generalization of the relation (20.291) between $1/\alpha_{\mu}$ and $1/\alpha_0$ can be found only numerically [5]. In the infrared limit of μ_0 , for which one usually chooses the electron mass $\mu_0 = m_e$, the coupling starts out at the stable fixed point $g_0 = \alpha = e^2/4\pi$, this being the experimental fine-structure constant. Such a theory is called infrared-stable. With increasing mass scale μ , the scale-dependent coupling constant α_{μ} keeps growing logarithmically until α_{μ} reaches the so-called Landau singularity at the scale parameter

$$\mu = \mu_L = \mu_0 \exp\left(\frac{3\pi}{2\alpha}\right) \approx m_e e^{280}. \quad (20.295)$$

This is an extremely large mass scale where many other forces dominate the electromagnetic ones.

The electromagnetic correlation functions possess poles at the corresponding high energy-momentum square $q^2 = \mu_L^2$, as was first discovered by Landau. The lowest-order amplitude for the exchange of a photon between two electrons

$$\frac{\alpha}{q^2} \quad (20.296)$$

is modified at large order to the renormalized amplitude

$$\frac{\alpha}{q^2} \frac{1}{1 - \frac{\alpha}{3\pi} \ln \frac{q^2}{m_e^2}}. \quad (20.297)$$

From the spectral representation of any correlation function we deduce that the pole at $q^2 = 0$ represents a state in the Hilbert space with positive norm. This is the state vector of the photon. The denominator of the amplitude (20.297) has also a second pole. Since the first has a positive slope as q^2 passes through zero, the second one at $q^2 = \mu_L^2$ must have a negative slope. In the Hilbert space, a pole with a negative slope of the inverse amplitude implies that the state at $q^2 = \mu_L^2$ must have a negative norm. Such states are commonly called *ghosts*. Thus the particles represented by Landau poles at $q^2 = \mu_L^2$ are really *Landau ghosts*.

Such states will also be found in the quantization of gravity to be discussed later in Chapter 30. They will have a range of the order of Planck length. They will be overwhelmed by stronger forces reaching out much farther than that. This will be discussed after Eq. (30.55).

Notes and References

More details on the subject of this chapter can be found in the textbook:

H. Kleinert and V. Schulte-Frohlinde, *Critical Phenomena in ϕ^4 -Theory*, World Scientific, Singapore, 2001 (<http://klnrt.de/b8>).

See also the paper

H. Kleinert, J. Phys. B **46**, 175401 (2013) (<http://klnrt.de/403>).

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21

Critical Properties of Nonlinear σ -Model

The $4 - \varepsilon$ -expansion of $O(N)$ -symmetric ϕ^4 -theories is not the only technique to study critical phenomena of three-dimensional systems with $O(N)$ -symmetry. A great deal can be learned about such systems by ignoring the size fluctuations of the fields and focussing attention only upon the Goldstone modes. We have explained in Chapter 9 that, in the limit of very low temperature or strongly negative mass parameter m^2 , the fields ϕ_a , ($a = 1, \dots, N$) in a $(\phi_a^2)^2$ -theory

$$\mathcal{A} = \int d^d x \left[\frac{1}{2} (\partial \phi_a)^2 + \frac{m^2}{2} \phi_a^2 + \frac{g}{4} (\phi_a^2)^2 \right] \quad (21.1)$$

acquire an infinite mass

$$M^2 = -2m^2 \rightarrow \infty \quad (21.2)$$

and are practically frozen at a fixed size

$$\phi_a^2 = |\phi|^2. \quad (21.3)$$

The Goldstone modes of the $O(N)$ -symmetric ϕ^4 field-theories are the main excitations of the system. They take place in the ordered phase, and they appear in the directions of ϕ_a , which fluctuate easily. If these directions are denoted by the unit vectors $n_a = \phi_a / \phi$, the euclidean action describing these fluctuations can be written as

$$\mathcal{A} = \frac{1}{2t} \int d^D x (\partial n_a)^2, \quad n_a^2 = 1, \quad (21.4)$$

where $1/t = |\phi|^2$. The partition function is defined by functionally integrating over the Boltzmann factor $e^{-\mathcal{A}}$ for all directions at each space point.

21.1 Introductory Remarks

The functional measure of these integrations is

$$\begin{aligned} \int \mathcal{D}\mathbf{n} &= \prod_{x,a} \int_{-\infty}^{\infty} \frac{d^N n_a(x)}{S_N} \delta^{(D)}(n_a^2 - 1) \\ &= \prod_{x,a} \int \frac{d^{N-1} n_a(x)}{S_N}, \end{aligned} \quad (21.5)$$

where $S_N = 2\pi^{N/2}/\Gamma(N/2)$ is the surface of a sphere in an N -dimensional space. The partition function is therefore

$$Z = \int \left[\frac{\mathcal{D}\mathbf{n}}{S_N} \right] e^{-\mathcal{A}[\mathbf{n}]}.$$
 (21.6)

As mentioned above, this is the continuum version of the so-called classical $O(N)$ -Heisenberg model of magnetism on a lattice

$$Z = \prod_{\mathbf{x},a} \left[\int \frac{d\mathbf{n}(\mathbf{x})}{S_N} \right] \exp \left\{ \frac{1}{2T} \sum_{\mathbf{x},i} [(\nabla_i n_a(\mathbf{x} + \mathbf{i}))^2 + 2D] \right\},$$
 (21.7)

where $\nabla_i n(\mathbf{x}) = n(\mathbf{x} + \mathbf{i}) - n(\mathbf{x})$ are the differences of $n^a(\mathbf{x})$ between sites. Because of this connection, we shall rename g as t and speak about it as a temperature. In Chapter 9 we have solved this model exactly in the limit $N \rightarrow \infty$, and the reader is referred to this chapter to recapitulate some of the results.

We shall now calculate the partition function (21.6) perturbatively for arbitrary N . For this we select a particular orientation $(0, \dots, 1)$ of the direction vector of the field ϕ_a , and consider the first $N - 1$ components

$$\pi_a(x) \equiv n_a(x); \quad a = 1, \dots, N - 1$$
 (21.8)

as independent fields of the system. The N th component is then determined from the others by the unit length of ϕ_a for $a = (1, \dots, N)$. It is commonly called σ :

$$n_N(x) = \sqrt{1 - \pi_a^2(x)} \equiv \sigma(x),$$
 (21.9)

and we can write the action of the nonlinear σ -model as

$$\mathcal{A} = \frac{1}{2t} \int d^D x \left[(\partial \pi_a)^2 + \left(\partial \sqrt{1 - \pi_a^2} \right)^2 \right].$$
 (21.10)

This action is scale invariant for $D = 2$ dimensions, where the field π_a has a vanishing naive dimension. The theory is renormalizable by power counting. Below $D = 2$ dimensions, the fluctuations are so violent that massless excitations do not exist. All Goldstone modes become massive at all temperatures. The dimension $D = 2$ is called the *lower critical dimension*.

For the action (21.4), the measure of integration is found by performing in (21.5) the integral over $n_N(x)$ after which we remain with

$$\int \frac{\mathcal{D}^{N-1}\boldsymbol{\pi}}{\sqrt{1 - \boldsymbol{\pi}^2}} = \prod_{x,a=1}^{N-1} \int \frac{d\pi_a(x)}{\sqrt{1 - \pi_a^2(x)}}.$$
 (21.11)

This can also be written as

$$\prod_{x,a=1}^{N-1} \int \mathcal{D}^{N-1}\pi_a \exp \left\{ -\frac{1}{2a^D} \int d^D x \log(1 - \pi_a^2(x)) \right\},$$
 (21.12)

where we have assumed the path integral to be set up on an underlying simple lattice of spacing a , such that we may write the products over all space points as exponentials of sums, which are turned into integrals:

$$\prod_x f(x) = \exp \left[\sum_x \log f(x) \right] = \exp \left[\frac{1}{a^D} \int d^D x \log f(x) \right]. \quad (21.13)$$

Then the partition function (21.6) of the nonlinear σ -model becomes

$$Z = \prod_{x,a=1}^{N-1} \left[\int \mathcal{D}^{N-1} \pi_a \right] \exp \left\{ -\frac{1}{2t} \int d^D x \left[(\partial \pi_a)^2 + \left(\partial \sqrt{1 - \pi_a^2} \right)^2 \right] \right. \\ \left. - \frac{1}{2a^D} \int d^D x \sum_{a=1}^{N-1} \log [1 - \pi_a^2(x)] \right\}. \quad (21.14)$$

Note that the original $O(N)$ -invariance of the Lagrangian (21.228) under transformation

$$\delta n_a = \omega_{ab} \delta n_b, \quad (21.15)$$

with $\omega_{ab} = -\omega_{ba}$, is present in (21.4) for transformations

$$\begin{aligned} \delta \pi_a &= \omega_{ab} \delta \pi_b + \omega_{aN} \sqrt{1 - \pi_c^2}, \\ \delta \sqrt{1 - \pi_c^2} &= -\omega_{aN} \delta \pi_a. \end{aligned} \quad (21.16)$$

21.2 Perturbation Theory

For a perturbation calculation of (21.14) we identify the free action as

$$\mathcal{A}_0 = \frac{1}{2t} \int d^D x (\partial \pi_a)^2, \quad (21.17)$$

and consider the remaining terms as interactions:

$$\begin{aligned} \mathcal{A}_{\text{int}} &= \int d^D x \left\{ \frac{1}{2t} \left[\frac{1}{4} (\partial \pi_a^2) (\partial \pi_b^2) - \frac{3}{16} (\partial \pi_a^2) \partial (\pi_b^2)^2 + \dots \right] \right. \\ &\quad \left. - \frac{1}{2a^D} \pi_a^2(x) - \frac{1}{4a^D} (\pi_a^2)^2 - \frac{1}{6a^D} (\pi_a^2)^3 - \dots \right\}. \end{aligned} \quad (21.18)$$

The functional integration is limited to the regime $\pi^2 < 1$, to be covered twice, once for $\sigma = +\sqrt{1 - \pi^2}$ and once for $\sigma = -\sqrt{1 - \pi^2}$. The perturbation expansion is a power series in t . For small t , the fluctuations will take place in the neighborhood of $\pi^2 \sim 0$. One may therefore replace the restricted integrations over each field component $\pi_a(x)$ by an unrestricted one covering the entire field axis from $-\infty$ to ∞ . Thereby we commit only a very small error of the order of $e^{-1/t}$. With this replacement, the free propagator is

$$\begin{aligned} \langle \pi_a(x) \pi_b(y) \rangle &= \delta_{ab} \int \frac{d^D k}{(2\pi)^D} \frac{t}{k^2} e^{ik(x-y)} \\ &\equiv \delta_{ab} G_0(x-y). \end{aligned} \quad (21.19)$$

In order to avoid problems with singularities at $k = 0$ (infrared singularities), it is useful to place the system into an external field pointing along the preferred field direction $(\phi_1, \dots, \phi_N) \propto (0, \dots, 1)$:

This corresponds to putting the Heisenberg model of magnetism into an external magnetic field. This field serves to stabilize the selected preferred field direction. Expanding also $\mathcal{A}_{\text{ext}}$ in powers of π_a , this replacement produces a pion mass term in the action

which changes the free propagator into

where

It also adds a further set of interactions

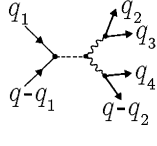
the first being a trivial shift in the energy. In momentum space, the lowest interactions in (21.18) can be written as follows

2-point

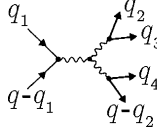
4-point

$$\begin{array}{c} q_1 \\ \nearrow \\ q - q_1 \end{array} \begin{array}{c} \nearrow \\ \searrow \\ q - q_2 \end{array} \begin{array}{c} \nearrow \\ \searrow \\ q_2 \end{array} = -\frac{1}{4a^D} \int \bar{d}^D q_1 \int \bar{d}^D q_2 \int \bar{d}^D q \pi_a(q_1) \pi_a(q - q_1) \pi_b(-q_2) \pi_b(q_2 - q), \quad (21.27)$$

6-point



$$= -\frac{1}{16t} \int d^D q_4 \cdots \int d^D q (q^2 + m^2) \times \pi_a(q_1) \pi_a(q-q_1) \pi_b(-q_2) \pi_b(-q_3) \pi_c(-q_4) \pi_c(q_2 + q_3 + q_4 - q), \quad (21.28)$$

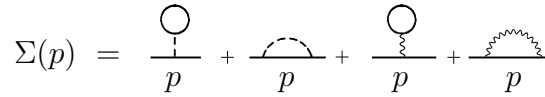


$$= -\frac{1}{6a^D} \int d^D q_1 \cdots \int d^D q_4 \int d^D q \times \pi_a(q_1) \pi_a(q-q_1) \pi_b(-q_2) \pi_b(-q_3) \pi_c(-q_4) \pi_c(q_2 + q_3 + q_4 - q). \quad (21.29)$$

The dashed line stands for a factor $q^2 + m^2$, while the wiggly lines represent a local interaction. In addition, these lines indicate the contraction of the $O(N)$ -exponents of the pairs of π -lines emerging from its ends.

From the magnetic interaction (21.20) we obtain once more the lower two-point interaction with a prefactor $m^2/8t$, and the lower four-point interaction with a prefactor $m^2/16t$, etc..

We shall now study the renormalization of the propagator to lowest order in perturbation theory. The self-energy contains two contractions involving the four-point function:



$$\Sigma(p) = \frac{\text{circle with vertical line}}{p} + \frac{\text{dashed line with semi-circle}}{p} + \frac{\text{circle with vertical wiggly line}}{p} + \frac{\text{wiggly line with semi-circle}}{p}. \quad (21.30)$$

Let us calculate the first two diagrams using (21.26) and closing two lines by a propagator. Alternatively, we may calculate the expectation

$$\frac{1}{8t} \int d^D q_1 \int d^D q_2 \int d^D q (q^2 + m^2) \langle \pi_c(p) \pi_a(q_1) \pi_a(q-q_1) \pi_b(-q_2) \pi_b(q_2-q) \pi_d(-p) \rangle$$

by forming all resulting Wick contractions, removing the disconnected diagrams, and amputating the external legs. This gives

$$\begin{aligned} & 2 \int d^D q_1 \int d^D q_2 \int d^D q (q^2 + m^2) \left\{ (N-1) \delta_{ca} \delta^{(D)}(p+q_1) \delta_{ad} \delta^{(D)}(q-q_1-p) \frac{\delta^{(D)}(-q)}{q^2 + m^2} \right. \\ & \quad \left. + 2 \delta_{ca} \delta^{(D)}(p+q_1) \delta_{ab} \frac{\delta^{(D)}(q-q_1-q_2)}{(q-q_1)^2 + m^2} \delta^{(D)}(q_2-q-p) \right\} \\ & = \delta_{cd} \frac{1}{2} \int d^D q \left\{ (N-1) \frac{m^2}{q^2 + m^2} + 2 \frac{q^2 + m^2}{(p+q)^2 + m^2} \right\}. \end{aligned} \quad (21.31)$$

By rewriting

$$\int d^D q \frac{q^2 + m^2}{(q+p)^2 + m^2} = \int d^D q \frac{(q+p)^2 + m^2 - 2p(q+p) + p^2}{(q+p)^2 + m^2}, \quad (21.32)$$

we can drop the $p(q+p)$ -term, since it is odd in $(q+p)$, and (21.32) becomes

$$\int d^D q \frac{q^2 + m^2}{(q+p)^2 + m^2} = \int d^D q + p^2 \int d^D q \frac{1}{q^2 + m^2}. \quad (21.33)$$

On a lattice, the first integral is equal to

$$\frac{1}{Na^D} \sum_q = \frac{1}{a^D}, \quad (21.34)$$

where N is the number of cells in the underlying lattice. Hence we can identify

$$\int d^D q = \frac{1}{a^D}. \quad (21.35)$$

This term in (21.33) is precisely cancelled by the contribution of the two-point interaction (21.26), and we arrive at

$$\sigma_{cd}(p) = \delta_{cd} \left[\frac{1}{2} (N-1) m^2 + p^2 \right] L, \quad (21.36)$$

where L is the one-loop integral

$$L \equiv \int d^D q \frac{1}{q^2 + m^2}. \quad (21.37)$$

The two-point vertex function is therefore at the one-loop level

$$\Gamma_{cd}^{(2)}(p) = \delta_{cd} \left\{ \frac{1}{t} (p^2 + m^2) + \left[\frac{1}{2} (N-1) m^2 + p^2 \right] L \right\}. \quad (21.38)$$

A one-loop effective action would have a free-field part

$$\mathcal{A}_{\text{eff}}[\pi] = \int d^d x \pi_c(x) \Gamma_{cd}^{(2)}(-i\partial) \pi_d(x). \quad (21.39)$$

The resulting two-point vertex function is thus

$$\Gamma_{cd}^{(2)}(p) = \delta_{cd} \left\{ \frac{1}{t} (p^2 + m^2) + \left[\frac{1}{2} (N-1) m^2 + p^2 \right] L \right\} + \mathcal{O}(t). \quad (21.40)$$

The corresponding effective action has a free-field part

$$\mathcal{A}_{\text{eff}}[\pi] = \int d^D x \Pi_c(x) \Gamma_{cd}^{(2)}(-i\partial) \Pi_d(x), \quad (21.41)$$

and reads in x -space

$$\mathcal{A}_{\text{eff}} = \frac{1}{2} \int d^D x \left\{ \left[\frac{1}{t} + L \right] (\partial \Pi_a)^2 - \frac{h}{t} \left[1 + \frac{1}{2} (N-1) t L \right] \Pi_a^2 \right\}. \quad (21.42)$$

These are the same field expressions as in the original free-field action, except that t and h^2 are replaced by the renormalized values,

$$\begin{aligned}\frac{1}{t} &\rightarrow \frac{1}{t} + L \\ h &\rightarrow h \left[1 + \frac{1}{2}(N-1)tL \right].\end{aligned}\quad (21.43)$$

The surprising feature of this theory is that, due to the $O(N)$ -symmetry, the renormalized action to all orders can be described in terms of only two renormalization constants, one for the wave function renormalization

$$\pi_R = Z_\pi^{-1/2} \pi \quad (21.44)$$

and another for the temperature renormalization

$$t_R = Z_t^{-1} t. \quad (21.45)$$

The symmetry forces us to introduce the renormalized magnetic field h as

$$h_R = Z_t^{-1} Z_\pi^{1/2} h \equiv Z_h h. \quad (21.46)$$

This will soon be demonstrated to any order on general grounds. Supposing, for a moment, that this is true. Then we write the renormalized free part of the effective action as

$$\mathcal{A}_{\text{eff}} = \frac{1}{2t_R} \int d^D x \left[(\partial \pi_R)^2 + h_R \pi_R^2 \right]. \quad (21.47)$$

Comparison with (21.43) gives

$$\begin{aligned}Z_t Z_\pi^{-1} &= (1 - tL), \\ Z_\pi^{-1/2} &= \left(1 + \frac{N-1}{2} tL \right),\end{aligned}\quad (21.48)$$

and hence

$$\begin{aligned}Z_\pi &= 1 - (N-1)tL + \dots, \\ Z_t &= 1 - (N-2)tL + \dots,\end{aligned}\quad (21.49)$$

$$Z_h = Z_t^{-1} Z_\pi^{1/2} = 1 + \frac{N-3}{2} tL + \dots. \quad (21.50)$$

Thus the temperature is renormalized as follows

$$\frac{1}{t_R} = \frac{1}{t} - (N-2)L + \dots. \quad (21.51)$$

For the simplest case of an $O(2)$ -model, this implies *no* first-order renormalization of the temperature at all, i.e., the coupling strength of the π_a -fields is unchanged by fluctuations. This property turns out to hold at *all* orders in t .

Obviously, this result depends crucially on the way the two renormalization factors in (21.42) are distributed over wave function and temperature. It is therefore worthwhile to go through the general renormalization in some detail.

Let us point out a property of this field theory in $D = 1$ dimension where we may interpret x as an imaginary time τ , and $\pi_a(x)$ as a position variable $x_a(\tau)/R$ of a point particle on the surface of a sphere of radius $R = 1/\sqrt{t}$ in N dimensions. The comparison will be presented in Section 21.8

21.3 Symmetry Properties of the Renormalized Effective Action

The $O(N)$ -symmetry of the theory implies the existence of a Ward-Takahashi identity which has to be fulfilled by the generating functional of all correlation functions:

$$Z[j_a, h] = \int \frac{\mathcal{D}\pi}{\sqrt{1 - \pi^2}} \exp \left\{ -\frac{1}{t} \int d^D x (\partial \pi_a)^2 + \left(\partial \sqrt{1 - \pi_a^2} \right)^2 - j_a \pi_a - h \sqrt{1 - \pi_a^2} \right\}. \quad (21.52)$$

Under a rotation in each of the (N, a) -planes for $a = 1, \dots, N - 1$, by an angle $\omega_{aN} \equiv \omega_a$:

$$\delta \pi_a = \omega_a \sqrt{1 - \pi_a^2}, \quad (21.53)$$

$$\delta \sqrt{1 - \pi_a^2} = -\omega_a \pi_a, \quad (21.54)$$

the source terms go over into

$$\begin{aligned} & \int d^D x \left\{ j_a \pi_a h \sqrt{1 - \pi_a^2} + \left[j_a \sqrt{1 - \pi_a^2} - h \pi_a \right] \omega_a \right\} \\ &= \int d^D x \left[(j_a - h \omega_a) \pi_a + (h + j_a \omega_a) \sqrt{1 - \pi_a^2} \right]. \end{aligned} \quad (21.55)$$

This implies that $Z[j_a, h]$ must be invariant under the replacement

$$j_a \rightarrow j_a + h \omega_a, \quad (21.56)$$

$$h \rightarrow h - j_a \omega_a, \quad (21.57)$$

which changes $Z[j_a, h]$ by

$$\delta Z[j_a, h] = \left[\left(h \frac{\partial}{\partial j_a} - \partial_a \frac{\partial}{\partial h} \right) Z \right] \omega_a. \quad (21.58)$$

This change has to vanish for any ω_a .

In order to find the consequences for the connected correlation functions, we go over to their generating functional

$$W[j_a, h] = -t \log Z[j_a, h]. \quad (21.59)$$

Defining the effective fields as usual by the functional derivatives of $W[j_a, h]$ with respect to the currents,

$$\Pi_a \equiv -\frac{\partial W}{\partial j_a}, \quad (21.60)$$

the effective energy at a fixed magnetic field h is given by the Legendre transform

$$\Gamma[\Pi_a, h] = W[j_a, h] + \int d^D x \Pi_a(x) j_a(x), \quad (21.61)$$

which contains the information on the currents in the derivative

$$j_a = \frac{\partial \Gamma}{\partial \Pi_a}. \quad (21.62)$$

The symmetry property (21.58) of $Z[j_a, h]$ can then be expressed as

$$\int d^D x \left[h(x) \Pi_a(x) + \frac{\delta \Gamma}{\delta h(x)} \frac{\delta \Gamma}{\delta \Pi_a(x)} \right] = 0. \quad (21.63)$$

We now separate $\Gamma[\Pi_a, h]$ into an h -free part $\Gamma^{(0)}[\Pi_a]$, and a part containing h . Since h is small, we may keep only the linear term in h , and continue with

$$\Gamma[\Pi_a, h] = \Gamma^{(0)}[\Pi_a] + \int d^D x h(x) \Gamma^{(1)}[\Pi_a](x) + \dots \quad (21.64)$$

For the first two expansion terms, Eq. (21.63) implies

$$\int d^D x \Gamma^{(1)}[\Pi_a](x) \frac{\delta \Gamma^{(0)}[\Pi_a]}{\delta \Pi_a(x)} = 0, \quad (21.65)$$

$$\int d^D x' \left\{ \Pi_a(x') + \Gamma^{(1)}[\Pi_a](x') \frac{\delta \Gamma^{(1)}[\Pi_a](x)}{\delta \Pi_a(x')} \right\} = 0. \quad (21.66)$$

For further discussion, we shall consider only the case of two dimensions, where the action is scale invariant and renormalizable by power counting. We focus attention upon the divergent part of the effective action, which also satisfies the differential equations (21.65), (21.66). Since the theory is renormalizable, the infinities appear only in quite restricted functional forms, the terms which have the same form as those in the original, i.e., $\int d^2 x (\partial \Pi_a)^2$ and $\int d^2 x (\Pi_a^2)^n$. Thus we only need to search for solutions of (21.65) among quite restricted local functionals $\Gamma^{(1)}[\Pi_a](x)$. First there is the restriction (21.66). Moreover, the search for possible expansion coefficients $\Gamma^{(1)}[\Pi_a](x)$ can be restricted even more. Since h has the dimension two, $\Gamma^{(1)}[\Pi_a](x)$ must be dimensionless. This implies that, in a further functional expansion of $\Gamma^{(1)}[\Pi_a](x)$,

$$\begin{aligned} \Gamma^{(1)}[\Pi_a](x) &= \Gamma^{(1)}[0](x) + \int d^2 y \Gamma^{(1)'}[0](x, y) \delta \Pi_a(y) \\ &\quad + \frac{1}{2} \int d^2 y d^2 z \Gamma^{(1)''}[0](x, y) \delta \Pi_a(y) \delta \Pi_a(z) + \dots \end{aligned} \quad (21.67)$$

The only bilocal coefficients permitted on dimensional grounds are $\delta^{(2)}$ -functions, so that $\Gamma^{(1)}[\Pi_a](x)$ can only receive contributions from local *functions* of $\Pi_a(x)$:

$$\Gamma^{(1)}[\Pi_a](x) = \gamma^{(1)}(\Pi_a(x)). \quad (21.68)$$

Then Eq. (21.66) implies that

$$\frac{\partial \gamma^{(1)}}{\partial \Pi_a} \gamma^{(1)} + \Pi_a = 0, \quad (21.69)$$

which can be integrated right away to give

$$\gamma^{(1)}(\Pi_a(x)) = \sqrt{B - \Pi_a^2(x)}. \quad (21.70)$$

The h -free term $\Gamma^{(0)}[\Pi_a]$ must reflect the $O(N)$ -invariance. Hence it must have the form

$$\Gamma^{(0)}[\Pi_a] = \int d^D x A \left\{ \frac{1}{2} (\partial \Pi_a)^2 + \frac{1}{2} \left(\partial \sqrt{C - \Pi_a^2} \right)^2 \right\}, \quad (21.71)$$

with some arbitrary constants A and C .

The point is now that due to the identity (21.65), the constants C and B are not independent. Indeed, since

$$\begin{aligned} \frac{\delta \Gamma^{(0)}}{\delta \Pi_a} &= -\partial^2 \Pi_a + \frac{\delta}{\delta \Pi_a} \frac{1}{2} \int d^2 x \frac{(\Pi_c \partial_i \Pi_c)^2}{C - \Pi_d^2} \\ &= -\partial^2 \Pi_a + \frac{\partial_i \Pi_a \partial_i \Pi_c}{C - \Pi_d^2} + \frac{\Pi_a}{(C - \Pi_d^2)} (\Pi_c \partial_i \Pi_c)^2 - \partial_i \left[\frac{\Pi_a}{\sqrt{C - \Pi_d^2}} \frac{\Pi_c \partial_i \Pi_c}{\sqrt{C - \Pi_d^2}} \right] \\ &= -\partial^2 \Pi_a + \frac{\Pi_a}{\sqrt{C - \Pi_d^2}} \partial_i^2 \sqrt{C - \Pi_d^2}, \end{aligned} \quad (21.72)$$

we can write (21.65) as

$$\int d^2 x \sqrt{B - \Pi_a^2} \left[-\partial^2 \Pi_a + \frac{\Pi_a}{\sqrt{C - \Pi_d^2}} \partial^2 \sqrt{C - \Pi_d^2} \right] = 0. \quad (21.73)$$

Partial integrations on the first term brings this to

$$\int d^2 x \left[-\Pi_a \partial^2 \sqrt{B - \Pi_c^2} + \sqrt{\frac{B - \Pi_c^2}{C - \Pi_d^2}} \partial^2 \sqrt{C - \Pi_c^2} \right] = 0, \quad (21.74)$$

and we conclude that the two constants B and C must be identical. The terms in the effective action with divergences have therefore the general form

$$\Gamma^{(0)}[\Pi_a] = \frac{1}{t} \int d^2 x \left\{ \frac{A}{2} (\partial_i \Pi_a)^2 + \frac{A}{2} \left(\partial_i \sqrt{B - \Pi_a^2} \right)^2 - h \sqrt{B - \Pi_a^2} \right\}. \quad (21.75)$$

This can be brought to the original form by introducing renormalized quantities

$$\Gamma^{(0)}[\Pi_a] = \frac{1}{t_R} \int d^2x \left\{ \frac{1}{2} (\partial_i \Pi_{Ra})^2 + \frac{1}{2} \left(\partial_i \sqrt{1 - \Pi_{Ra}^2} \right)^2 - h_R \sqrt{1 - \Pi_{Ra}^2} \right\}. \quad (21.76)$$

If we rewrite (21.75) as

$$\begin{aligned} \Gamma^{(2)}[\Pi_a] = & \frac{AB}{t} \int d^2x \left\{ \frac{1}{2} [\partial(B^{1/2}\Pi_a)]^2 \right. \\ & \left. + \frac{1}{2} [\partial\sqrt{1 - (B^{-1/2}\Pi_a)^2}]^2 - hA^{-1}B^{-1/2}\sqrt{1 - (B^{-1/2}\Pi_a)^2} \right\}, \end{aligned} \quad (21.77)$$

we identify

$$\Pi_{Ra} = B^{-1/2}\Pi_a, \quad (21.78)$$

$$\frac{1}{t_R} = \frac{AB}{t}, \quad (21.79)$$

$$h_R = A^{-1}B^{-1/2}h, \quad (21.80)$$

implying a renormalizability of the theory in terms of the two renormalization constants:

$$Z_t = AB, \quad (21.81)$$

$$Z_\pi = B. \quad (21.82)$$

21.4 Critical Behavior in $N=2+\epsilon$ Dimensions

Just as in the ϕ^4 -theory of Chapter 18, where we studied the renormalization group in $4 - \epsilon$ dimensions, we shall now consider $2 + \epsilon$ dimensions for $\epsilon > 0$. The naive scale dimension of t is $\mu^{-\epsilon}$, where μ is a mass. We therefore go over to a dimensionless renormalized temperature by replacing in Eq. (21.51)

$$\frac{1}{t_R} \rightarrow \frac{\mu^\epsilon}{t_R}. \quad (21.83)$$

Then the renormalization equations for t_R reads

$$\frac{\mu^\epsilon}{t_R} = \frac{1}{t} - (N - 2)L = \frac{1}{t} Z_t. \quad (21.84)$$

We now calculate L in $2 + \epsilon$ dimensions. According to Eqs. (11.140) and (11.137), the integral diverges near $\epsilon = 0$ as follows:

$$\begin{aligned} L = \int \frac{d^D q}{(2\pi)^D} \frac{1}{q^2 + h} &= S_D \frac{1}{2} \Gamma\left(1 + \frac{\epsilon}{2}\right) \Gamma\left(-\frac{\epsilon}{2}\right) h^{\epsilon/2} \\ &= -S_D \frac{1}{\epsilon} h^{\epsilon/2} + \mathcal{O}(\epsilon^1). \end{aligned} \quad (21.85)$$

We use once more the mass scale μ and remove from this integral the divergent expression

$$L_{div} = -S_D \mu^\epsilon \frac{1}{\epsilon}. \quad (21.86)$$

Then (21.85) can be written as

$$\frac{\mu^\epsilon}{t_R} = \frac{1}{t} + \frac{1}{2}(N-2)S_D \mu^\epsilon, \quad (21.87)$$

or

$$t = \mu^{-\epsilon} t_R \left[1 + \frac{1}{\epsilon}(N-2)S_D t_R \right]. \quad (21.88)$$

From (21.87) we calculate the β -function

$$\beta(t_R) \equiv t_R^{-1} \mu \partial_\mu t_R = -t_R^2 \mu \partial_\mu t_R^{-1}|_{t,\epsilon} = \epsilon t_R - (N-2)S_D t_R^2 + \dots \quad (21.89)$$

This has an ultraviolet-stable fixed point at

$$t_R^c = \frac{\epsilon}{(N-2)} + \dots \quad (21.90)$$

21.5 Critical Exponents

We now use the above results to calculate the critical exponents at the one-loop level. We first consider the exponent ν governing the way in which the correlation length ξ goes to infinity as t_R approaches the critical point t_R^c from above:

$$\xi \propto (t_R - t_R^c)^{-\nu}. \quad (21.91)$$

The following analysis is very similar to that in Chapter 20, except for one important difference: the physical variable that depends directly on the temperature of the system is now $t_R(\mu)$. In the ϕ^4 -theory of Chapter 20, it was $m^2(\mu) \propto T/T_c - 1 \equiv \tau$. By analogy, we set here $\tau = t/t_c - 1$, so that the behavior (21.91) amounts to the power behavior of the correlation length $\xi \propto \tau^{-\nu}$.

The most direct way to calculate the critical exponent ν is based on the observation that physically observable quantities cannot have anomalous dimensions. Since the coherence length ξ is such a quantity, it satisfies $\mu \partial_\mu \xi(t) = 0$, and after expressing ξ in terms of the renormalized temperature t_R , which depends itself on μ via (21.84), we obtain the renormalization group equation

$$\left[\mu \partial_\mu + \beta(t_R) \frac{\partial}{\partial t_R} \right] \xi(t_R, \mu) = 0, \quad (21.92)$$

this being an analog of the Eq. (20.34) without the γ - and γ_m -terms. Now, dimensional analysis implies that ξ must depend on the two arguments as follows

$$\xi(t_R, \mu) = \mu^{-1} \bar{\xi}(t_R), \quad (21.93)$$

so that for $\bar{\xi}(t_R)$, the differential equation becomes

$$\left[-1 + \beta(t_R) \frac{\partial}{\partial t_R} \right] \bar{\xi}(t_R) = 0. \quad (21.94)$$

This is solved by

$$\bar{\xi}(t_R) = \text{const} \times \exp \left\{ \int_0^{t_R} dt \frac{1}{\beta(t)} \right\}. \quad (21.95)$$

We may choose the correlation length ξ at zero temperature to coincide with μ^{-1} , which amounts to the initial condition

$$\bar{\xi}(0) = 1. \quad (21.96)$$

The integral is singular at $t = 0$, and a subtraction is necessary to extract a finite result. For this we make use of the explicit form of the singularity, $\beta(t) \approx \epsilon t$, found in (21.89), and rewrite (21.95) as follows

$$\bar{\xi}(t_R) = \text{const} \times t_R^{1/\epsilon} \exp \left\{ \int_0^{t_R} dt \left[\frac{1}{\beta(t)} - \frac{1}{\epsilon t} \right] \right\}. \quad (21.97)$$

For $t_R \rightarrow t_R^c$, this equation behaves like

$$\begin{aligned} \bar{\xi}(t_R) &\approx \text{const} \times (t_R^c)^{1/\epsilon} \exp \left\{ \int_0^{t_R} dt \frac{1}{\beta'(t_R^c)(t - t_R^c)} \right\} \\ &\approx \text{const} \times (t_R^c)^{1/\epsilon} (t_R - t_R^c)^{1/\beta'(t_R^c)}. \end{aligned} \quad (21.98)$$

From this we identify the critical exponent of the coherence length as

$$\nu = -1/\beta'(t_R^c). \quad (21.99)$$

In Eq. (21.89) we found

$$\beta'(t_R^c) = \epsilon Z(N-2) S_D t_R, \quad (21.100)$$

which is equal to $-\epsilon$ at $t_R = t_R^c$. Thus

$$\nu = \epsilon^{-1}. \quad (21.101)$$

This result is independent of N . It should be compared to the result of the $O(N)$ -symmetric ϕ^4 -theory of Chapter 18, where we obtained in $4 - \epsilon$ dimensions [recall Eq. (20.186)]

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)}\epsilon. \quad (21.102)$$

The relation between the two expansion parameters ϵ is $\epsilon = 2 - \varepsilon$. In three dimensions, where $\epsilon = 1$ and $\varepsilon = 1$, the result (21.102) at $N \rightarrow \infty$ agrees with (21.101).

Since both models describe the same physical system, they should have the same critical exponents. However, the expressions (21.99) and (21.102) have quite a different N -dependence. This shows that none of the two results can really be trusted in three dimensions. Apparently, the parameter $\epsilon = 1$ is too large in either case to justify using the lowest-order term in the ϵ -expansion.

Let us calculate the critical exponent β of Eq. (20.164) that is observed in the temperature behavior of the spontaneous magnetization M in the ordered phase. It is defined by the power law in which the renormalized expectation of the field $\sigma = \sqrt{1 - \pi^2}$ goes to zero as t_R approaches the critical point [recall Eq. (20.154)]:

$$M \equiv \langle \sigma_R \rangle \equiv \Sigma_R \propto (-\tau)^\beta; \quad t_R \rightarrow t_R^c - 0. \quad (21.103)$$

Since $\sigma = \sqrt{1 - \pi^2}$ has obviously a vanishing engineering dimension, the magnetization $M = \sigma$ can depend only on $t_R(\mu)$. Moreover, due to the $O(N)$ -symmetry, Σ is renormalized in the same way as π was in Eq. (21.44), such that we have

$$\sigma_R = Z_\pi^{-1/2} \langle \sigma \rangle. \quad (21.104)$$

and

$$\Sigma_R = Z_\pi^{-1/2} \Sigma. \quad (21.105)$$

Explicitly, this follows from Eqs. (21.75) and (21.78). There the field Σ has gone over into $\sqrt{B - \Pi_a^2}$, which is equal to $B^{-1/2} \sqrt{1 - \Pi_{Ra}^2}$, thus confirming (21.105) [recalling (21.82)].

Writing the magnetization $M(t_R, \mu)$ as $M(t_R(\mu))$, we see that it satisfies the renormalization group equation

$$\left[\beta(t_R) \frac{\partial}{\partial t_R} + \gamma_\pi(t_R) \right] M(t_R) = 0, \quad (21.106)$$

where

$$\gamma_\pi(t_R) = Z_\pi^{-1/2} \mu \partial_\mu Z_\pi^{1/2}. \quad (21.107)$$

According to (21.49) and (21.87), the lowest-order result is

$$\gamma_\pi(t_R) = \frac{(N-1)}{2S_D t_R}. \quad (21.108)$$

Equation (21.106) is then solved by

$$M(t_R) = \exp \left[- \int_0^t dt' \frac{\gamma_\pi(t')}{\beta(t')} \right]. \quad (21.109)$$

Near the critical point t_R^c , this behaves like

$$M(t_R) \sim (-\tau)^{-\gamma_\pi(t_R^c)/\beta'(t_R^c)} \sim \xi^{-\gamma_\pi(t_R^c)}. \quad (21.110)$$

Recalling the definition (20.163) we identify the critical exponent of spontaneous magnetization [not to be confused with the β -function (21.89)] as

$$\beta = \frac{\gamma_\pi(t_R^c)}{\beta'(t_R^c)}. \quad (21.111)$$

We shall denote $\gamma_\pi(t_R^c)$ and $\beta'(t_R^c)$ by γ^* and β'^* , respectively, so that $\beta = -\gamma^*/\beta'^*$. Inserting the lowest-order ϵ -expansions, $\gamma^* \approx (N-1)\epsilon/2$, $\beta'^* \approx -\epsilon/(N-2)$, we obtain

$$\beta = \frac{N-1}{2(N-2)} + \mathcal{O}(\epsilon). \quad (21.112)$$

This should be compared with the β -exponent of the $O(N)$ -symmetric ϕ^4 -theory. Taking the hyperscaling relation (20.164), inserting $D = 4 - \epsilon$ and the ϵ -expansions

$$\eta = \frac{N+2}{2(N+8)^2} \epsilon^2 + \dots, \quad (21.113)$$

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)} \epsilon + \frac{(N+2)(N^2+23N+60)}{8(N+8)^3} \epsilon^2 + \dots, \quad (21.114)$$

from Eqs. (20.185) and (20.186), we see that

$$\beta = \frac{1}{2} + \mathcal{O}(\epsilon). \quad (21.115)$$

Only the $N = \infty$ limits agree with each other, the low- N exponents are quite different, indicating again that, in three dimensions, both $\epsilon = 1$ and $\epsilon = 1$ are somewhat too large to give an roughly reliable result in either expansion.

It should be realized that due to the vanishing naive dimensions of the Goldstone fields $\pi(x)$, the critical exponents derived in $D = 2 + \epsilon$ dimensions are now quite different from those derived from the ϕ^4 -theory in $D = 4 - \epsilon$ in Chapter 20. In order to find all scaling results in $D = 2 + \epsilon$ dimensions, we start from the renormalization group equation obeyed by the general N -point function

$$\left\{ \mu \partial_\mu + \beta(t_R) \frac{\partial}{\partial t_R} + n \gamma_\pi(t_R) + \gamma_h(t_R) h_R \partial_{h_R} \right\} \Gamma^{(n)}(p, t_R, h_R, \mu) = 0, \quad (21.116)$$

where [compare with (20.30) and (20.33)]

$$\begin{aligned} \gamma_h &\equiv \frac{h}{h_R} \mu \partial_\mu \frac{h_R}{h} = \frac{h}{h_R} \mu \partial_\mu \left(Z_t^{-1} Z_\pi^{1/2} \right) |_{t,h} \\ &= \frac{h}{h_R} \left[\mu \partial_\mu \left(\mu^{-\epsilon} \frac{t_R}{t} \right) Z_\pi^{1/2} + \frac{1}{2} Z_t^{-1} Z_\pi^{1/2} \mu \partial_\mu \log Z_\pi \right] \\ &= \frac{h}{h_R} \left\{ \mu^{-\epsilon} Z_t^{-1} Z_\pi^{1/2} \left[-\epsilon + \frac{1}{t_R} \beta(t_R) \right] + Z_t^{-1} Z_\pi^{1/2} \gamma_\pi \right\} \\ &= h \left[-\epsilon + \frac{\beta(t_R)}{t_R} + \gamma_\pi \right]. \end{aligned} \quad (21.117)$$

Near the critical point where $\beta(t_R)$ vanishes, this implies

$$\frac{h_R(\mu)}{h_R(\mu_1)} \propto \left(\frac{\mu}{\mu_1}\right)^{\gamma_\pi^* - \epsilon}. \quad (21.118)$$

Together with

$$\mu \frac{d}{d\mu} t_R(\mu) \approx \beta'^* \times (t_R - t_R^c), \quad (21.119)$$

we have

$$t_R(\mu) - t_R^c \propto \left(\frac{\mu}{\mu_1}\right)^{\beta'^*} = \left(\frac{\mu}{\mu_1}\right)^{-1/\nu}, \quad (21.120)$$

from which we conclude that μ_1 goes to zero near the critical point as follows:

$$\left(\frac{\mu}{\mu_1}\right) \propto \mu \xi. \quad (21.121)$$

This implies that $h_R(\mu_1)$ vanishes according to the relation

$$\frac{h_R(\mu)}{h_R(\mu_1)} \propto \xi^{-\nu(\gamma_\pi^* - \epsilon)} \propto (\mu \epsilon)^{\gamma_\pi^* - \epsilon}. \quad (21.122)$$

Therefore, the general vertex function satisfies the scaling relation

$$\Gamma^{(n)}(p, t_R(\mu), h_R(\mu), \mu) = \exp \left\{ -n \int_{\mu_1}^{\mu} \frac{d\mu'}{\mu'} \gamma_\pi(\mu') \Gamma^{(n)}(p, t_R(\mu_1) h_R(\mu_1), \mu_1) \right\}. \quad (21.123)$$

Since the naive dimension of $\Gamma^{(n)}$ and h_R are D and 2, respectively, we can rescale the right-hand side and get in the critical regime

$$\left(\frac{\mu_1}{\mu}\right)^{D+n\gamma_\pi^*} \Gamma^{(n)} \left(p \frac{\mu}{\mu_1}, t_R^c, h_R(\mu_1) \left(\frac{\mu}{\mu_1}\right)^2, \mu \right), \quad (21.124)$$

thus arriving at a scaling relation

$$\Gamma^{(n)}(p, t_R, h_R, \mu) \approx \xi^{-D} (\mu \xi)^{n\gamma_\pi^*} \Gamma^{(n)}(p \xi, t_R^c, h_R(\mu) (\mu \xi)^{D-\gamma_\pi^*}, \mu). \quad (21.125)$$

In a similar fashion we derive the scaling relation for the vertex functions in the presence of background fields Π and Σ [in analogy with (20.92) and (20.93)]. Since both fields appear $O(N)$ -symmetrically, we can suppress one of them and write:

$$\Gamma^{(n)}(p, t_R, \Sigma(\mu), \mu) = \xi^{-D-n\gamma_\pi^*} \Gamma^{(n)}(p \mu \xi, t_R^c, \Sigma/\mu, \xi^{\gamma_\pi^*}, \mu). \quad (21.126)$$

From this we may derive all critical exponents of the system and relate them to γ_π^* and ν . The exponent β of magnetization calculated in (21.111) satisfies the hyperscaling relation

$$\beta = \gamma_\pi^* \nu = \frac{\nu}{2}(D - 2 + \eta), \quad (21.127)$$

which is the same as that derived from an ε -expansion in Eq. (20.164).

Let us also find the critical exponent α of the specific heat C [recall (20.145)]. Since C measures the second temperature derivative of $\Gamma^{(0)}$, and since $\Gamma^{(0)} \propto \xi^D \propto \tau^{D\nu}$, we obtain the hyperscaling relation

$$\alpha = 2 - D\nu, \quad (21.128)$$

just as before in (20.147).

The critical exponent γ of the susceptibility [see (20.152)] is obtained by differentiating $\Gamma^{(0)}$ twice with respect to the field strength

$$\xi^{-1} \propto \frac{\partial^2 \Gamma^{(0)}}{\partial \Sigma^2} \propto \xi^{-D+2\gamma_\pi^*} \propto \tau^{-\nu(2\gamma_\pi^*-D)}. \quad (21.129)$$

Hence

$$\gamma = -\nu(2\gamma_\pi^* - D) = \nu(2 - \eta), \quad (21.130)$$

as before in (20.153). Alternatively, we could have used $\xi \propto d^2 \Gamma^{(0)} / dh_R^2$, with the same result.

For the exponent δ of the critical magnetization [see (20.154)], we differentiate $\Gamma^{(0)}$ with respect to Σ and see that h_R must behave like

$$h_R \propto \frac{\partial \Gamma^{(0)}}{\partial \Sigma} \propto \xi^{-D+\gamma_\pi^*} (\Sigma \xi^{\gamma_\pi^*})^\delta. \quad (21.131)$$

If this relation is supposed to remain nontrivial for $\tau \rightarrow 0$, we have the condition

$$-D + \gamma_\pi^* + \gamma_\pi^* \delta = 0, \quad (21.132)$$

or

$$\delta = -1 + \frac{D}{\gamma_\pi^*} = \frac{D + 2 - \eta}{D - 2 + \eta}, \quad (21.133)$$

just as in (20.157). The same critical exponent would, of course, follow from the relation

$$\Sigma_R \propto \frac{\partial h^0}{\partial h_R} \sim h_R^{1/\delta}. \quad (21.134)$$

Thus, even though the derivation was completely different, all scaling relations are exactly the same as those found in the $O(N)$ -symmetric ϕ^4 -theory. The basic reason is that, since $\xi^{\gamma^*} \propto \tau^\beta$ and $\xi^{-D+\gamma^*} \propto \tau^{\delta\beta}$, the equation of state

$$\begin{aligned} j &= \xi^{-D+\gamma^*} v'(t_R^c, \Sigma \xi^{\gamma^*}, \mu) \\ &= \tau^{\delta\beta} f\left(\frac{\Sigma}{\tau^\beta}\right) \end{aligned} \quad (21.135)$$

follows Widom's general scaling form (20.173)

$$\frac{h}{M^\delta} = f\left(\frac{\tau}{M^{1/\beta}}\right). \quad (21.136)$$

21.6 Two- and Three-Loop Results

For completeness, let us also write down the result up to the three loop level. The two-loop diagrams are shown in Fig. 21.1. We have omitted the corresponding diagrams involving the $1/a^D$ terms, for brevity. The three loop diagrams are quite numerous. In order to display them we drop the dashed and wiggly lines and show only the topological structure in Fig. 21.2. The two renormalization constants have the following $1/\epsilon$ -singularities

$$\begin{aligned} Z_t &= 1 + \frac{N-2}{\epsilon} t_R + \left[\frac{(N-2)^2}{\epsilon^2} + \frac{N-2}{2\epsilon} \right] t_R^2 \\ &\quad + \left[\frac{(N-2)^3}{\epsilon^3} + \frac{7(N-2)^2}{6\epsilon^2} + \frac{(N-2)(N+2)}{12\epsilon} \right] t_R^3 + \dots, \end{aligned} \quad (21.137)$$

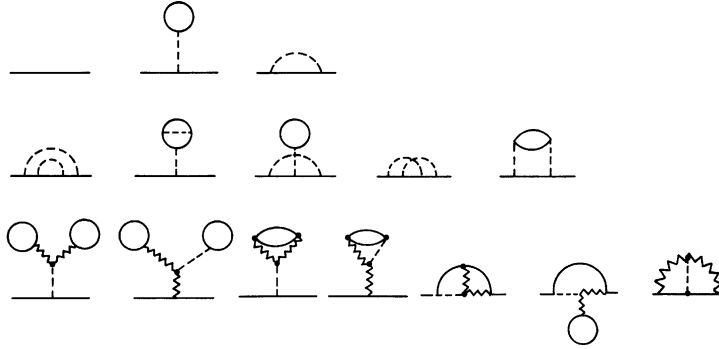


FIGURE 21.1 Two-loop diagrams

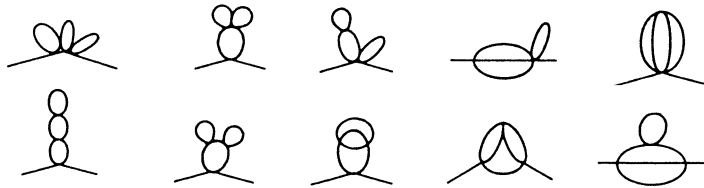


FIGURE 21.2 Three-loop diagrams

$$Z_\pi = 1 + \frac{N-1}{\epsilon} t_R + \frac{(N-1)(N-\frac{3}{2})}{\epsilon^2} t_R^2 + \left[-\frac{N-1}{3\epsilon^3} \left(-3N^2 + \frac{19}{2}N - \frac{15}{2} \right) + \frac{(N-1)(N-2)}{3\epsilon^2} + \frac{(N-2)(N-1)}{4\epsilon} \right] t_R^3 + \dots \quad (21.138)$$

From this one finds the functions $\beta(t_R)$ and $\gamma_\pi(t_R)$ [recalling (21.89) and (21.107)]

$$\begin{aligned} \beta(t_R) &= \frac{\epsilon t_R}{1 + t_R \frac{\partial}{\partial t_R} \log Z_t} \\ &= \epsilon t_R - (N-2)t_R^2 - (N-2)t_R^3 - \frac{1}{4}(N-2)(N+2)t_R^4 + \dots, \end{aligned} \quad (21.139)$$

$$2\gamma_\pi(t_R) = \beta(t_R) \frac{d \log Z_\pi}{dt_R} = (N-1)t_R + \frac{3}{4}(N-1)(N-2)t_R^3 + \dots \quad (21.140)$$

The critical coupling t_R^c defined by $\beta(t_R^c) = 0$ has the ϵ -expansion

$$t_R^c = \frac{\epsilon}{N-2} - \frac{\epsilon^2}{(N-2)^2} + \frac{6-N}{4} \frac{\epsilon^3}{(N-2)^3} + \dots, \quad (21.141)$$

and the critical exponents are

$$\nu^{-1} = -\beta'(t_R^c) = \epsilon + \frac{\epsilon^2}{N-2} + \frac{\epsilon^3}{2(N-2)} + \dots, \quad (21.142)$$

$$\eta = -\epsilon + 2\gamma_\pi(t_R^c) = \frac{\epsilon}{N-2} - (N-1) \frac{\epsilon^2}{(N-2)^2} + \frac{N(N-1)}{2} \frac{\epsilon^3}{(N-2)^3} + \dots \quad (21.143)$$

From the scaling relation $\beta = \nu(D-2+\eta)/2$ we obtain the critical exponent magnetization

$$\beta = \frac{N-1}{2(N-2)} - \frac{(N-1)}{(N-2)^2} \epsilon + \frac{3}{2} \frac{N-1}{(N-2)^3} \epsilon^2 + \dots \quad (21.144)$$

These ϵ -expansions show a very poor convergence at $\epsilon = 1$, where they are supposed to describe the three-dimensional situation. Moreover, the series for ν^{-1} has no alternating signs, indicating that it may not even be Borel-resummable [13]. One might nevertheless attempt a Borel-Padé resummation. Consider, for example, the case of $N = 3$ (vector model) where

$$\nu^{-1} = \epsilon + \epsilon^2 + \frac{1}{2}\epsilon^3 + \dots \quad (21.145)$$

This is the Borel transformation of the function

$$B_\nu(t) = \epsilon t + \epsilon^2 \frac{t^2}{2!} + \epsilon^3 \frac{t^3}{2 \cdot 3!} + \dots, \quad (21.146)$$

from which one obtains

$$\nu^{-1} = \int_0^\infty e^{-t} B_\nu(t) dt. \quad (21.147)$$

Let us take a simple $[1, 2]$ -Padé approximation for $B_\nu(t)$. This is a ratio of a polynomial of degree one in the numerator and of degree two in the denominator, which has the same small- t expansion as in (21.146). It reads

$$B_\nu(t) = \frac{\epsilon t}{1 - \frac{\epsilon}{2}t + \frac{\epsilon^2}{6}t^2}, \quad (21.148)$$

and it is easy to verify that it has the expansion (21.145). Inserted into (21.147) we obtain at $\epsilon = 1$:

$$\nu^{-1} = \int_0^\infty e^{-t} \frac{t}{1 - \frac{t}{2} + \frac{t^2}{6}} \approx 1.25. \quad (21.149)$$

Note that the $[1, 1]$ -approximant would have a pole for $t > 0$ preventing its use.

To resum similarly the series (21.143) for η , we may use a $[2, 1]$ -Padé-approximation:

$$\begin{aligned} B_\eta(t) &= \epsilon t - \frac{2\epsilon^2 t^2}{2!} + 3\epsilon^3 \frac{t^3}{3!} + \dots \\ &= \epsilon t \frac{1 - \epsilon t/2}{1 + \epsilon t/2}, \end{aligned} \quad (21.150)$$

to find at $\epsilon = 1$:

$$\eta = \int_0^\infty e^{-t} t \frac{1 - t/2}{1 + t/2} = 0.11. \quad (21.151)$$

These results may be compared with the well-known critical exponents of the three-dimensional classical Heisenberg model:

$$\nu^{-1} \approx 1.39, \quad (21.152)$$

$$\eta \approx 0.04. \quad (21.153)$$

The numbers for ν^{-1} agree reasonably well with each other considering the arbitrariness of the resummation procedure. The numbers for η agree insofar as they are both small.

The ϵ -expansions have been driven to order ϵ^4 with an entirely different technique using perturbation expansions in $1/N$ [2]. The results for the fourth-order contributions to the series (21.139), (21.140), (21.142), and (21.143) are

$$\beta_5 = \frac{N-2}{12} \left[(N^2 - 22N + 34) - 18(N-3)\zeta(3) \right] t_R^5, \quad (21.154)$$

$$2\gamma_{\pi 4} = \frac{(N-1)(N-2)}{12} [-4(N-5) + 3(N-3)\zeta(3)] t_R^4, \quad (21.155)$$

$$t_R^{c4} = \frac{1}{12} \left[(N^2 - 7N + N^2) - 18(N-3)\zeta(3) \right] \frac{\epsilon^4}{(N-2)^4}, \quad (21.156)$$

$$\nu_4^{-1} = - \left[30 - 14N + N^2 + (54 - 18N)\zeta(3) \right] \frac{\epsilon^4}{4(N-2)^3}, \quad (21.157)$$

$$\eta_4 = -(N-1) \left[-6 + 2N + N^2 + (-12 + N + N^2)\zeta(3) \right] \frac{\epsilon^4}{4(N-2)^4}. \quad (21.158)$$

The additional terms do not improve the critical exponents if only Padé-Borel resummation techniques are used. Another, more powerful method is needed to extract precise numbers.

21.7 Variational Resummation of ϵ -Expansions

Having seen the difficulties in extracting accurate critical exponents from the above ϵ -expansions, we decide to resum the above series using information from the $4 - \epsilon$ - expansions of the ϕ^4 -theories. This becomes possible by rewriting the latter as power series in the variable $\tilde{\epsilon} \equiv 2(4 - D)/(D - 2)$. The initial five expansion coefficients of these functions are known from ϵ -expansions of critical exponents in $O(N)$ -symmetric ϕ^4 -theory in $D = 4 - \epsilon$ dimensions. The first four expansion coefficients of the strong-coupling expansions are determined from (21.142), (21.143), (21.157), and (21.158). Recall that the critical exponent ν , that governs the divergence of the coherence length as $\xi \propto |T - T_c|^{-\nu}$, is obtained from a seven-loop treatment of the classical Heisenberg model with $N = 3$ to be $\nu = 0.7073 \pm 0.0030$ [4]. In $D = 4 - \epsilon$ dimensions, a five-loop expansion [5] extrapolated to $\epsilon = 1$ had previously led to $\nu = 0.7050 \pm 0.0055$. Apart from the expansion coefficients, the latter results incorporate information on the large-order growth contained in the tip of the left-hand cut in the complex coupling-constant plane. Results are very close to those obtained from strong-coupling ϕ^4 -theory using the six-loop expansions available in [8].

It is generally accepted that, as a consequence of the *universality hypothesis* of critical phenomena of all systems with equal Goldstone bosons, the same critical exponents should be obtainable from renormalization group studies of $O(N)$ nonlinear σ -models in $D = 2 + \epsilon$ dimensions at $\epsilon = 1$. The fact that the latter expansions have remained, up to now, rather useless for any practical calculation is their non-Borel character. That has led some authors doubt the use of such expansions around the lower critical dimension altogether [9]. This would be quite unfortunate, since it would jeopardize other interesting theories such as Anderson's theory of localization [10]. A basis of these doubts is the increasing relevance of higher derivatives with respect to ϵ [11]. Hopes for the utility of these expansions are, however, not completely lost since the argument involves an interchange of limits in the analytic continuation in ϵ , and of increasing the powers of ϵ [12].

In this Section we can confirm these positive hopes by extracting from the equations (21.142), (21.143), (21.157), and (21.158), supplemented by the five-loop ϵ -expansions around four dimensions, very accurate critical exponents ν for the classical Heisenberg model as well as for the universality classes $O(N)$ with $N = 0, 1, 2$. After evaluating the series for ν^{-1} at $\epsilon = 1$, we find from the ϵ -expansion of the three-

dimensional $O(3)$ -model the diverging successive values $\nu^{-1} = (1, 2, 2.5, 3.25)$. Also Padé approximations do not help, the best of them, the $[1,2]$ -approximation, giving the too large value $\nu = 2$. So far, the only result which is not far from the true value has been obtained via the Padé-Borel transform [1]

$$P^{[1,2]}(\epsilon, t) = \frac{\epsilon t}{1 - \epsilon t/2 + \epsilon^2 t^2/6}. \quad (21.159)$$

From this one obtains the ϵ -dependent critical exponent

$$\nu^{-1}(\epsilon) = \int_0^\infty dt e^{-t} P^{[1,2]}(\epsilon, t), \quad (21.160)$$

whose value at $\epsilon = 1$ is $\nu^{-1}(1) \approx 1.252$, corresponding to $\nu \approx 0.799$, still much too large to be reliable. The other Padé-Borel approximations are singular and thus of no use at all, as shown in Fig. 21.3.

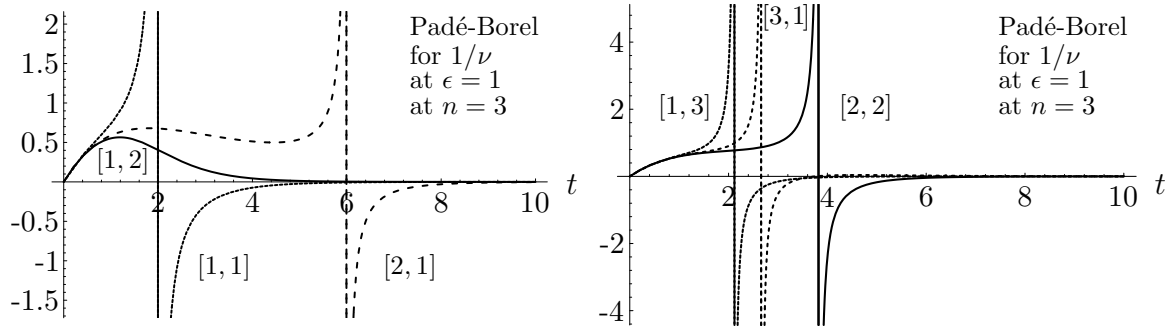


FIGURE 21.3 Integrands of the Padé-Borel transform (21.160) for the Padé approximants $[1,1]$, $[2,1]$, $[1,2]$ and for $[1,3]$, $[3,1]$, $[2,2]$ at $\epsilon = 1$. Only the last is integrable, yielding $\nu^{-1} \approx 1.25183 \approx 1/.79883$.

The full ϵ -dependence of the power series (21.157) and the Padé-Borel-approximation (21.160) can be seen in Fig. 21.4.

A direct evaluation of the series for the anomalous dimension η yields the worse values $(2, -2, 4, -5)$. Here the nonsingular Borel-Padé approximations $[2,1]$, $[1,2]$, and $[1,1]$ yield 0.147, 0.150, and 0.139, rather than the correct value 0.032. The full ϵ -dependence of the power series (21.158) and the Padé-Borel-approximation $[2,1]$ are also shown in Fig. 21.4.

21.7.1 Strong-Coupling Theory

The remedy for these problems comes from the theory developed in Ref. [18]. It allows us to extract the strong-coupling properties of a ϕ^4 -theory from divergent perturbation expansions. In particular, we found power behavior for the renormalization constants at large couplings, and from this all critical exponents of the system. By using the known expansion coefficients of the renormalization constants

in three dimensions up to six loops, we derived extremely accurate values for the critical exponents. The method is a systematic extension [15, 6] to arbitrary orders of the Feynman-Kleinert variational approximation to path integrals [17]. For an anharmonic oscillator, this so-called *Variational Perturbation Theory* (VPT) [18] yields expansions which converge uniformly in the coupling strength and exponentially fast, like $e^{-\text{const} \times L^{1/3}}$ in the order L of the approximation, as was observed some time ago [19, 20] and proved in [20, 21, 22]. In the present book, VPT was applied in Chapter 3 which reviews briefly its historic development. The extension to field theory shows the same type of convergence, with the power $1/3$ replaced by $1 - \omega$, where ω is the critical exponent governing the approach to scaling. This field-theoretic development will be combined here with an earlier interpolation procedure [23] to resum the non-Borel expansions (21.142) and (21.157).

Let us briefly recall the interpolation procedure called field theoretic variational perturbation theory (VPT) by which a divergent weak-coupling expansion of the type $E_L(g_0) = \sum_{n=0}^L a_n g_0^n$ can be combined with a strong-coupling expansion $E_M(g_0) = g_0^{p/q} \sum_{m=0}^M b_m (g_0^{-2/q})^m$. Previously treated examples [23] were the anharmonic oscillator with parameters $p = 1/3$, $q = 3$ for the energy eigenvalues, and the Fröhlich polaron with $p = 1$, $q = 1$ for the ground-state energy and $p = 4$, $q = 1$ for the mass. As described in detail in the textbook [2], in Chapter 19, the first step is to rewrite the weak-coupling expansion with the help of an auxiliary scale parameter κ as

$$E_L(g_0) = \kappa^p \sum_{n=0}^L a_n \left(\frac{g_0}{\kappa^q} \right)^n, \quad (21.161)$$

where κ is eventually set equal to 1. We shall see below that the quotient p/q parametrizes the *leading power behavior* in g_0 of the strong-coupling expansion, whereas $2/q$ characterizes the *approach* to the leading power behavior. In a second step we replace κ by the identical expression

$$\kappa \rightarrow \sqrt{K^2 + \kappa^2 - K^2} \quad (21.162)$$

containing a dummy scaling parameter K . The series (21.161) is then reexpanded in powers of g_0 up to the order L , thereby treating $\kappa^2 - K^2$ as a quantity of order g_0 . The result is most conveniently expressed in terms of dimensionless parameters

$$\hat{g}_0 \equiv g_0/K^q \quad (21.163)$$

and

$$\sigma \equiv (1 - \hat{\kappa}^2)/\hat{g}_0. \quad (21.164)$$

Then the replacement (21.162) amounts to

$$\kappa \longrightarrow K(1 - \sigma \hat{g}_0)^{1/2}, \quad (21.165)$$

so that the reexpanded series reads explicitly

$$W_L(\hat{g}_0, \sigma) = K^p \sum_{n=0}^L \varepsilon_n(\sigma) (\hat{g}_0)^n, \quad (21.166)$$

with the coefficients

$$\varepsilon_n(\sigma) = \sum_{j=0}^n a_j \binom{(p-qj)/2}{n-j} (-\sigma)^{n-j}. \quad (21.167)$$

For any fixed g_0 , we form the first and second derivatives of $W_L(g_0, K)$ with respect to K , calculate the K -values of the extrema and the turning points, and select the smallest of these as the optimal scaling parameter K_L . The function $W_L(g_0) \equiv W_L(g_0, K_L)$ constitutes the L th variational approximation $E_L(g_0)$ to the function $E(g_0)$. This is the essence of VPT.

It is easy to take this approximation to the strong-coupling limit $g_0 \rightarrow \infty$. For this we observe that (21.166) has the scaling form

$$W_L(g_0, K) = K^p w_L(\hat{g}_0, \hat{\kappa}^2). \quad (21.168)$$

For dimensional reasons, the optimal K_L increases with g_0 like $K_L \approx g_0^{1/q} c_L$, so that $\hat{g}_0 = c_L^{-q}$ and $\sigma = 1/\hat{g}_0 = c_L^q$ remain finite in the strong-coupling limit, whereas $\hat{\kappa}^2$ goes to zero like $1/[c_L(g_0/\kappa^q)^{1/q}]^2$. Hence

$$W_L(g_0, K_L) \approx g_0^{p/q} c_L^p w_L(c_L^{-q}, 0). \quad (21.169)$$

Here c_L plays the role of the variational parameter to be determined by the optimal extremum or turning point of $c_L^p w_L(c_L^{-q}, 0)$. The full strong-coupling expansion is obtained by expanding $w_L(\hat{g}_0, \hat{\kappa}^2)$ in powers of $\hat{\kappa}^2 = (g_0/\kappa^q \hat{g}_0)^{-2/q}$. The result is

$$W_L(g_0) = g_0^{p/q} \left[b_0(\hat{g}_0) + b_1(\hat{g}_0) \left(\frac{g_0}{\kappa^q} \right)^{-2/q} + b_2(\hat{g}_0) \left(\frac{g_0}{\kappa^q} \right)^{-4/q} + \dots \right] \quad (21.170)$$

with

$$b_n(\hat{g}_0) = \frac{1}{n!} w_L^{(n)}(\hat{g}_0, 0) \hat{g}_0^{(2n-p)/q}, \quad (21.171)$$

where $w_L^{(n)}(\hat{g}_0, \hat{\kappa}^2)$ is the n th derivative of $w_L(\hat{g}_0, \hat{\kappa}^2)$ with respect to $\hat{\kappa}^2$. Explicitly:

$$\frac{1}{n!} w_L^{(n)}(\hat{g}_0, 0) = \sum_{l=0}^L (-1)^{l+n} \sum_{j=0}^{l-n} a_j \binom{(p-qj)/2}{l-j} \binom{l-j}{n} (-\hat{g}_0)^j. \quad (21.172)$$

The optimal variational energy (21.170) is found by going for each g_0 to the value of $\kappa(g_0)$ where $w_L^{(n)}(\hat{g}_0, 0)$ is minimal (or has a saddle point, if a minimum does not exist).

The optimal variational energy has a strong-coupling expansion in powers of $(g_0/\kappa^q)^{-2/q}$. That can be derived as follows: We expand the reduced coupling (21.163) into a strong-coupling series

$$\hat{g}_0 = \gamma_0 + \gamma_1 \left(\frac{g_0}{\kappa^q} \right)^{-2/q} + \gamma_2 \left(\frac{g_0}{\kappa^q} \right)^{-4/q} + \dots, \quad (21.173)$$

TABLE 21.1 Coefficients $b_n(\hat{g}_0)$ in the strong-coupling expansion (21.170), and the associated γ_i in (21.173).

n	b_n	$-\gamma_{N-1}$
2	$\bar{b}_2 + \gamma_1 \bar{b}'_1 + \frac{1}{2} \gamma_1^2 \bar{b}''_0$	$\bar{b}'_1 / \bar{b}''_0$
3	$\bar{b}_3 + \gamma_2 \bar{b}'_1 + \gamma_1 \bar{b}_2 + \gamma_1 \gamma_2 \bar{b}''_0 + \frac{1}{2} \gamma_1^2 \bar{b}''_1 + \frac{1}{6} \gamma_1^3 \bar{b}^{(3)}_0$	$(\bar{b}'_2 + \gamma_1 \bar{b}''_1 + \frac{1}{2} \gamma_1^2 \bar{b}^{(3)}_0) / \bar{b}''_0$
4	$\bar{b}_4 + \gamma_3 \bar{b}'_1 + \gamma_2 \bar{b}'_2 + \gamma_1 \bar{b}'_3 + (\frac{1}{2} \gamma_1^2 + \gamma_1 \gamma_3) \bar{b}''_0$ $+ \gamma_1 \gamma_2 \bar{b}''_1 + \frac{1}{2} \gamma_1^2 \bar{b}''_2 + \frac{1}{2} \gamma_1^2 \gamma_2 \bar{b}^{(3)}_0 + \frac{1}{6} \gamma_1^3 \bar{b}^{(3)}_1 + \frac{1}{24} \gamma_1^4 \bar{b}^{(4)}_0$	$(\bar{b}'_3 + \gamma_2 \bar{b}''_1 + \gamma_1 \bar{b}''_2 + \gamma_1 \gamma_2 \bar{b}^{(3)}_0$ $+ \frac{1}{2} \gamma_1^2 \bar{b}^{(3)}_1 + \frac{1}{6} \gamma_1^3 \bar{b}^{(4)}_0) / \bar{b}''_0$

and insert this into (21.172) to obtain a strong-coupling series of $w_L^{(n)}(\hat{g}_0, 0)$ in powers of $(g_0/\kappa^q)^{-2/q}$. This is optimized as follows: We first treat the leading strong-coupling coefficient $b_0(\hat{g}_0)$ and identify the optimal value of γ_0 . Then we optimize the partial sums $W_L(g_0)$ with the expansion (21.173), by varying $\gamma_1, \gamma_2, \dots$. In this way we find the optimal equations for $b_n(\hat{g}_0)$'s listed in Table 21.1.

It was demonstrated in [23] how one can find a variational perturbation series for functions for which one knows L weak-coupling and M strong-coupling expansion coefficients. We must merely extend further the set of initial coefficients $a_1, \dots, a_L$ by M yet unknown ones $a_{L+1}, \dots, a_{L+M}$, and determine the latter via a fit of the resulting strong-coupling coefficients $b_0, \dots, b_{M-1}$ to the former.

21.7.2 Interpolation

The interpolation procedure will now be applied to the perturbation expansion (21.157) in $2 + \epsilon$ dimensions, considering it as the *strong-coupling expansion* of a series in the variable $\tilde{\epsilon} = 2(4 - D)/(D - 2) = 4(1 - \epsilon/2)/\epsilon = \epsilon/(1 - \epsilon/2)$:

$$\begin{aligned} \nu^{-1} = & 4\tilde{\epsilon}^{-1} - 8\frac{N-4}{N-2}\tilde{\epsilon}^{-2} + 16\frac{N-4}{N-2}\tilde{\epsilon}^{-3} \\ & - 32 \left\{ [52 + 108\zeta(3)] - [16 + 36\zeta(3)]N + N^2 \right\} \frac{\tilde{\epsilon}^{-3}}{(N-2)^3} + \dots \end{aligned} \quad (21.174)$$

The weak-coupling expansion of this series is [5]

$$\begin{aligned} \nu^{-1} = & 2 - \frac{N+2}{N+8}\tilde{\epsilon} + (20 + 3N + N^2) \frac{(2+N)\tilde{\epsilon}^2}{2(8+N)^3} \\ & + [-2240 - 624N - 212N^2 - 9N^3 - 2N^4 + 8 \cdot 12(8+N)(22+5N)\zeta(3)] \frac{(2+N)\tilde{\epsilon}^3}{8(8+N)^5} \\ & + [5(568576 + 382144N + 103920N^2 + 9532N^3 + 1142N^4 + 21N^5 + 4N^6) \\ & + 80(-249600 - 148960N - 42912N^2 - 6516N^3 - 350N^4 + 3N^5) \zeta(3) + 80 \cdot 18(8+N)^3(22+5N)\zeta(4) \\ & - 80 \cdot 80(8+N)^2(186 + 55N + 2N^2) \zeta(5)] \frac{(2+N)}{160(8+N)^7} \tilde{\epsilon}^4 \\ & + [945(-105091072 - 106771456N - 47635968N^2 - 11768576N^3 - 1835504N^4 - 122812N^5 \end{aligned} \quad (21.175)$$

$$\begin{aligned}
& -6270 N^6 - 45 N^7 - 8 N^8 \Big] . \\
& +15120 \Big(57911296 + 46323968 N + 17913728 N^2 + 3869024 N^3 + 514592 N^4 + 46900 N^5 + 1902 N^6 - 37 N^7 \Big) \zeta(3) + \\
& +15120 \Big(-47874048 - 40615936 N - 11928064 N^2 - 1525888 N^3 - 89408 N^4 - 3200 N^5 - 128 N^6 \Big) \zeta^2(3) \\
& +945 \Big(101376 + 61056 N + 13392 N^2 + 1278 N^3 + 45 N^4 \Big) \zeta(4) \\
& +256 \cdot 945 (8+N)^2 \Big(345552 + 193822 N + 48749 N^2 + 6506 N^3 + 235 N^4 \Big) \zeta(5) \\
& +945 \cdot 56448 (8+N)^3 \Big(526 + 189 N + 14 N^2 \Big) \zeta(7) \Big] \frac{(N+2)\tilde{\varepsilon}^5}{120960 (8+N)^9} + \dots .
\end{aligned}$$

Their M -dependence is plotted in Fig. 21.4 as a function of the variable $x = M^{-2}$ which makes them lie approximately on a straight line intercepting the ν -axis at $\nu_\infty = 0.705$. This extrapolated value is in excellent agreement with the previous determinations [3, 7], whose numerical forms are for $N = 3, 4, 5, 1$:

$$N = 3 : \nu^{-1} = 2 - 0.45455 \tilde{\varepsilon} + 0.071375 \tilde{\varepsilon}^2 + 0.15733 \tilde{\varepsilon}^3 - 0.52631 \tilde{\varepsilon}^4 + 1.5993 \tilde{\varepsilon}^5 \quad (21.176)$$

$$N = 4 : \nu^{-1} = 2 - 0.5 \tilde{\varepsilon} + 0.0833333 \tilde{\varepsilon}^2 + 0.147522 \tilde{\varepsilon}^3 - 0.499944 \tilde{\varepsilon}^4 + 1.47036 \tilde{\varepsilon}^5, \quad (21.177)$$

$$N = 5 : \nu^{-1} = 2 - 0.538462 \tilde{\varepsilon} + 0.0955849 \tilde{\varepsilon}^2 + 0.135442 \tilde{\varepsilon}^3 - 0.469842 \tilde{\varepsilon}^4 + 1.34491 \tilde{\varepsilon}^5, \quad (21.178)$$

$$N = 1 : \nu^{-1} = 2 - 0.333333 \tilde{\varepsilon} + 0.0493827 \tilde{\varepsilon}^2 + 0.158478 \tilde{\varepsilon}^3 - 0.539937 \tilde{\varepsilon}^4 + 1.78954 \tilde{\varepsilon}^5. \quad (21.179)$$

Extending these series by four more terms

$$a_6 \tilde{\varepsilon}^6 + a_7 \tilde{\varepsilon}^7 + a_8 \tilde{\varepsilon}^8 + a_9 \tilde{\varepsilon}^9, \quad (21.180)$$

we calculate the strong-coupling coefficients (21.171) by extremizing (21.170) with (21.173), after identifying g_0 with $\tilde{\varepsilon}$ and the parameters (p, q) with $(-2, 2)$. Then the coefficients a_6, a_7, a_8, a_9 are determined to make $b_0(\hat{g}_0), b_1(\hat{g}_0), b_2(\hat{g}_0), b_3(\hat{g}_0)$ agree with (21.182). The technique of doing this is described in detail in Ref. [23].

In order to see how the result improves with the number M of additional terms in (21.173), we go through this procedure successively for $M = 1, 2, 3, 4$. The successive additional expansion coefficients for the $O(N)$ universality classes with $N = 3, 4, 5, 1$ are listed in Tables 21.2–21.5, respectively. The four resulting curves for $\nu^{-1}(\varepsilon)$ are shown in Figs. 21.4–21.8. For $N = 3$, the successive critical exponents ν at $\varepsilon = 1$ taken from Fig. 21.4 are

$$(\nu_1, \nu_2, \nu_3, \nu_4) = (0.87917, 0.75899, 0.731431, 0.712152). \quad (21.181)$$

The other $O(N)$ universality classes are displayed analogously.

TABLE 21.2 Coefficients of the successive extension of the expansion coefficients in Eq. (21.180) for $n = 3$. They emerge from the $M = 1, 2, 3, 4$ strong-coupling coefficients (4, 8, -16, 160) of Eq. (21.182).

n	a_6	a_7	a_8	a_9
1	-203.827			
2	-5.67653	17.6165		
3	-4.25622	9.04109	-15.7331	
4	-3.80331	6.87304	-10.0012	12.35521

TABLE 21.3 Coefficients of the successive extension of the expansion coefficients in Eq. (21.180) for $n = 4$. They emerge from the $M = 1, 2, 3, 4$ strong-coupling coefficients (4, 0, 0, 221.096) of Eq. (21.182).

n	a_6	a_7	a_8	a_9
1	-147.508			
2	-7.91064	37.1745		
3	-4.59388	12.3044	-27.0837	
4	-3.72613	7.47851	-12.2129	16.9547

TABLE 21.4 Coefficients of the successive extension of the expansion coefficients in Eq. (21.180) for $n = 5$. They emerge from the $M = 1, 2, 3, 4$ strong-coupling coefficients (8, -8/3, 16/3, 106.131) of Eq. (21.182).

n	a_6	a_7	a_8	a_9
1	-108.648			
2	-10.1408	60.7217		
3	-4.75598	15.1045	-38.9689	
4	-3.57909	7.84272	-14.1142	21.6045

TABLE 21.5 Coefficients of the successive extension of the expansion coefficients in Eq. (21.180) for $n = 1$. They emerge from the $M = 1, 2, 3, 4$ strong-coupling coefficients (4, -24, 48, 3825.54) of Eq. (21.182).

n	a_6	a_7	a_8	a_9
1	-413.921			
2	-5.25285	12.1104		
3	-442759	12450066	-196950675	
4	-5.7343	13.7134	-25.226	38.0976

Since the ϵ -expansion (21.157) is singular at $N = 2$, we expect difficulties with our procedure for $N < 2$. Indeed, the determination of the expansion coefficients in Table 21.5 shows a large irregularity for $M = 3$, and the successive approximations for ν^{-1} in Fig. 21.8 show no sign of convergence with increasing M .

Finally, we plot our highest ($M = 4$) approximations for $N = 3, 4, 5$ together with the large- N approximations for $N = \infty, 20, 10, 6$ in Fig. 21.7. We see the trend for increasing N , which shows that the latter for $N = 6$ is still far from the exact curve. This can also be seen in Fig. 3 of Ref. [24].

The same calculation is done for the critical exponent η . In the variable $\tilde{\epsilon}$, the series (21.158) reads

$$\begin{aligned} \eta = & \frac{\tilde{\epsilon}^{-1}}{N-2} - 2n \frac{\tilde{\epsilon}^{-2}}{(N-2)^2} + 8n(N-1) \frac{\tilde{\epsilon}^{-3}}{(N-2)^3} \\ & + 16(N-1) \left[(6-2n^2) + [12-n-n^2] \zeta(3) \right] \frac{\tilde{\epsilon}^{-4}}{(N-2)^4} + \dots \end{aligned} \quad (21.182)$$

The weak-coupling expansion is [5]

$$\begin{aligned} \eta/\epsilon^2 = & \frac{2+N}{2(N+8)^2} + (272+56N-N^2) \frac{(2+N)\epsilon}{8(N+8)^4} \\ & + \left\{ 46144 + 17920N + 1124N^2 - 230N^3 - 5N^4 - 32 \cdot 12(22+5N)\zeta(3) \right\} \frac{(2+N)\epsilon^2}{32(N+8)^6} \\ & + \left\{ 5655552 + 2912768N + 262528N^2 - 121472N^3 - 27620N^4 - 946N^5 - 13N^6 \right. \\ & \left. + 16(N+8) \left(-171264 - 68672N - 1136N^2 + 1220N^3 + 10N^4 + N^5 \right) \zeta(3) \right. \\ & \left. + 128 \cdot 9(N+8)^3(22+5N)\zeta(4) + 128 \cdot 40(N+8)^2(186+55N+2N^2)\zeta(5) \right\} \frac{(2+N)\epsilon^3}{128(N+8)^8} + \dots, \end{aligned} \quad (21.183)$$

whose numerical expressions are for $N = 3, 4, 5, 1$:

$$N = 3: \quad \eta/\epsilon^2 = 5/242 + 0.0183987\tilde{\epsilon} - 0.0166488\tilde{\epsilon}^2 + 0.032432\tilde{\epsilon}^3, \quad (21.184)$$

$$N = 4: \quad \eta/\epsilon^2 = 1/48 + 0.0173611\tilde{\epsilon} - 0.0157657\tilde{\epsilon}^2 + 0.029057\tilde{\epsilon}^3, \quad (21.185)$$

$$N = 5: \quad \eta/\epsilon^2 = 7/338 + 0.0161453\tilde{\epsilon} - 0.0148734\tilde{\epsilon}^2 + 0.0259628\tilde{\epsilon}^3, \quad (21.186)$$

$$N = 1: \quad \eta/\epsilon^2 = 1/54 + 0.01869\tilde{\epsilon} - 0.0176738\tilde{\epsilon}^2 + 0.0386577\tilde{\epsilon}^3. \quad (21.187)$$

Extending these series by four more terms

$$a_6 \tilde{\epsilon}^6 + a_7 \tilde{\epsilon}^7 + a_8 \tilde{\epsilon}^8 + a_9 \tilde{\epsilon}^9, \quad (21.188)$$

we calculate the strong-coupling coefficients (21.171) by extremizing (21.170) with (21.173), after identifying g_0 with $\tilde{\epsilon}$ and the parameters (p, q) with $(-2, 2)$. Then the coefficients a_6, a_7, a_8, a_9 are determined to make $b_0(\hat{g}_0), b_1(\hat{g}_0), b_2(\hat{g}_0), b_3(\hat{g}_0)$ agree with (21.182). The technique of doing this is described in detail in Ref. [23].

In order to see how the result improves with the number M of additional terms in (21.173), we go through this procedure successively for $M = 1, 2, 3, 4$. The successive additional expansion coefficients for the $O(N)$ universality classes with $N = 3, 4, 5, 1$ are listed in Tables 21.2–21.5, respectively. The four resulting curves for $\nu^{-1}(\epsilon)$ are shown in Figs. 21.4–21.8. For $N = 3$, the successive critical exponents ν at $\epsilon = 1$ taken from Fig. 21.4 are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.87917, 0.75899, 0.731431, 0.712152)$. Their M -dependence is plotted on the right-hand side of Fig. 21.4 as a function of the variable $x = M^{-2}$ which makes them lie approximately on a straight line intercepting the ν -axis at $\nu_\infty = 0.705$. This extrapolated value is in excellent agreement with the previous determination [7] from ϕ^4 -theories, and somewhat smaller than the seven-loop result in [3, 6].

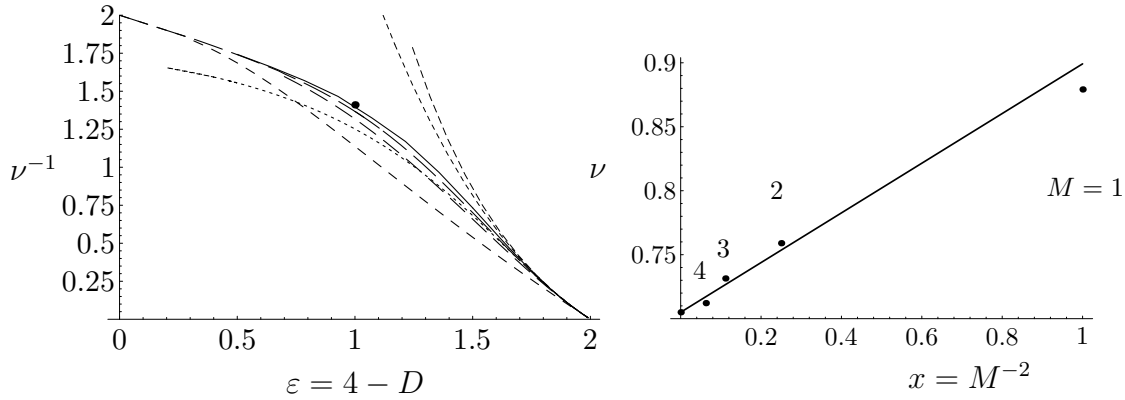


FIGURE 21.4 Inverse of the critical exponent ν for the classical Heisenberg model in $O(3)$ -universality class, plotted as a function of $\epsilon = 4 - D$. The solid curve is obtained from variational interpolation of the five-loop ϵ -expansion of the ϕ^4 -theory around $D = 4$ dimensions and the four-loop ϵ -expansion (21.157) of the nonlinear σ -model around 2 dimensions. Long-dashed curves show the successive approximations which make use of the strong-coupling expansion (21.182) only up to the first, second, and third order. Short-dashed curves display the first three and four terms of the ϵ -expansion and its Padé [1,2]-Borel approximations (the lowest curve). The dot shows the seven-loop result in $D = 3$ dimensions, $\nu = 0.7096$. The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.87917, 0.75899, 0.731431, 0.712152)$. These are extrapolated to infinite order on the right-hand plot, yielding $\nu = 0.705$.

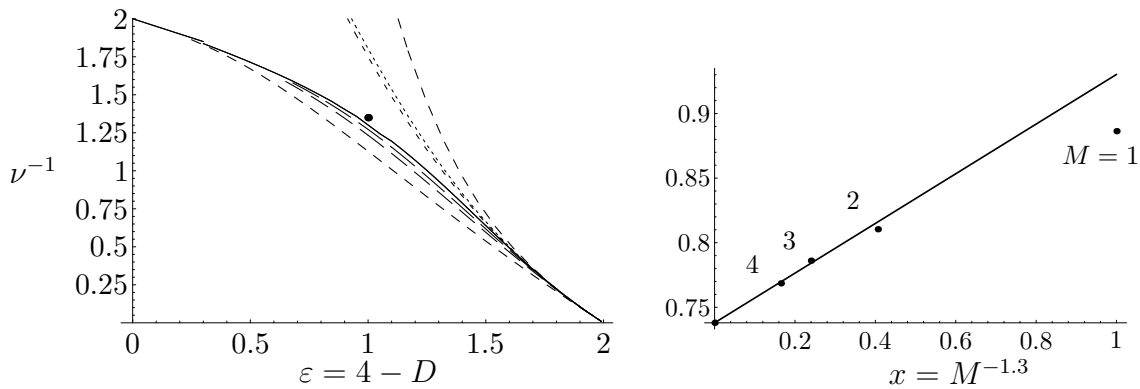


FIGURE 21.5 Analog plot to Fig. 21.4. Short-dashed curves display the first three and four terms of the ϵ -expansion and its Padé [1,2]-Borel approximations (lowest curve). The dot shows the seven-loop result in $D = 3$ dimensions, $\nu = 0.7096$. The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.88635, 0.810441, 0.786099, 0.768565)$. These are extrapolated on the right-hand plot to infinite order, yielding $\nu = 0.7381$.

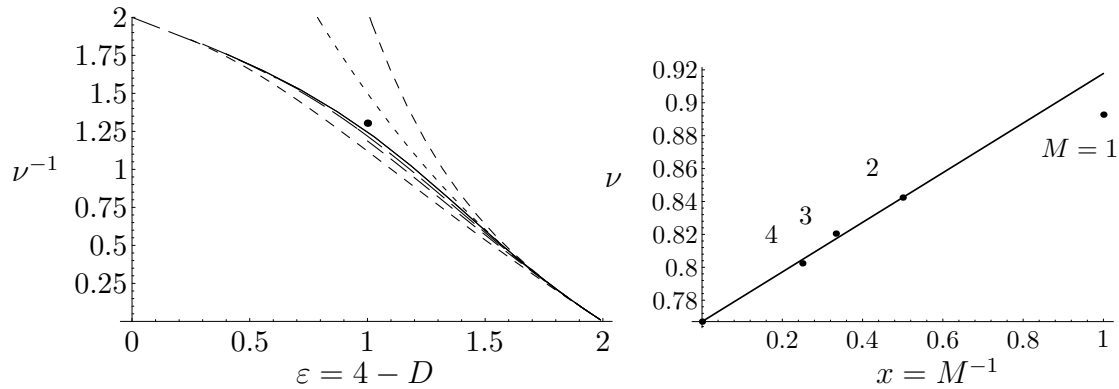


FIGURE 21.6 Analog plot to Fig. 21.4. There is no Padé-Borel approximation. The dot shows the seven-loop result in $D = 3$ dimensions, $\nu = 0.767$. The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.89278, 0.842391, 0.820491, 0.8024160)$. These are extrapolated on the right-hand plot to infinite order, yielding $\nu = 0.767$.

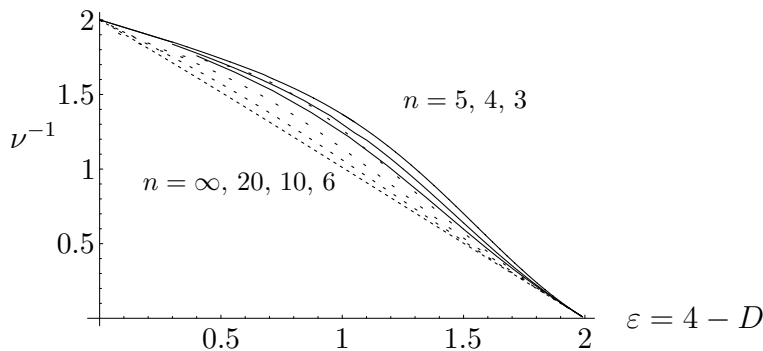


FIGURE 21.7 Highest approximations ($M = 4$) for $n = 3, 4, 5$ (counting from the top), and the $1/n$ -expansions to order $1/n^2$ for $n = \infty, 20, 10, 6$ (counting from the bottom). The sixth-order result is obviously still far from the exact one.

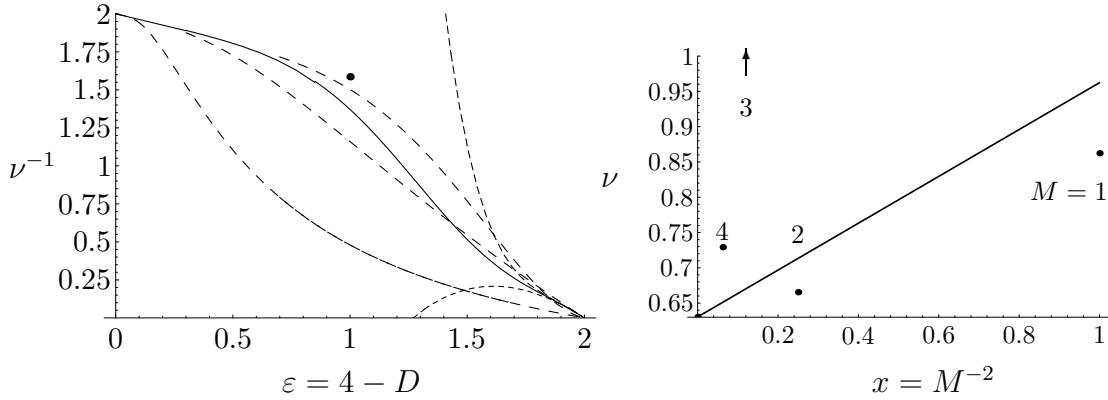


FIGURE 21.8 Analog plot to Fig. 21.4, for the $O(1)$ -universality class (the Ising model). There is no Padé-Borel approximation. The dot shows the seven-loop result in $D = 3$ dimensions, $\nu = 0.6304$. The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.862357, 0.665451, 2.08686, 0.802416)$. Their position with respect to the accurate value $\nu = 0.767$ is shown on the right-hand plot, with the failure to converge up to order $M = 4$.

21.8 Relation of σ -Model to Quantum Mechanics of a Point Particle on a Sphere

In $D=1$ dimension, the coordinate x may be identified as a time t , and the field variable $\pi_\mu(t)$ as a normalized position variable $x^\mu(t)$ of a massive point particle on the surface of a sphere. Then the action (21.228) for $t = 2/R$ describes the quantum mechanics of this system. It has the general geometric form

$$\mathcal{A} = \frac{1}{2} \int dt g_{\mu\nu}(x) \dot{x}^\mu(t) \dot{x}^\nu(t), \quad \mu, \nu = 1, \dots, D, \quad (21.189)$$

with a metric

$$g_{\mu\nu} = R^2 \left(\delta_{\mu\nu} + \frac{x^\mu x^\nu}{1 - \mathbf{x}^2} \right). \quad (21.190)$$

The Christoffel symbol, defined via the inverse metric $g^{\lambda\kappa} = (g^{-1})^{\lambda\kappa}$ as

$$\Gamma_{\mu\nu}{}^\kappa \equiv \frac{1}{2} g^{\lambda\kappa} (\partial_\mu g_{\nu\lambda} + \partial_\nu g_{\mu\lambda} - \partial_\lambda g_{\mu\nu}), \quad (21.191)$$

has for (21.190) the simple form

$$\Gamma_{\mu\nu}{}^\kappa = \frac{1}{R^2} g_{\mu\nu} x^\kappa. \quad (21.192)$$

The curvature tensor

$$R_{\mu\nu\lambda}{}^\kappa \equiv \partial_\mu \Gamma_{\nu\lambda}{}^\kappa - \partial_\nu \Gamma_{\mu\lambda}{}^\kappa + \Gamma_{\mu\lambda}{}^\tau \Gamma_{\nu\tau}{}^\kappa - \Gamma_{\nu\lambda}{}^\tau \Gamma_{\mu\tau}{}^\kappa \quad (21.193)$$

is found to satisfy

$$R_{\mu\nu\lambda\kappa} = g_{\kappa\sigma} R_{\mu\nu\lambda}{}^{\sigma} = \frac{1}{R^2} \left[(\delta_{\nu\lambda} \delta_{\mu\kappa} - \delta_{\mu\lambda} \delta_{\nu\kappa}) + \frac{1}{1 - \mathbf{x}^2} (x^{\nu} x^{\lambda} \delta_{\mu\kappa} + \delta_{\nu\lambda} x^{\mu} x^{\kappa} - x^{\mu} x^{\lambda} \delta_{\nu\kappa} - \delta_{\mu\lambda} x^{\nu} x^{\kappa}) \right]. \quad (21.194)$$

Using (21.190), this can be expressed in the characteristic form for homogeneous spaces:

$$R_{\mu\nu\lambda\kappa} = \frac{1}{R^2} (g_{\mu\kappa} g_{\nu\lambda} - g_{\mu\lambda} g_{\nu\kappa}). \quad (21.195)$$

The Ricci tensor and curvature scalar are [recall (4.365)]

$$R_{\mu\nu} = \delta^{\lambda}{}_{\kappa} R_{\mu\lambda\nu}{}^{\kappa} = (D - 2) g_{\mu\nu}, \quad R = g^{\mu\nu} R_{\mu\nu} = \frac{(D - 1)(D - 2)}{R^2}. \quad (21.196)$$

The path integral associated with the action (21.228) can be solved exactly by time slicing [25]. The resulting time evolution amplitude has an energy spectrum given by the eigenvalues of the Hamilton operator

$$H = \frac{\hbar^2}{2MR^2} L^2, \quad (21.197)$$

where $\hbar^2 L^2$ is the square of the angular momentum operator in N dimensions under which the sphere is rotationally invariant. The eigenvalues of L^2 are $l(l + N - 2)$ with $l = 0, 1, 2, \dots$. The spectrum of H coincides with that of the curved-space Schrödinger operator

$$H = -\frac{\hbar^2}{2MR^2} \Delta, \quad (21.198)$$

where Δ is the Laplace-Beltrami operator

$$\Delta = \frac{1}{\sqrt{g}} \partial_{\mu} \sqrt{g} g^{\mu\nu} \partial_{\nu} \quad (21.199)$$

on the surface of a sphere.

Let us investigate whether the above formal evaluation of Feynman diagrams in the nonlinear σ -model produces the same energy spectrum. The answer is negative: the spectrum emerging from the σ -model turns out to be the spectrum of a particle *near* the surface of a sphere. That spectrum is obtained by time-slicing naively the continuous path integral

$$Z = \int \mathcal{D}n^a \mathcal{D}\lambda e^{-\frac{1}{2} \int d\tau \{ \dot{n}_a^2 + \lambda [(n^a)^2 - 1] \}}, \quad (21.200)$$

in which a particle moves initially through an N -dimensional euclidean space. It is restricted to a $D = N - 1$ -dimensional sphere by a δ -function $\delta^D((n^a(x))^2 - 1)$ at every spacetime point x . In the time-sliced version, the particle lies on the surface only at the points where the δ -function forces it to do so. The intermediate sections

of the paths, however, runs from each point on the surface straight through the N -dimensional space to the next point on the surface, thereby leaving slightly the surface. This is why this path integral describes a particle *near* the surface of a sphere. The difference between the two energies is explained in Ref. [25].

The spectrum *near* the surface of a sphere in N dimensions is

$$E_l = \frac{\hbar^2}{2R^2} (L_2^2)_l, \quad (21.201)$$

with eigenvalues $(L_2^2)_l = (l + N/2 - 1)^2 - 1/4$ for $l = 0, 1, 2, \dots$. These have their origin in a large-argument expansion of a Bessel function

$$I_{l+N/2-1}(z/\epsilon) \approx \sqrt{\frac{2\pi z}{\epsilon}} e^{z/\epsilon} \left[1 - \epsilon \frac{(L_2^2)_l}{2z} + \dots \right]. \quad (21.202)$$

They appear in the time slices of width ϵ of the exponential $e^{-\frac{1}{2} \int d\tau \{ \dot{n}_a^2 + \lambda [(n^a)^2 - 1] \}}$ when transforming the cartesian coordinates n_a into the spherical coordinates in an N -dimensional space. On the sphere, the Hamiltonian operator (21.197) gives the energy spectrum

$$E_l = \frac{\hbar^2}{2R^2} (L^2)_l, \quad (21.203)$$

where $(L^2)_l = l(l + N - 1)$ for $l = 0, 1, 2, \dots$. The difference between the energies near and on the sphere has the l -independent value

$$\Delta E_l = \frac{\hbar^2}{2R^2} \frac{(N-1)(N-3)}{4}. \quad (21.204)$$

The lowest-order calculation of the renormalization constants in the nonlinear σ -model shows that this calculation procedure produces a spectrum of the type (21.201).

To see this we consider the renormalized action (21.47) and observe that the squared mass of the π -field is modified by the factor Z_h of Eq. (21.50). For the mass m itself, this implies

$$m_R = m \left(1 + \frac{\hbar}{R^2} \frac{N-3}{4} L + \dots \right), \quad (21.205)$$

where we have replaced t by $1/R^2$ and reinserted $\hbar$, thus returning to proper physical units. The Feynman integral (21.37) for L can easily be performed for $D = 1$ using the formula $\int dp/(p^2 + m^2) = \pi$, yielding $L = 1/2m$ [compare also (11.123)]. The mass receives therefore an explicit correction

$$m_R = m + \frac{\hbar}{2R^2} \frac{N-3}{4} + \dots \quad (21.206)$$

The quantum mechanical ground state energy of a harmonic oscillator of frequency m_R is $m_R\hbar/2$. The ground state energy of the $N - 1$ harmonically fluctuating variables $x_a(\tau)$ is therefore

$$E = (N - 1) \frac{m_R \hbar}{2} = (N - 1) \frac{m \hbar}{2} + \frac{\hbar^2}{2R^2} \frac{(N - 1)(N - 3)}{8} + \dots \quad (21.207)$$

In the limit $m \rightarrow 0$, we remain with the ground state energy (21.201) *near* the sphere.

21.9 Generalization of the Model

There exists a simple generalization of a point particle on a surface of a sphere: the *spinning top*. In fact, the ordinary spinning top in three dimensions is equivalent to a point particle on the surface of a sphere in four dimensions [26].

The action of a symmetric spinning top with moments of inertia I is

$$\mathcal{A} = \frac{1}{2I} \int dt (\omega_1^2 + \omega_2^2 + \omega_3^2), \quad (21.208)$$

where ω_i are the angular velocities of the spinning top. If $g = e^{-i\phi(t)\sigma/2}$ denote the 2×2 -rotation matrices specifying the orientation of the top, they are defined by

$$\omega_i = i \text{tr}(\sigma_i g^{-1} \partial_t g). \quad (21.209)$$

Alternatively we can write

$$\mathcal{A} = \int dt \frac{1}{I} \text{tr}[(g^{-1} \partial_t g)^2]. \quad (21.210)$$

This system has a field theoretic analog in a generalized nonlinear σ -model defined by the action

$$\mathcal{A} = \frac{1}{t} \int d^D x \text{tr}[g^{-1} \partial_\mu g g^{-1} \partial^\mu g]. \quad (21.211)$$

The partition function (21.14) including an external magnetic field of the type (21.20) becomes for this action

$$Z = \int \mathcal{D}g \exp \left\{ -\frac{1}{t} \int d^D x \text{tr}[g^{-1} \partial_\mu g g^{-1} \partial^\mu g] + h \text{tr}[D(g) + D^*(g)] - \frac{1}{2a^D} \int d^D x \log \det g \right\}, \quad (21.212)$$

where $D(g)$ is some matrix representation of the group elements g . In general, we may assume g to be elements of any Lie group which can be represented as exponentials

$$g = e^{-i\pi_a G_a}, \quad (21.213)$$

where the generators G_a close under commutation relations, with antisymmetric structure constants f_{abc} :

$$[G_a, G_b] = i f_{abc} G_c. \quad (21.214)$$

From the exponential form we find the partial derivatives $g^{-1} \partial_\mu g$ as

$$g^{-1} \partial_\mu g = e^{i\pi_a G_a} \frac{1}{d\pi_a} \left[e^{-i(\pi_a + d\pi_a) G_a} - e^{-i\pi_a G_a} \right] \frac{\partial_\mu \pi_a}{\partial_\mu}. \quad (21.215)$$

The exponential $e^{i\pi_a G_a} e^{-i(\pi_a + d\pi_a) G_a}$ is expanded into a *Neumann-Liouville* or *Dyson-series* [recall (1.247)]. Abbreviating $\pi_a G_a$ by $\not{\pi}$, this gives

$$\begin{aligned} e^{i\not{\pi}} e^{-i(\not{\pi} + d\not{\pi})} &= 1 - i \int_0^1 d\sigma e^{i\sigma \not{\pi}} d\not{\pi} e^{-i\sigma \not{\pi}} + \mathcal{O}(d\not{\pi}^2) \\ &= 1 - i \left\{ d\not{\pi} + \frac{i}{2!} [\not{\pi}, d\not{\pi}] + \frac{i}{3!} [\not{\pi}, [\not{\pi}, d\not{\pi}]] + \dots \right\}. \end{aligned} \quad (21.216)$$

In this way we find

$$g^{-1} \partial_\mu g = -i G_a \left(\partial_\mu \pi_a + \frac{1}{2} \pi_b \partial_\mu \pi_c f_{abc} + \frac{1}{6} \pi_b \pi_c \partial_\mu \pi_d f_{bde} f_{efa} + \dots \right). \quad (21.217)$$

Normalizing the generators to

$$\text{tr}(G_a G_b) = \frac{1}{2} \eta_{ab}, \quad \eta_{ab} \equiv f_{acd} f_{bcd}, \quad (21.218)$$

we obtain

$$\text{tr}[g^{-1} \partial_\mu g g^{-1} \partial^\mu g] = \frac{1}{2} g_{ab}(\pi) \partial_\mu \pi_a \partial^\mu \pi_b, \quad (21.219)$$

with the metric in field space

$$g_{ab}(\pi) = \delta_{ab} - \frac{1}{12} f_{acd} f_{bce} \pi_d \pi_e - \frac{1}{360} f_{acd} f_{cpe} f_{phf} f_{bhk} \pi_d \pi_e \pi_f \pi_k + \dots \quad (21.220)$$

From this we calculate the connection

$$\Gamma_{abc} = -\frac{1}{12} f_{cad} f_{bde} \pi_e + \dots, \quad (21.221)$$

and the curvature tensor (21.193) as

$$R_{abcd} = \frac{1}{12} (f_{ach} f_{bdh} - f_{bch} f_{adh}) + \dots \quad (21.222)$$

The expansion (21.220) starts therefore out like

$$g_{\mu\nu} = \delta_{\mu\nu} - R_{adbe} \pi_d \pi_e + \dots \quad (21.223)$$

The commutation relations (21.214) are satisfied by the adjoint representation

$$(G_a)_{bc} = -if_{abc}, \quad (21.224)$$

which allows us to rewrite (21.225) as

$$R_{abcd} = \frac{1}{12}f_{abe}f_{ecd} + \dots \quad (21.225)$$

In the tensor form of the adjoint representation, the generators are

$$(G_{ab})_{cd} = if_{abe}f_{ecd}, \quad (21.226)$$

so that we may identify $R_{abcd} = -i(G_{ab})_{cd}$. In the case of the Lorentz group, the generators (21.226) become $(G_{ab})_{cd} = i(g_{ac}g_{bd} - g_{bc}g_{ad})$ as in Eq. (4.65), and (21.225) coincides with (21.195).

The perturbation expansion and critical behavior of this theory can be discussed in complete analogy with the previous $O(N)$ -sigma model. One separates the action (21.228) in the coordinates $\pi^a(t)$ into free and interacting parts as

$$\mathcal{A} = \frac{1}{2} \int dt \delta_{ab} \dot{\pi}^a(t) \dot{\pi}^b(t), \quad a, b = 1, \dots, N-1, \quad (21.227)$$

$$\mathcal{A}^{\text{int}} = \frac{1}{2} \int dt R_{adbe} \dot{\pi}^a(t) \dot{\pi}^b(t) \pi^d(t) \pi^e(t), \quad (21.228)$$

and obtains the first-order correction to the free-particle energy density

$$E^{(1)} = \langle \mathcal{A}^{\text{int}} \rangle = -\frac{1}{2} R_{adbe} \langle \dot{\pi}^a(t) \dot{\pi}^b(t) \rangle \langle \pi^d(t) \pi^e(t) \rangle. \quad (21.229)$$

With a small infrared regulator mass m , the correlation function is

$$\langle \pi^a(t) \pi^b(t') \rangle = \delta^{ab} \int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{iqt} \frac{1}{q^2 + m^2} = \frac{\delta^{ab}}{2m} e^{-m|t-t'|}. \quad (21.230)$$

At equal times, this yields

$$\langle \pi^a(t) \pi^a(t) \rangle = \delta^{ab} \frac{1}{2m}, \quad \langle \dot{\pi}^a(t) \dot{\pi}^b(t) \rangle = -\delta^{ab} \frac{m}{2}, \quad (21.231)$$

the latter in dimensional regularization where $\int dk/2\pi = 0$ allows us to omit the Jacobian in the measure of path integration. Inserting this into (21.232), we obtain

$$E^{(1)} = \langle \mathcal{A}^{\text{int}} \rangle = \frac{1}{8} R. \quad (21.232)$$

Notes and References

For a derivation of the critical exponents of the $O(N)$ nonlinear σ -model see [1].

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- [25] See Sections 8.9 and 10.4 in Re. [6].
- [26] See Section 1.15 and Chapter 8 in the textbook [6] on p. 739.

*It is simplicity that makes the uneducated
more effective than the educated.*
ARISTOTELES (384 BC–322 BC)

22

Functional-Integral Calculation of Effective Action. Loop Expansion

The functional-integral formula for $Z[j]$ can be employed for a rather direct evaluation of the effective action of a theory. Diagrammatically, the result will be the loop expansion organized by powers of the Planck quantum $\hbar$ [1].

22.1 General Formalism

Consider the generating functional of all Green functions

$$Z[j] = e^{iW[j]/\hbar}, \quad (22.1)$$

where $W[j]$ is the generating functional of all *connected* Green functions. The vacuum expectation of the field, the average

$$\Phi(x) \equiv \langle \phi(x) \rangle, \quad (22.2)$$

is given by the first functional derivative

$$\Phi(x) = \delta W[j] / \delta j(x). \quad (22.3)$$

This can be inverted to yield $j(x)$ as an x -dependent functional of $\Phi(x)$:

$$j(x) = j[\Phi](x), \quad (22.4)$$

which may be used to form the Legendre transform of $W[j]$:

$$\Gamma[\Phi] \equiv W[j] - \int d^4x j(x) \Phi(x), \quad (22.5)$$

where $j(x)$ on the right-hand side is replaced by (22.4). The result is the *effective action* of the theory.

The first functional derivative of the effective action gives back the current

$$\frac{\delta \Gamma[\Phi]}{\delta \Phi(x)} = -j(x). \quad (22.6)$$

This equation justifies the name effective action for the functional $\Gamma[\Phi]$. In the absence of an external current $j(x)$, the effective action $\Gamma[\Phi]$ is extremal on the physical field expectation value (22.2). Thus it plays exactly the same role for the fully interacting quantum theory as the action does for the classical field configurations.

The Legendre transformation (22.5) can be inverted to recover the generating functional $W[j]$ from the effective action:

$$W[j] = \Gamma[\Phi] + \int d^4x j(x)\Phi(x). \quad (22.7)$$

Let us compare this with the functional-integral formula for the generating functional $Z[j]$:

$$Z[j] = \frac{\int \mathcal{D}\phi(x) e^{(i/\hbar)\{\mathcal{A}[\phi] + \int d^4x j(x)\phi(x)\}}}{\int \mathcal{D}\phi(x) e^{(i/\hbar)\mathcal{A}_0[\phi]}}. \quad (22.8)$$

Using (22.1) and (22.5), this implies a functional-integral formula for the effective action $\Gamma[\Phi]$:

$$e^{\frac{i}{\hbar}\{\Gamma[\Phi] + \int d^4x j(x)\Phi(x)\}} = \mathcal{N} \int \mathcal{D}\phi(x) e^{(i/\hbar)\{\mathcal{A}[\phi] + \int d^4x j(x)\phi(x)\}}, \quad (22.9)$$

where $\mathcal{N}$ is a normalization factor:

$$\mathcal{N} = \left\{ \int \mathcal{D}\phi(x) e^{(i/\hbar)\mathcal{A}_0[\phi]} \right\}^{-1}. \quad (22.10)$$

We have explicitly displayed the fundamental quantum of action $\hbar$, which is a measure for the size of quantum fluctuations.

There are many physical systems for which quantum fluctuations are rather small, except in the immediate vicinity of certain critical points. For these systems, it is desirable to develop a method of solving (22.9) for $\Gamma[\Phi]$ as a series expansion in powers of $\hbar$, taking into account successively increasing quantum fluctuations.

In the limit $\hbar \rightarrow 0$, the path integral over the field $\phi(x)$ in (22.8) is dominated by the classical solution $\phi_{\text{cl}}(x)$ which extremizes the exponent

$$\left. \frac{\delta \mathcal{A}}{\delta \phi} \right|_{\phi=\phi_{\text{cl}}(x)} = -j(x). \quad (22.11)$$

At this level we therefore identify

$$W[j] = \Gamma[\Phi] + \int d^4x j(x)\Phi(x) = \mathcal{A}[\phi_{\text{cl}}] + \int d^4x j(x)\phi_{\text{cl}}(x). \quad (22.12)$$

Of course, $\phi_{\text{cl}}(x)$ is a functional of $j(x)$, so that we may write it more explicitly as $\phi_{\text{cl}}[j](x)$. By differentiating $W[j]$ with respect to j , we have from Eqs. (22.3) and (22.7):

$$\Phi(x) = \frac{\delta W}{\delta j} = \frac{\delta \Gamma}{\delta \Phi} \frac{\delta \Phi}{\delta j} + \Phi + j \frac{\delta \Phi}{\delta j}. \quad (22.13)$$

Inserting the classical field equation (22.11), this becomes

$$\Phi(x) = \frac{\delta \mathcal{A}}{\delta \phi_{\text{cl}}} \frac{\delta \phi_{\text{cl}}}{\delta j} + \phi_{\text{cl}} + j \frac{\delta \phi_{\text{cl}}}{\delta j} = \phi_{\text{cl}}. \quad (22.14)$$

Thus, to this approximation, $\Phi(x)$ coincides with the classical field $\phi_{\text{cl}}(x)$. For the ϕ^4 -theory with $O(N)$ -symmetry, the action is

$$\mathcal{A}[\phi] = \int d^4x \left[\frac{1}{2} (\partial \phi_a)^2 - \frac{m^2}{2} \phi_a^2 - \frac{g}{4!} (\phi_a^2)^2 \right]. \quad (22.15)$$

Replacing the $\phi_a \rightarrow \phi_{\text{cl}a} + \delta \phi_s = \Phi_a + \delta \phi$ on the right-hand side of Eq. (22.12), we therefore obtain the lowest-order result for the effective action (which is of zeroth order in $\hbar$):

$$\Gamma[\Phi] \approx \mathcal{A}[\Phi] = \int d^4x \left[\frac{1}{2} (\partial \Phi_a)^2 - \frac{m^2}{2} \Phi_a^2 - \frac{g}{4!} (\Phi_a^2)^2 \right]. \quad (22.16)$$

It equals the fundamental action, and is also referred to as the mean field approximation to the effective action.

We have shown in Chapter 13 that all vertex functions can be obtained from the derivatives of $\Gamma[\Phi]$ with respect to Φ at the equilibrium value of Φ for $j = 0$. We begin by assuming that $m^2 > 0$.¹ Then $\Gamma[\Phi]$ has an extremum at $\Phi_a \equiv 0$, and there are only two types of non-vanishing vertex functions $\Gamma^{(n)}(x_1, \dots, x_n)$: For $n = 2$, we obtain the lowest-order two-point function

$$\begin{aligned} \Gamma^{(2)}(x_1, x_2)_{ab} &\equiv \left. \frac{\delta^2 \Gamma}{\delta \Phi_a(x_1) \delta \Phi_b(x_2)} \right|_{\Phi_a=0} = \left. \frac{\delta^2 \mathcal{A}}{\phi_a(x_1) \phi_b(x_2)} \right|_{\phi_a=\Phi_a=0} \\ &= (-\partial^2 - m^2) \delta_{ab} \delta^{(4)}(x_1 - x_2). \end{aligned} \quad (22.17)$$

This determines the inverse of the propagator:

$$\Gamma_{ab}^{(2)}(x_1, x_2) = [i\hbar G^{-1}]_{ab}(x_1, x_2). \quad (22.18)$$

Thus we find in this zeroth-order approximation that $G_{ab}(x_1, x_2)$ is equal to the free propagator:

$$G_{ab}(x_1, x_2) = G_{0ab}(x_1, x_2). \quad (22.19)$$

For $n = 4$, we find the lowest-order four-point function

$$\Gamma_{abcd}^{(4)}(x_1, x_2, x_3, x_4) \equiv \frac{\delta^4 \Gamma}{\delta \Phi_a(x_1) \delta \Phi_b(x_2) \delta \Phi_c(x_3) \delta \Phi_d(x_4)} = g T_{abcd}, \quad (22.20)$$

where

$$T_{abcd} = \frac{1}{3} (\delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc}) \quad (22.21)$$

¹Also the case $m^2 < 0$ corresponds to a physical state in a different phase and will be discussed separately. In fact, the phase transition is the reason for the nonexistence of tachyon particles, i.e., of particles that move faster than the speed of light. See the pages 1123, 1294 and 1311.

is the fundamental vertex [compare (22.16)] for the local interaction of strength g .

The effective action has the virtue that all diagrams of the theory can be obtained from tree diagrams built from propagators $G_{ab}(x_1, x_2)$ and vertex functions. This was explained in Chapter 13. In lowest approximation, we recover precisely the subset of all original Feynman diagrams with a tree-like topology. These are the diagrams which do not involve any loop integration. Since the limit $\hbar \rightarrow 0$ corresponds to the classical equations of motion with no quantum fluctuations, we conclude: Classical field theory corresponds to tree diagrams.

The use of the initial action as an approximation to the effective action neglecting fluctuations is often referred to as *mean-field theory*.

22.2 Quadratic Fluctuations

In order to find the $\hbar$ -correction to this approximation we expand the action in powers of the fluctuations of the field around the classical solution

$$\delta\phi(x) \equiv \phi(x) - \phi_{\text{cl}}(x), \quad (22.22)$$

and perform a perturbation expansion. The quadratic term in $\delta\phi(x)$ is taken to be the free-field action, the higher powers in $\delta\phi(x)$ are the interactions. Up to second order in the fluctuations $\delta\phi(x)$, the action is expanded as follows:

$$\begin{aligned} \mathcal{A}[\phi_{\text{cl}} + \delta\phi] + \int d^4x j(x)[\phi_{\text{cl}}(x) + \delta\phi(x)] \\ = \mathcal{A}[\phi_{\text{cl}}] + \int d^4x j(x)\phi_{\text{cl}}(x) + \int d^4x \left\{ j(x) + \frac{\delta\mathcal{A}}{\delta\phi(x)} \Big|_{\phi=\phi_{\text{cl}}} \right\} \delta\phi(x) \\ + \int d^4x d^4y \delta\phi(x) \frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)} \Big|_{\phi=\phi_{\text{cl}}} \delta\phi(y) + \mathcal{O}((\delta\phi)^3). \end{aligned} \quad (22.23)$$

The curly bracket term linear in the variation $\delta\phi$ vanishes due to the extremality property of the classical field ϕ_{cl} expressed by the field equation (22.11). Inserting this expansion into (22.9), we obtain the approximate expression

$$Z[j] \approx \mathcal{N} e^{(i/\hbar)\{\mathcal{A}[\phi_{\text{cl}}] + \int d^4x j\phi_{\text{cl}}\}} \int \mathcal{D}\delta\phi \exp \left\{ \frac{i}{\hbar} \int d^4x d^4y \delta\phi(x) \frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)} \Big|_{\phi=\phi_{\text{cl}}} \delta\phi(y) \right\}. \quad (22.24)$$

We now observe that the fluctuations in $\delta\phi$ will be of average size $\sqrt{\hbar}$ due to the $\hbar$ -denominator in the Fresnel integrals over $\delta\phi$ in (22.24). Thus the fluctuations $(\delta\phi)^n$ are on the average of relative order $\hbar^{n/2}$. If we ignore corrections of the order $\hbar^{3/2}$, the fluctuations remain quadratic in $\delta\phi$ and we may calculate the right-hand side of (22.24) as

$$\begin{aligned} \mathcal{N} e^{(i/\hbar)\{\mathcal{A}[\phi_{\text{cl}}] + \int d^4x j(x)\phi_{\text{cl}}(x)\}} \left[\det \frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)} \Big|_{\phi=\phi_{\text{cl}}} \right] \\ = (\det iG_0)^{1/2} e^{(i/\hbar)\{\mathcal{A}[\phi_{\text{cl}}] + \int d^4x j(x)\phi_{\text{cl}}(x) + i(\hbar/2)\text{Tr} \log[\delta^2\mathcal{A}/\delta\phi(x)\delta\phi(y)|_{\phi=\phi_{\text{cl}}}\}]} \quad (22.25) \end{aligned}$$

Comparing this with the left-hand side of (22.9), we find that to first order in $\hbar$ the effective action may be recovered by equating

$$\Gamma[\Phi] + \int d^4x j(x)\Phi(x) = \mathcal{A}[\phi_{\text{cl}}] + \int d^4x j\phi_{\text{cl}} + \frac{i\hbar}{2} \text{Tr} \log \frac{\delta^2 \mathcal{A}}{\delta\phi(x)\delta\phi(y)}(\phi_{\text{cl}}). \quad (22.26)$$

In the limit $\hbar \rightarrow 0$, the trace log term disappears and (22.26) reduces to the classical action.

To include the $\hbar$ -correction into $\Gamma[\Phi]$, we expand $W[j]$ as

$$W[j] = W_0[j] + \hbar W_1[j] + \mathcal{O}(\hbar^2). \quad (22.27)$$

Correspondingly, the field Φ differs from Φ_{cl} by a correction of the order $\hbar^2$:

$$\Phi = \phi_{\text{cl}} + \hbar\phi_1 + \mathcal{O}(\hbar^2). \quad (22.28)$$

Inserting this into (22.26), we find

$$\begin{aligned} \Gamma[\Phi] + \int d^4x j\Phi &= \mathcal{A}[\Phi - \hbar\phi_1] + \int d^4x j\Phi - \hbar \int d^4x j\phi_1 + \frac{i}{2}\hbar \text{Tr} \log \frac{\delta^2 \mathcal{A}}{\delta\phi\delta\phi} \Big|_{\phi=\Phi-\hbar\phi_1} \\ &\quad + \mathcal{O}(\hbar^2). \end{aligned}$$

Expanding the action up to the same order in $\hbar$ gives

$$\begin{aligned} \Gamma[\Phi] &= \mathcal{A}[\Phi] + \hbar \left\{ \frac{\delta \mathcal{A}[\Phi]}{\delta\Phi} - j \right\} \phi_1 + \int d^4x j\Phi + \frac{i}{2}\hbar \text{Tr} \log \frac{\delta^2 \mathcal{A}}{\delta\phi\delta\phi} \Big|_{\phi=\Phi} \\ &\quad + \mathcal{O}(\hbar^2). \end{aligned} \quad (22.29)$$

But because of (22.11), the curly-bracket term is only of the order $\mathcal{O}(\hbar^2)$, so that we find the one-loop form of the effective action

$$\begin{aligned} \Gamma[\Phi] &= \int d^4x \left[\frac{1}{2}(\partial\Phi)^2 - \frac{m^2}{2}\Phi^2 - \frac{g}{4!}\Phi^4 \right] \\ &\quad + \frac{i}{2}\hbar \text{Tr} \log \left[-\partial^2 - m^2 - \frac{g}{2}\Phi^2 \right], \end{aligned} \quad (22.30)$$

where we dropped the infinite additive constant $\frac{i}{2}\hbar \text{Tr} \log [-\partial^2 - m^2]$.

If we generalize this to an $O(N)$ -invariant theory with N components ϕ_a ($a = 1, \dots, N$), this expression becomes

$$\begin{aligned} \Gamma[\Phi] = \Gamma_0[\Phi] + \Gamma_1[\Phi] &= \int d^4x \left[\frac{1}{2}(\partial\Phi_a)^2 - \frac{m^2}{2}\Phi_a^2 - \frac{g}{4!}(\Phi_a^2)^2 \right] \\ &\quad + \frac{i}{2}\hbar \text{Tr} \log \left[-\partial^2 - m^2 - \frac{g}{6}(\delta_{ab}\Phi_c^2 + 2\Phi_a\Phi_b) \right]. \end{aligned} \quad (22.31)$$

What is the graphical content of the set of all Green functions at this level? In this discussion we shall assume that $N = 1$. For $j = 0$, we find that the minimum

of $\Gamma[\Phi]$ lies at $\Phi = \Phi^0 \equiv \Phi_j = 0$, just as in the mean-field approximation. Around this minimum, we may expand the trace log in powers of Φ , and obtain

$$\frac{i}{2}\hbar \text{Tr} \log \left(-\partial^2 - m^2 - \frac{g}{2}\Phi^2 \right) = \frac{i}{2}\hbar \text{Tr} \log \left(-\partial^2 - m^2 \right) + \frac{i}{2}\hbar \text{Tr} \log \left(1 + \frac{i}{-\partial^2 - m^2} g \frac{\Phi^2}{2} \right). \quad (22.32)$$

The second term can be expanded in powers of Φ^2 as follows:

$$-i\frac{\hbar}{2} \sum_{n=1}^{\infty} \left(-i\frac{g}{2} \right)^n \frac{1}{n} \text{Tr} \left(\frac{i}{-\partial^2 - m^2} \Phi^2 \right)^n.$$

If we insert

$$G_0 = \frac{i}{-\partial^2 - m^2}, \quad (22.33)$$

then (22.32) can be written as

$$i\frac{\hbar}{2} \text{Tr} \log \left(-\partial^2 - m^2 \right) - i\frac{\hbar}{2} \sum_{n=1}^{\infty} \left(-i\frac{g}{2} \right)^n \frac{1}{n} \text{Tr} \left(G_0 \Phi^2 \right)^n. \quad (22.34)$$

More explicitly, the terms with $n = 1$ and $n = 2$ read:

$$\begin{aligned} & -\frac{\hbar}{2}g \int d^4x d^4y \delta^{(4)}(x-y) G_0(x,y) \Phi^2(y) \\ & + i\hbar \frac{g^2}{16} \int d^4x d^4y d^4z \delta^4(x-z) G_0(x,y) \Phi^2(y) G_0(y,z) \Phi^2(z) + \dots \end{aligned} \quad (22.35)$$

The expansion terms correspond obviously to the Feynman diagrams

$$\begin{array}{c} \text{---} \diagup \quad \text{---} \diagup \quad \text{---} \diagup \quad \text{---} \diagup \\ \bigcirc \quad + \quad \bigcirc \quad + \quad \bigcirc \quad + \quad \bigcirc \quad + \dots \end{array} \quad (22.36)$$

Thus, the series (22.34) is a sum of all diagrams with one loop and any number of fundamental Φ^4 -vertices.

To systemize the entire expansion (22.34), the leading trace log expression may be pictured by a single-loop diagram

$$i\frac{\hbar}{2} \text{Tr} \log \left(-\partial^2 - m^2 \right) = \bigcirc. \quad (22.37)$$

The subsequent two diagrams in (22.36) contribute corrections to the vertices $\Gamma^{(2)}$ and $\Gamma^{(4)}$ in (22.17) and (22.20). The remaining ones produce higher vertex functions and lead to more involved tree diagrams. Note that only the first two corrections

are formally divergent, all other Feynman integrals converge. In momentum space, the corrections are, from (22.35),

$$\Gamma^{(2)}(q) = q^2 - m^2 - \hbar \frac{g}{2} \int \frac{d^4 k}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\eta} \quad (22.38)$$

$$\Gamma^{(4)}(q_i) = g - i \frac{g^2}{2} \left[\int \frac{d^4 k}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\epsilon} \frac{i}{(q_1 + q_2 - k)^2 - m^2 + i\eta} + 2 \text{ perm} \right]. \quad (22.39)$$

The convergence of all higher diagrams in the expansion (22.36) is ensured by the renormalizability of the theory. Indeed, up to $n = 4$, a counter term may be written down for each infinity that has the same form as those in the original Lagrangian (22.15). In euclidean form, we may write (22.38) and (22.39) as

$$\Gamma^{(2)}(q) = - \left(q^2 + m^2 + \hbar \frac{g}{2} D_1 \right), \quad (22.40)$$

$$\Gamma^{(4)}(q_i) = g - \hbar \frac{g^2}{2} [I(q_1 + q_2) + 2 \text{ perm}], \quad (22.41)$$

where D_1 and $I(q)$ are the Feynman integrals [compare (11.26) and (11.29)]

$$D_1 = \int d^4 k_E \frac{1}{k_E^2 + m^2} \quad (22.42)$$

and

$$I(q) = \int d^4 k_E \frac{1}{(k_E^2 + m^2)} \frac{1}{[(k + q)_E^2 + m^2]}. \quad (22.43)$$

The integrals can be calculated in D dimensions by separating them into a directional and a size integral as

$$\begin{aligned} \int d^D k &= \int \frac{d^D k}{(2\pi)^D} = \frac{S_D}{(2\pi)^D} \int dk k^{D-1} \\ &\equiv \frac{S_D}{2} \int dk^2 (k^2)^{D/2-1}. \end{aligned} \quad (22.44)$$

We further simplify all calculations by performing a Wick rotation of all energy integrals $\int dk_0$ into $i \int_{-\infty}^{\infty} dk_4$. Then the integrals $\int d^4 k$ become what are called euclidean integrals $i \int d^4 k_E$ where $k_E^\mu = (\mathbf{k}, k_4)$, and $k^2 = k_0^2 - \mathbf{k}^2$ becomes $-k_E^2 = -(\mathbf{k}^2 + k_4^2)$. By the same token we introduce the euclidean version $\Gamma_E[\Phi] = -i\Gamma[\Phi]$ of the effective action (22.30) whose functional derivatives are vertex functions $\Gamma^{(n)}$.

We further introduce renormalized fields

$$\phi_R(x) \equiv Z_\phi^{-1/2} \phi(x), \quad (22.45)$$

where $Z_\phi^{1/2}$ is a *field renormalization constant*. It serves to absorb infinities arising in the momentum integrals. The renormalized vertex functions are obtained by calculating all vertex functions in $D = 4 - \epsilon$ dimensions and fixing the renormalization

constants order by order in perturbation theory. Alternatively, we can add to the bare action suitable counter terms. In either way, we arrive at finite expressions.

If we regularize the integrals dimensionally in $4 - \epsilon$ dimensions, the counterterms take the forms calculated in Section 11.5, and the expression (22.40) becomes

$$\begin{aligned} \Gamma_R^{(2)}(q) = & - \left\{ q^2 + m^2 + \hbar \frac{g}{2} S_D \mu^{-\epsilon} m^2 \times \right. \\ & \left. \times \left[\frac{1}{2} \Gamma(2 - \epsilon/2) \Gamma(-1 + \epsilon/2) \left(\frac{m^2}{\mu^2} \right)^{-\epsilon/c} + \frac{1}{\epsilon} \right] \right\}, \end{aligned} \quad (22.46)$$

while (22.41) is renormalized to

$$\Gamma_R^{(4)}(q_i) = g - \hbar \frac{g^2}{2} \{ [I(q_1 + q_2) + 2 \text{ perm}] - 3I(0) \}. \quad (22.47)$$

The Feynman integral $I(q)$ has, after subtracting the $1/\epsilon$ -pole in Eq. (22.43), the small- ϵ behavior [compare (11.176)]

$$I_R(q) = -\frac{1}{2} S_D \mu^{-\epsilon} \left[1 + L^m(q) + \log \frac{q^2}{\mu^2} \right] + \mathcal{O}(\epsilon), \quad (22.48)$$

with

$$\begin{aligned} L^m(q) &= \int_0^1 dx \log \left[x(1-x) + \frac{m^2}{q^2} \right] \\ &= -2 + \log \frac{m^2}{q^2} + \frac{\sqrt{q^2 + 4m^2}}{\sqrt{q^2}} \log \frac{\sqrt{q^2 + 4m^2} + \sqrt{q^2}}{\sqrt{q^2 + 4m^2} - \sqrt{q^2}}. \end{aligned} \quad (22.49)$$

As far as the original effective action (22.30) to order $\hbar$ is concerned, we may add the counter terms as

$$\begin{aligned} \Gamma[\Phi] &= \int d^4x \left\{ \frac{1}{2} (\partial\Phi)^2 - \frac{m^2}{2} \Phi^2 - \frac{g}{4!} \Phi^4 \right\} - i \frac{\hbar}{2} \text{Tr} \log \left(-\partial^2 - m^2 - \frac{g}{2} \Phi^2 \right) \\ &+ \frac{g}{4} \int \frac{d^4q}{(2\pi)^4} \frac{1}{q^2 + m^2} \int d^4x \Phi^2(x) - \frac{g^2}{16} \int \frac{d^4q}{(2\pi)^4} \frac{1}{(q^2 + m^2)} \int d^4x \Phi^4. \end{aligned} \quad (22.50)$$

The divergent integrals in the last two terms can be evaluated with any regularization method, and (22.50) becomes

$$\begin{aligned} \Gamma[\Phi] &= \int d^4x \left\{ \frac{1}{2} (\partial\Phi)^2 - \frac{m^2}{2} \Phi^2 - \frac{g}{4!} \Phi^4 \right\} + i \frac{\hbar}{2} \text{Tr} \log \left(-\partial^2 - m^2 - \frac{g}{2} \Phi^2 \right) \\ &- c^{m^2} \frac{m^2}{2} \Phi^2 - c^g \frac{g^2}{4!} \Phi^4. \end{aligned} \quad (22.51)$$

The third line may be written as

$$- \frac{\hbar g}{4} (m^2)^{1-\epsilon/2} c_1 \Phi^2 + \frac{\hbar g^2}{16} (m^2)^{-\epsilon/2} c_2 \Phi^4, \quad (22.52)$$

with the constants

$$c_1 = m^{\epsilon-2} \int d^D p_E \frac{1}{p_E^2 + m^2}, \quad (22.53)$$

$$c_2 = m^\epsilon \int d^D p_E \frac{1}{(p_E^2 + m^2)^2}. \quad (22.54)$$

We evaluate these integrals using the formulas [2]

$$\int d^D k_E \frac{1}{k_E^2 + m^2} = S_D \frac{\Gamma(D/2)\Gamma(1-D/2)}{2\Gamma(1)} \frac{1}{(m^2)^{1-D/2}}, \quad (22.55)$$

and

$$\int d^D k_E \frac{1}{(k_E^2 + m^2)^2} = S_D \frac{\Gamma(D/2)\Gamma(2-D/2)}{2\Gamma(1)} \frac{1}{(m^2)^{2-D/2}}. \quad (22.56)$$

Further, by integrating (22.55) over m^2 , we find

$$\int d^D k_E \log(k_E^2 + m^2) = S_D \frac{\Gamma(D/2)\Gamma(1-D/2)}{D\Gamma(1)} (m^2)^{D/2}. \quad (22.57)$$

In the so-called minimal subtraction scheme in $4 - \epsilon$ dimensions, only the singular $1/\epsilon$ pole parts of the two integrals are selected for the subtraction in (22.50). In the neighborhood of $\epsilon = 0$, (22.53) and (22.54) become

$$c_1 = -S_D \frac{2}{\epsilon} + \mathcal{O}(\epsilon), \quad (22.58)$$

$$c_2 = S_D \frac{1}{\epsilon} \left(1 - \frac{\epsilon}{2}\right) + \mathcal{O}(\epsilon). \quad (22.59)$$

Hence we can choose as counter terms the singular terms in (22.52):

$$-\frac{\hbar g \mu^{-\epsilon}}{4} m^2 S_D \left(-\frac{1}{\epsilon}\right) \Phi^2, \quad \frac{\hbar g^2 \mu^{-\epsilon}}{16} S_D \frac{1}{\epsilon} \Phi^4. \quad (22.60)$$

These make the effective action (22.51) finite for any mass m .

Note, however, that an auxiliary mass parameter μ must be introduced to define these expressions. If the physical mass m is nonzero, μ can be chosen to be equal to m . But for $m = 0$, we must use an arbitrary nonzero auxiliary mass μ as the renormalization scale.

Observe that up to the order $\hbar$, there is no divergence that needs to be absorbed in the gradient term $\int d^D x (\partial\Phi)^2$ of the effective action (22.51). These come in as soon as we carry the same analysis to one more loop order.

Let us calculate the effective potential in the critical regime for a constant field Φ at the one-loop level. It is defined by $v(\Phi) = -\Gamma_E[\Phi]/VT$. The argument in the

trace log term is now diagonal in momentum space and the calculation reduces to a simple momentum integral. It follows directly from (22.51) and reads

$$v(\Phi) = \frac{m^2}{2}\Phi^2 + \frac{g}{4!}\Phi^4 + \frac{\hbar}{2} \int \frac{d^D q_E}{(2\pi)^D} \log \left(1 + \frac{g}{2} \frac{\Phi^2}{q_E^2 + m^2} \right) - \frac{\hbar g}{4} (m^2)^{1-\epsilon/2} c_1 \Phi^2 + \frac{\hbar g^2}{16} (m^2)^{-\epsilon/2} c_2 \Phi^4. \quad (22.61)$$

The expansions in powers of ϵ have an important property which has direct consequences for the strong-coupling limit that is measured in critical phenomena. For small ϵ , Eq. (22.47) can be rewritten as

$$\Gamma_R^{(2)} = \left(q_E^2 + m^2 + \frac{\hbar}{4} \mu^{-\epsilon} g S_D \log \frac{m_E^2}{\mu^2} \right), \quad (22.62)$$

which is, to the same order in g , equal to

$$\Gamma_R^{(2)}(q) = \left[q_E^2 + \left(\frac{m^2}{\mu^2} \right)^{1+\frac{\hbar}{4} \mu^{-\epsilon} g S_D} \mu^2 \right]. \quad (22.63)$$

This means that the vertex function at $q = 0$ has a mass term that depends on the mass m of the ϕ -field via a power law:

$$\Gamma_R^{(2)}(0) = \left(\frac{m^2}{\mu^2} \right)^\gamma \mu^2. \quad (22.64)$$

The power γ depends on the coupling strength g like

$$\gamma = 1 + \frac{\hbar}{4} \mu^{-\epsilon} g S_D. \quad (22.65)$$

The important point is that this power γ is measurable as an experimental quantity called the *susceptibility*. It is called the *critical exponent* of the susceptibility.

If the effective action is calculated to order $\hbar^2$, then the gradient term in the effective action is modified and becomes

$$\Gamma[\Phi] = \int d^d x \Phi_R(x) \Gamma_R(\hat{q}) \Phi_R(x), \quad (22.66)$$

where $\Phi_R(x) = Z_\phi^{-1/2} \Phi(x)$, and Z_ϕ is the field renormalization constant introduced in (22.45). It is divergent for $\epsilon \rightarrow 0$ in $D = 4 - \epsilon$ dimensions. In the critical limit $m^2 \rightarrow 0$, the renormalization is power-like $\Phi_R(x) \rightarrow (\mu/\mu_0)^{-\eta/2} \Phi(x)$, and Eq. (22.63) becomes

$$\Gamma_R^{(2)}(q) = - \left[(q^2)^{2-\eta} \mu^\eta + \left(\frac{m^2}{\mu^2} \right)^\gamma \mu^2 \right]. \quad (22.67)$$

The power η is called the *anomalous dimension* of the field Φ .

From (22.67) we extract that the coherence length of the system ξ behaves like

$$\xi = \mu^{-1}(m^2)^{-\nu}, \quad (22.68)$$

where

$$\nu \equiv \gamma/(2 - \eta) \quad (22.69)$$

is the *critical exponent of the coherence length*.

Another power behavior is found for $\Gamma_R^{(4)}(\mathbf{0})$:

$$\begin{aligned} \Gamma_R^{(4)}(\mathbf{0}) &\xrightarrow{m \rightarrow 0} g \left(1 + \frac{3}{4} \hbar g \mu^{-\epsilon} S_D \log \frac{m^2}{\mu^2} \right) + \mathcal{O}(m^2) \\ &= g \left(\frac{m^2}{\mu^2} \right)^{\hbar \frac{3}{4} g \mu^{-\epsilon} S_D}. \end{aligned} \quad (22.70)$$

Also this power behavior is measurable, and defines the critical index β via the so-called *scaling relation*

$$\gamma - 2\beta \equiv \frac{3}{4} \hbar g \mu^{-\epsilon} S_D, \quad (22.71)$$

so that

$$\beta = \frac{1}{2} - \frac{1}{4} \hbar g \mu^{-\epsilon} S_D. \quad (22.72)$$

The higher powers of Φ are accompanied by terms which are more and more singular in the limit $m \rightarrow 0$. From the Feynman integrals in (22.34) we see that the diagrams in (22.36) behave like $m^{4-\epsilon-n}$ for $m \rightarrow 0$, and so do the associated effective action terms Φ^n .

The coefficients of the dimensionless quantities $(\Phi^2/\mu^{2-\epsilon}) \equiv (\tilde{\Phi}^2)^n$ or $(g\Phi^2/\mu^2)^n \equiv (\hat{\Phi}^2)^n$ have the general form $(m^2/\mu^2)^{\gamma-2n\beta}$, so that the effective potential can be written as

$$v(\Phi) = \mu^{4-\epsilon} \left(\frac{m^2}{\mu^2} \right)^\gamma \frac{\Phi^2}{\mu^{2-\epsilon}} f(x), \quad (22.73)$$

with

$$x \equiv \left(\frac{m^2}{\mu^2} \right)^{-2\beta} \frac{\Phi^2}{\mu^{2-\epsilon}} \equiv t^{-2\beta} \frac{\Phi^2}{\mu^{2-\epsilon}} = t^{-2\beta} \tilde{\Phi}^2, \quad (22.74)$$

where we have abbreviated

$$t \equiv \frac{m^2}{\mu^2}. \quad (22.75)$$

For small Φ , the function $f(x)$ has a Taylor expansion in even powers of Φ , corresponding to the diagrams in Eq. (22.36):

$$f(x) = 1 + \sum_{n=1}^{\infty} f_n x^n = 1 + \sum_{n=1}^{\infty} f_n \left(t^{-2n\beta} \tilde{\Phi}^2 \right)^n. \quad (22.76)$$

If we start the sum at $n = -1$, we also get the general form of the vacuum energy

$$v(0) = \mu^{4-\epsilon} \left(\frac{m^2}{\mu^2} \right)^{\gamma+2\beta}. \quad (22.77)$$

The exponent $\gamma + 2\beta$ is equal to $D\nu$, where ν is the exponent defined in (22.69).

By differentiating this energy twice with respect to m^2 , we obtain the temperature behavior of the specific heat

$$C \propto \left(\frac{m^2}{\mu^2} \right)^{D\nu-2} = \left(\frac{m^2}{\mu^2} \right)^{-\alpha}, \quad (22.78)$$

which yields the important critical exponent $\alpha = 2 - D\nu$ that governs the singularity of the famous λ -peak in superfluid helium at $T_c \approx 2.7$ Kelvin. This is the most accurately determined critical exponent of any many-body systems. Such an accuracy was achieved by performing the measurement in a micro-gravity environment on a satellite [3].

We can also rewrite (22.73) in the form

$$v(\Phi) = \mu^{4-\epsilon} \frac{S_D}{\lambda} \left(\frac{m^2}{\mu^2} \right)^{\gamma} \frac{g\Phi^2}{\mu^2} \bar{f}(y), \quad (22.79)$$

where

$$\bar{f}(y) = 1 + \sum_{n=1}^{\infty} \bar{f}_n y^n = 1 + \sum_{n=1}^{\infty} \bar{f}_n \left(t^{-2\beta} \left(\frac{g\Phi^2}{\mu^2} \right) \right)^n, \quad (22.80)$$

and

$$y \equiv \frac{\lambda}{S_D} x = g\mu^{-\epsilon} x = \left(\frac{m^2}{\mu^2} \right)^{-2\beta} \left(\frac{g\Phi^2}{\mu^2} \right) = t^{-2\beta} \hat{\Phi}^2. \quad (22.81)$$

In the limit $m^2 \rightarrow 0$, the expansions (22.76) and (22.80) are divergent since the coefficients grow like $n!$. A sum can nevertheless be calculated with the technique of Variational Perturbation Theory (VPT). This was used before in Chapter 3, whose first citation reviews briefly its development.

22.3 Massless Theory and Widom Scaling

Let us evaluate the zero-mass limit of $v(\Phi)$. Since m^2 always accompanies the coupling strength in the denominator, the limit $m^2 \rightarrow 0$ is equivalent to the limit $g \rightarrow \infty$, i.e., to the strong-coupling limit.

The strong-coupling limit deserves special attention. The theory in this limit is referred to as the *critical theory*. This name reflects the relevance of this limit for the behavior of physical systems at a critical temperature where fluctuations are of infinite range.

We shall see immediately that for large y , $f(y)$ behaves like a pure power of y : $f(y) \rightarrow y^{(\delta-1)/2}$, so that

$$v(\Phi) \rightarrow \mu^{4-\epsilon} \frac{1}{4!} \frac{S_D}{\lambda} \left(\frac{g\Phi^2}{\mu^2} \right)^{(\delta+1)/2}. \quad (22.82)$$

Without fluctuation corrections, δ has the value 3, and (22.82) reduces properly to the mean-field potential $g\Phi^4/4!$.

With the general leading large- Φ -behavior, the potential in the form (22.79) is the so-called *Widom scaling expression* that depends on $y^{-1/2\beta} \propto m^2/\Phi^{1/\beta}$ [5] in the following general way:

$$v(\Phi) \propto \Phi^{\delta+1} w(m^2/\Phi^{1/\beta}). \quad (22.83)$$

From this effective potential we may derive the general Widom form of the equation of state. After adding a source term $H\Phi$ and going to the extremum, we obtain $H(\Phi) = \partial v(\Phi)/\partial \Phi$ with the general behavior

$$H(\Phi) \propto \Phi^\delta h(m^2/\Phi^{1/\beta}). \quad (22.84)$$

Recalling (22.83), we identify the general form of the potential (22.73) as being

$$v(\Phi) \rightarrow \mu^{4-\epsilon} \frac{1}{4!} \frac{S_D}{\lambda} \left(\frac{g\Phi^2}{\mu^2} \right)^{(\delta+1)/2} \hat{w}(\tau), \quad (22.85)$$

where $\tau \equiv (m^2/\mu^2)/(\Phi/\mu^{1-\epsilon/2})^{1/\beta} \equiv t/(\tilde{\Phi}^2)^{1/\beta}$.

For small m^2 , $\hat{w}(\tau)$ has a series expansion in powers of $\tau^{\omega\nu}$:

$$\hat{w}(\tau) = 1 + c_1 \tau^{\omega\nu} + c_2 \tau^{2\omega\nu} + \dots, \quad (22.86)$$

or, since $t = \mu\xi^{-1/\nu}$,

$$\hat{w}(\tau) = 1 + \bar{c}_1 \xi^{-\omega} \Phi^{-\omega\nu/\beta} + \bar{c}_2 \xi^{-2\omega} \Phi^{-2\omega\nu/\beta} + \dots. \quad (22.87)$$

Here ω is the Wegner exponent [6] that governs the approach to scaling. Its numerical value is close to 0.8 [7].

Differentiating (22.85) with respect to Φ yields the following leading contribution to H :

$$\begin{aligned} H &= \partial_{\Phi} v(\Phi) = \frac{\delta+1}{4!} \mu^2 \left(\frac{g\Phi^2}{\mu^2} \right)^{(\delta-1)/2} \\ &= \frac{\delta+1}{4!} \mu^2 \left(\frac{\lambda \tilde{\Phi}^2}{S_D} \right)^{(\delta-1)/2}, \end{aligned} \quad (22.88)$$

where $\delta - 1 = \gamma/\beta$.

Note that the effective potential remains finite for $m = 0$. Then, $v(\Phi)$ becomes

$$v(\Phi) = \frac{g}{4!} \Phi^4 + \frac{\hbar}{2} \int \frac{d^D q}{(2\pi)^D} \log \left(1 + \frac{g}{2} \frac{\Phi^2}{q^2} \right) + \frac{\hbar g^2 \mu^{-\epsilon} S_D}{16 \epsilon} \Phi^4. \quad (22.89)$$

This displays an important feature: When expanding the logarithm in powers of Φ , the expansion terms correspond to increasingly divergent Feynman integrals

$$\int \frac{d^D q}{(2\pi)^D} \frac{1}{(q^2)^n}.$$

Contrary to the previously regularized divergencies coming from the large- q^2 regime, these divergencies are due to the $q = 0$ -singularity of the massless propagators $G_0(q) = i/q^2$. This means that they are IR-singularities.

Let us verify that the effective potential remains indeed finite for $m = 0$. Performing the momentum integral in (22.89), the potential becomes

$$v(\Phi) = \frac{g}{4!} \Phi^4 + \frac{\hbar}{4} S_D \left(-\frac{1}{\epsilon} \right) \left(\frac{g}{2} \Phi^2 \right)^{2-\frac{\epsilon}{2}} + \frac{\hbar g^2}{16} S_D \mu^{-\epsilon} \frac{1}{\epsilon} \Phi^4. \quad (22.90)$$

With the goal of expanding this for a small- ϵ expansion, we divide the coupling constant and field by a scale parameter involving μ . Then $g\mu^{-\epsilon}$ and $\Phi/\mu^{1-\epsilon/2}$ are dimensionless quantities, on which the effective potential depends as follows:

$$v(\Phi) = \mu^{4-\epsilon} \left[\frac{g\mu^{-\epsilon}}{4!} \left(\frac{\Phi}{\mu^{1-\epsilon/2}} \right)^4 + \frac{\hbar}{4} S_D \left(-\frac{1}{\epsilon} \right) \times \left(\frac{g\mu^{-\epsilon}}{2} \frac{\Phi^2}{\mu^{2-\epsilon}} \right)^{2-\frac{\epsilon}{2}} \right] + \frac{\hbar g^2}{16} \frac{\mu^{-2\epsilon}}{\epsilon} S_D \left(\frac{\Phi}{\mu^{1-\epsilon/2}} \right)^4. \quad (22.91)$$

If we use the dimensionless coupling constant

$$\lambda \equiv S_D \hbar g \mu^{-\epsilon}, \quad (22.92)$$

and the reduced field $\tilde{\Phi} \equiv \Phi/\mu^{1-\epsilon/2}$ as new variables, then

$$v(\Phi) = \frac{\mu^{4-\epsilon}}{\hbar S_D} \left[\frac{\lambda}{4!} \tilde{\Phi}^4 + \frac{1}{4} \left(-\frac{1}{\epsilon} \right) \left(\frac{\lambda \tilde{\Phi}^2}{2} \right)^2 \times \left(1 - \frac{\epsilon}{2} \log \frac{\lambda \tilde{\Phi}^2}{2} \right) + \frac{\lambda^2}{16\epsilon} \tilde{\Phi}^4 \right]. \quad (22.93)$$

To zeroth order in ϵ , the prefactor is equal to $\mu^4 8\pi^2$. Thus the massless limit of the effective potential is well defined in $D = 4$ dimensions. There is, however, a special feature: The finiteness is achieved at the expense of an extra parameter μ .

The most important property of the critical potential is that it cannot be expanded in integer powers of Φ^2 . Instead, the expression (22.93) can be rewritten, correctly up to order λ^2 , as

$$v(\Phi) = \frac{\mu^{4-\epsilon}}{S_D} \frac{1}{6} \left\{ \left(\frac{\lambda}{2} \tilde{\Phi}^2 \right)^2 + \frac{3}{8} \left(\frac{\lambda}{2} \tilde{\Phi}^2 \right)^2 \log \frac{\lambda}{2} \tilde{\Phi}^2 \right\} = \frac{\mu^{4-\epsilon}}{S_D} \frac{1}{6\lambda} \left(\frac{\lambda}{2} \tilde{\Phi}^2 \right)^{2+\frac{3}{4}\lambda} + \mathcal{O}(\lambda^3). \quad (22.94)$$

This is the typical power behavior of a critical interaction. The power of $\tilde{\Phi}$ defines the *critical exponent of the interaction*, in general denoted by $1 + \delta$, so that up to the first order in the coupling strength, we identify

$$\delta = 3 + \frac{3}{2}\lambda. \quad (22.95)$$

At the mean-field level, δ is equal to 3.

22.4 Critical Coupling Strength

What is the coupling strength λ in the critical regime? The counter term proportional to Φ^4 in Eq. (22.89) implies that we are using renormalized quantities in all subtracted expressions. The relation between the bare coupling constant g_B and the renormalized one g is, to this one-loop order,

$$g_B = g + \frac{3}{2} \hbar g^2 \mu^{-\epsilon} \frac{S_D}{\epsilon} + \dots \quad (22.96)$$

For a given bare interaction strength g_B , the renormalized coupling depends on the parameter μ chosen for the renormalization procedure. Equivalently we may imagine having defined the field theory on a fine spatial lattice with a specific small lattice spacing $a \propto 1/\mu$. The renormalized coupling constant will then depend on the choice of a .

If we sum an infinite chain of such corrections, we obtain a geometric sum that is an expansion of the equation

$$g_B = \frac{g}{1 - \frac{3}{2} \hbar g \mu^{-\epsilon} \frac{S_D}{\epsilon}}, \quad (22.97)$$

which has (22.96) as its first expansion term. Equivalently we may write

$$\frac{1}{\hbar g_B \mu^{-\epsilon}} = \frac{1}{\hbar g \mu^{-\epsilon}} - \frac{3}{2} \frac{S_D}{\epsilon} + \dots \quad (22.98)$$

In this equation, we can go to the strong-coupling limit $g_B \rightarrow \infty$ by taking μ to the critical limit $\mu \rightarrow 0$, where we find that the renormalized coupling has a finite value

$$\frac{1}{\hbar g \mu^{-\epsilon}} = \frac{3 S_D}{2 \epsilon} + \dots \quad (22.99)$$

For the dimensionless coupling constant (22.92), this amounts to the strong-coupling limit

$$\lambda \equiv \hbar g \mu^{-\epsilon} S_D \rightarrow \frac{2}{3} \epsilon + \dots, \quad (22.100)$$

with the omitted terms being of higher order in ϵ . The approach to this limit starting from small coupling is obtained from (22.97) to be

$$\hbar g \mu^{-\epsilon} = \frac{1}{\frac{1}{\hbar g_B \mu^{-\epsilon}} + \frac{3 S_D}{2 \epsilon}}. \quad (22.101)$$

At a small bare coupling constant g_B , this starts out with the renormalized expression which is determined by the s -wave scattering length $\hbar g \mu^{-\epsilon} = 6 \times 4\pi \hbar^2 a_s / M$ [recall Eq. (9.266)]. In the strong-coupling limit of g_B , which is equal to the critical limit $\mu \rightarrow 0$, the value (22.99) is reached.

For the exponents γ, β , and δ in (22.65), (22.72), and (22.95), the strong-coupling limits are

$$\gamma = 1 + \frac{1}{6}\epsilon, \quad \beta = \frac{1}{2} - \frac{1}{6}\epsilon, \quad \delta = 3 + \epsilon. \quad (22.102)$$

They are approached for finite g_B like

$$\gamma = 1 + \frac{1}{4} \hbar g \mu^{-\epsilon}, \quad \beta = \frac{1}{2} - \frac{1}{4} \hbar g \mu^{-\epsilon}, \quad (22.103)$$

with the just discussed g_B -behavior of g .

If the omitted terms in (22.100) are calculated for all N and up to higher loop orders, one finds $\lambda = 2g^*$, where g^* is the strong-coupling limit $g_B \rightarrow \infty$ of the series in Eq. (15.18) of the textbook [2]. The other critical exponents may be obtained from the $\bar{g}_B \rightarrow \infty$ -limit of similar expansions for ν, η into $\alpha = 2 - \nu D$, $\beta = \nu(D - 2 + \eta)$, $\gamma = \nu(2 - \eta)$, and $\delta = (D + 2 - \eta)/(D - 2 + \eta)$. These can be extracted from Chapter 15 in Ref. [2].

All these series are divergent. But they can be resummed for $\epsilon = 1$ in the strong-coupling limit $\bar{g}_B \rightarrow \infty$. As an example, the series for $\bar{g}$ at $N = 2$ yields the limiting value $\bar{g} \rightarrow g^* \approx 0.503$ (see Fig. 17.1 in [2]). The typical dependence of $\bar{g}$ on $\bar{g}_B$ is displayed in Fig. 20.8 of [2]. For ν and η the corresponding plots are shown in Figs. 20.9 and 20.10 of [2]. We leave it as an exercise to compose from these the dependence of α, β , and δ as functions of $\bar{g}_B$.

It should be pointed out that the potential in the first line of (22.94) has another minimum, away from the origin, solving

$$\frac{\lambda}{3!}\tilde{\Phi}^3 + \frac{\lambda^2}{8}\tilde{\Phi}^3 \left(\log \frac{\lambda}{2}\tilde{\Phi}^2 - \frac{1}{2} \right) + \frac{\lambda^2}{16}\tilde{\Phi}^3 = 0. \quad (22.104)$$

The other minimum solves

$$\lambda \log \frac{\lambda}{2}\tilde{\Phi}^2 = -\frac{4}{3}, \quad (22.105)$$

which lies at

$$\tilde{\Phi}^2 = \frac{2}{\lambda} e^{-4/3\lambda}. \quad (22.106)$$

However such a solution found for small λ is not reliable. The higher loops to be discussed below and neglected up to this point will produce more powers of $\lambda \log(\lambda \tilde{\Phi}^2/2)$, and the series cannot be expected to converge at such a large λ . As a matter of fact, the approximate exponentiation performed in (22.94) does not show a minimum and will be seen, via the methods to be described later, to be the correct analytic form of the potential to all orders in λ for small enough ϵ and λ .

If we want to apply the formalism to a Bose-Einstein-condensate, we must discuss the case of a general $O(N)$ -symmetric version of the effective potential based on the action (22.31), into which we must insert the number $N = 2$. The equation for the bare coupling constant is then

$$g_B = g + \frac{N+8}{6} \hbar g^2 \mu^{-\epsilon} \frac{S_D}{\epsilon} + \dots, \quad (22.107)$$

rather than (22.96), so that the strong-coupling limit (22.100) becomes

$$\lambda \equiv S_D \hbar g \mu^{-\epsilon} \rightarrow \frac{6}{N+8} \epsilon + \dots, \quad (22.108)$$

with the other critical exponents (22.102):

$$\gamma = 1 + \frac{N+2}{2(N+8)}\epsilon, \quad \beta = \frac{1}{2} - \frac{3}{2(N+8)}\epsilon, \quad \delta = 3 + \frac{9}{N+8}\epsilon. \quad (22.109)$$

If we carry the loop expansion to higher order in $\hbar$, we find the perturbation expansion for the renormalized $\bar{g} = \hbar g_B \mu^{-\epsilon}/2S_D$ as function of the bare coupling $\bar{g}_B = \hbar g_B \mu^{-\epsilon}/2S_D$ [taken from Eq. (15.18) in Ref. [2], in particular the higher expansion terms]:

$$\begin{aligned} \frac{\bar{g}}{\bar{g}_B} = & 1 - \bar{g}_B \frac{8+N}{3} \epsilon^{-1} + \bar{g}_B^2 \left\{ \frac{(8+N)^2}{9} \frac{1}{\epsilon^2} + \frac{14+3N}{6} \frac{1}{\epsilon} \right\} \\ & + \bar{g}_B^3 \left\{ -\frac{(8+N)^3}{27} \frac{1}{\epsilon^3} - 4 \frac{(8+N)(14+3N)}{27} \frac{1}{\epsilon^2} \right. \\ & \left. - \frac{[2960+922N+33N^2+(2112+480N)\zeta(3)]}{648} \frac{1}{\epsilon} \right\} + \dots \end{aligned} \quad (22.110)$$

Given this $\bar{g}_B$ -dependence of $\bar{g}$, we find for γ the expansion

$$\begin{aligned} \gamma = & \frac{\bar{g}}{6}(N+2) - 5\frac{\bar{g}^2}{36}(N+2) + \frac{\bar{g}^3}{72}(N+2)(5N+37) \\ & - \frac{\bar{g}^4}{15552}(N+2) [-N^2 + 7578N + 31060 \\ & + 48\zeta(3)(3N^2 + 10N + 68) + 288\zeta(4)(5N + 22)] + \dots, \end{aligned} \quad (22.111)$$

in which $\bar{g}$ has the limiting value (22.110).

The expression $(m^2/\mu^2)^\gamma$ in the two-point function can be replaced by an expansion of m^2/m_B^2 in powers of $\bar{g}_B$ that can be taken from Eq. (15.15) in [2], again with $\bar{g}$ replaced by (22.110). This expansion can be resummed by Variational Perturbation Theory to obtain a curve of the type shown in Fig. 20.8–20.10 of [2]. This permits us to relate $t = m^2/\mu^2$ directly to $\mu^{-\epsilon}g_B$.

22.5 Resumming the Effective Potential

According to Eq. (22.79), the effective action in the condensed phase with negative m^2 has an expansion in powers of y :

$$\frac{v(\Phi)}{\mu^{4-\epsilon}} = t^\gamma \frac{\Phi^2}{\mu^{2-\epsilon}} (\bar{f}_0 + \bar{f}_1 y + \dots), \quad (22.112)$$

where

$$y = t^{-2\beta} g \Phi^2 / \mu^2 = t^{-2\beta} \hat{\Phi}^2. \quad (22.113)$$

From Eq. (22.80), we determine $\bar{f}_0 = \bar{f}_1 = 1$.

In the critical regime where t is small, y becomes large, and we must convert the small- y expansion into a large- y expansion. Near the strong-coupling limit, the Widom function (22.83) has an expansion in powers of $(m^2)^{\omega/\nu} \propto \xi^{-\omega}$ which contains the Wegner critical exponent $\omega \approx 0.8$ governing the *approach to scaling* [7]. The general expansion for strong couplings is

$$\frac{v(\Phi)}{\mu^{4-\epsilon}} = t^\gamma \frac{\Phi^2}{\mu^{2-\epsilon}} (t^{-2\beta} \hat{\Phi}^2)^{(\delta-1)/2} \left(b_0 + \sum_{m=1}^{\infty} \frac{b_m}{(t^{-2\beta} \hat{\Phi}^2)^{m\omega\nu/2\beta}} \right). \quad (22.114)$$

We may derive this from the rules of VPT in [2, 4], reviewed in some detail in Section 21.7. First we rewrite a variational ansatz for the right-hand side of Eq. (22.112) with the help of a dummy parameter $\kappa = 1$ as

$$w_N = \mu^2 t^\gamma \Phi^2 \kappa^p \left(\bar{f}_0 + \bar{f}_1 \frac{y}{\kappa^q} + \dots \right). \quad (22.115)$$

Next we exchange κ^p by the identical expression $\sqrt{K^2 + gr^p}$, where $r \equiv (k^2 - K^2)/K^2$. After this we form w_1 by expanding w_N up to order g , and setting $\kappa = 1$. This leads to

$$\begin{aligned} w_1 &= \mu^2 t^\gamma \Phi^2 K^p \left[\bar{f}_0 \left(1 - \frac{p}{2} + \frac{p}{2} \frac{1}{K^2} \right) + \bar{f}_1 \frac{y}{K^q} \right] \\ &= \mu^2 t^\gamma \Phi^2 W_1(y). \end{aligned} \quad (22.116)$$

The last term in the first line shows that, for large y , K has to grow like

$$K \propto y^{1/q}. \quad (22.117)$$

We now extremize w_1 with respect to K by finding the place where the derivative dw_1/dK vanishes. This determines K from the equation

$$t^\gamma \Phi^2 K^{p-1} \frac{p(2-p)}{2} \left[\bar{f}_0 \left(1 - \frac{1}{K^2} \right) - \bar{f}_1 c \frac{y}{K^q} \right] = 0, \quad (22.118)$$

where

$$c \equiv \frac{2(p-q)}{p(p-2)} \approx 0.32. \quad (22.119)$$

In the free-particle limit $y \rightarrow 0$, the solution is $K(0) = 1$, and

$$w_1 = \mu^2 t^\gamma \Phi^2 \bar{f}_0. \quad (22.120)$$

The last term in (22.118) shows once more that, for large y , K will be proportional to $y^{1/q}$. Moreover, it allows to sharpen relation (22.117) to the large- y behavior

$$K \rightarrow K_{\text{as}}(y) = (cy)^{1/q} \approx 0.648 y^{0.381}. \quad (22.121)$$

Then the leading large- y behavior of (22.97) is $\Phi^2 (cy)^{p/q} \propto (\Phi^2)^{p+1}$.

The first correction to the large- y behavior comes from the second term in the brackets of (22.118) which, by (22.113), should behave like

$$K^2 \rightarrow (c t^{-2\beta} g \Phi^2 / \mu^2)^{\omega\nu/2\beta} \approx (c t^{-2\beta} g \Phi^2 / \mu^2)^{0.76}. \quad (22.122)$$

Comparing this with (22.99) and (22.117), we find $p = 2(2 - \eta)/\omega$ and $q = 4\beta/\omega\nu$. For the $N = 2$ universality class these have the numerical values $p \approx 4.92$ and $q \approx 4 \times 0.32/(0.8 \times 0.66) \approx 2.63$. Solving (22.118), we see that, for small y , $K(y)$ has the diverging expansion

$$K(y) = 1 + 0.32 y - 0.165967 y^2 + 0.155806 y^3 + \dots, \quad (22.123)$$

so that W_1 has the diverging expansion

$$W_1 = 1 + y + 0.154436 y^3 + \dots. \quad (22.124)$$

From Eq. (22.82) we know that the power $p+1$ must be equal to $(\delta+1)/2$, so that

$$y^{p/q} = y^{(\delta-1)/2} = y^{(2-\eta)\nu/2\beta} \approx y^{1.87}. \quad (22.125)$$

If we insert (22.117) into (22.97), the extremal variational energy is

$$w_1(y) = \mu^2 t^\gamma \Phi^2 K^p \left(1 - \frac{p}{2} + \frac{y}{K^q} \right), \quad (22.126)$$

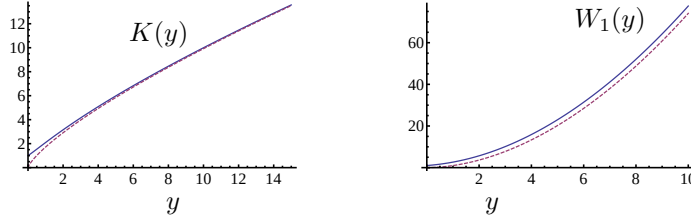


FIGURE 22.1 Solution of the variational equation (22.118) for $\bar{f}_1 = 1$. The dotted curves show the pure large- y behavior.

where $K = K(y)$ is the function of y plotted on the left in Fig. 22.1.

For large y , where $K(y)$ has the limiting behavior (22.121), W_1 becomes

$$\begin{aligned} W_1(y) &\rightarrow W_{\text{as}}(y) = K^p \left(1 - \frac{p}{2} + \frac{1}{c}\right) \\ &\approx 0.197 y^{1.87}. \end{aligned} \quad (22.127)$$

Near the limit, the corrections to (22.121) are

$$\begin{aligned} K(y) &= K_{\text{as}}(y) \left(1 + \sum_{m=1}^{\infty} \frac{h_m}{y^{m\omega\nu/2\beta}}\right) \\ &\approx 0.648 y^{0.381} \left(1 + \sum_{m=1}^{\infty} \frac{h_m}{y^{0.761m}}\right), \end{aligned} \quad (22.128)$$

with $h_1 \approx 0.909$, $h_2 \approx -0.155, \dots$. Inserting this into (22.116), we find

$$\begin{aligned} W_1(y) &= W_{\text{as}}(y) \left(1 + \sum_{m=1}^{\infty} \frac{b_m}{y^{m\omega\nu/2\beta}}\right) \\ &\approx 0.197 y^{1.87} \left(1 + \sum_{m=1}^{\infty} \frac{b_m}{y^{0.761m}}\right), \end{aligned} \quad (22.129)$$

with $b_1 \approx 3.510$, $b_2 \approx 4.65248, \dots$.

22.6 Fractional Gross-Pitaevskii Equation

We now extremize the effective action (22.51) with the two-loop corrected quadratic term (22.63). We consider the case of $N = 2$ where $\Phi^2 = \Psi^* \Psi$. Then we take the effective potential (22.126) with the extremal $K = K(y)$ as a function of y (plotted in Fig. 22.1). From this we form the derivative $\partial w_1(y)/\partial \Psi^*$ and obtain the time-independent *fractional Gross-Pitaevskii equation*:

$$(\hat{\mathbf{p}}^2)^{1-\eta/2} \Psi + \frac{\partial w_1(y)}{\partial \Psi^*} = 0. \quad (22.130)$$

If we use the weak-coupling limit of $w_1(y)$ and the gradient term, this reduces to the ordinary time-independent Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2M} \nabla^2 - \mu + g_S \Psi^\dagger \Psi \right] \Psi(x) = 0. \quad (22.131)$$

The relation of g_S with the previous coupling constant is

$$g_S/2 = g/4!. \quad (22.132)$$

Here μ is the chemical potential of the particles which is fixed by ensuring a given particle number N . In a harmonic trap, μ is replaced by $\mu + M\omega^2 \mathbf{x}^2/2$. Recalling the relation $m^2 = -2M\mu$ one has $m^2 = -2M M\omega^2 R_c^2 (1 - R^2/R_c^2)$. The oscillator energy $M\omega^2 R_c^2$ corresponds to a length scale $\ell_\mathcal{O}$ by the relation $M\omega^2 R_c^2 = \hbar^2/M\ell_\mathcal{O}^2$, so that m^2 may be written as $m^2 = \mu^2(R^2/R_c^2 - 1)$ with $\mu = 1/\ell_\mathcal{O}$.

In the strong-coupling limit, however, we arrive at the time-independent *fractional Gross-Pitaevskii equation*:

$$\left[(\hat{\mathbf{p}}^2)^{1-\eta/2} + \frac{\delta+1}{4\mu^\eta} g_c |\Psi(\mathbf{x})|^{\delta-1} \right] \Psi(\mathbf{x}) = 0. \quad (22.133)$$

By using the full effective action for all coupling strengths and masses m^2 we can derive the properties of the condensate at any coupling strength. Before reaching the strong-coupling limit, we may use Eq. (22.130) to calculate the field strength Ψ as a function of g_S . In this regime, the critical exponents $\eta, \alpha, \beta, \delta$ have not yet reached their strong-coupling values but must be replaced by the $\bar{g}_B$ -dependent precritical values calculated from (22.110) and the corresponding equations for $\eta, \alpha, \beta, \delta$.

In a trap, the mass term becomes weakly space-dependent. If the trap is rotationally symmetric, then m^2 will depend on $R = |\mathbf{x}|$ and the time-independent Gross-Pitaevskii equation has to be solved with $m^2(R) \propto 1 - R^2/R_c^2$. More specifically, the bare coupling constant on the right-hand side has to be determined in such a way that m^2/m_B^2 has the experimental size. If the experiments are performed in an external magnetic field B , the s -wave scattering length a_s has an enhancement factor $(B/B_c - 1)^{-1}$ and Eq. (22.110) can again be used. We can then calculate the density profile quite easily in the Thomas-Fermi approximation as done in Ref. [8].

In a rotating BEC we can calculate the different forms of the density profiles of vortices for various coupling strengths which can be varied from weak to strong by subjecting the BEC to different magnetic fields, raising it from zero up to the Feshbach resonance. The profiles are shown in Fig. 22.2. Note that the central region becomes more and more depleted at stronger couplings.

22.7 Summary

We have shown that the expansion of the effective action of a ϕ^4 -theory in even powers of the field strength $\Phi = \langle \phi \rangle$ can be resummed to obtain an expression that is valid for *any* field strength, even in the strong-coupling limit. It has the phenomenological scaling form once proposed by Widom, and can be used to calculate the shape of a BEC up to the Feshbach resonance, with and without rotation.

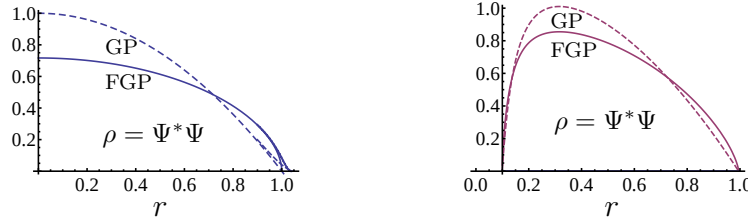


FIGURE 22.2 Condensate density from the Gross-Pitaevskii equation (22.131) (GP, dashed) and its fractional version (22.133) (FGP), both in the Thomas-Fermi approximation where the gradients are ignored. The FGP-curve shows a marked depletion of the condensate. On the right hand, a vortex is included. The zeros at $r \approx 1$ will be smoothened by the gradient terms in (22.133) and (22.133), as shown on the left-hand plots without a vortex. The curves can be compared with those in Ref. [10, 11, 12, 13, 14, 15].

Appendix 22A Effective Action to Order $\hbar^2$

Let us now find the next correction to the effective action [16]. Instead of truncating the expansion (22.23), we keep all terms, reorganizing only the linear and quadratic terms as in the passage to (22.23). This yields the exact expression

$$e^{\frac{i}{\hbar}\{\Gamma[\Phi]+j\Phi\}} = e^{\frac{i}{\hbar}W[j]} = e^{\frac{i}{\hbar}(\mathcal{A}[\phi_{\text{cl}}]+j\phi_{\text{cl}})-\frac{\hbar}{2}\text{Tr}\log\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}]}e^{\frac{i}{\hbar}\hbar^2W_2[\phi_{\text{cl}}]}, \quad (22A.1)$$

where $W_2[\phi_{\text{cl}}]$ is defined by

$$e^{\frac{i}{\hbar}\hbar^2W_2[\phi_{\text{cl}}]} = \frac{\int \mathcal{D}\phi e^{\frac{i}{\hbar}\{\frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}]\phi+I[\phi_{\text{cl}},\phi]\}}}{\int \mathcal{D}\phi e^{\frac{i}{\hbar}\{\frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}]\phi\}}}, \quad (22A.2)$$

and $\mathcal{R}$ is the remainder of the fluctuating action

$$\mathcal{R}[\phi_{\text{cl}},\phi] = \mathcal{A}[\phi_{\text{cl}}+\phi] - \mathcal{A}[\phi_{\text{cl}}] - \frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}]\phi. \quad (22A.3)$$

The subscript ϕ denotes functional differentiation and integration symbols. Adjacent space-time variables have been omitted, for brevity. We have renamed $\delta\phi(x)$ by $\phi(x)$.

Note that by construction, $\mathcal{R}$ is at least cubic in ϕ . Thus the path integral (22A.3) may be considered as the generating functional Z of a theory of a ϕ field, with a propagator

$$\mathcal{G}[\Phi_{\text{cl}}] = i\hbar\{\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}]\}^{-1},$$

and an interaction $\mathcal{R}$ that depends in a complicated manner on j via ϕ_{cl} . We know from previous sections, and will immediately verify this explicitly, that $\hbar^2W_2$ is indeed of order $\hbar^2$. Let us again set

$$\phi = \phi_{\text{cl}} + \hbar\phi_1. \quad (22A.4)$$

We shall express $W[j]$ in the form

$$W[j] = \mathcal{A}[\phi_{\text{cl}}] + \phi_{\text{cl}}j + \hbar\Delta_1[\phi_{\text{cl}}] \quad (22A.5)$$

and collect one- and two-loop corrections in the term

$$\Delta_1[\phi_{\text{cl}}] = \frac{i}{2}\text{Tr}\log i\hbar\mathcal{G}^{-1} + \hbar W_2[\phi_{\text{cl}}]. \quad (22A.6)$$

The functional $W[j]$ depends explicitly on j only via the second term, in all others the j dependence is due to $\phi_{\text{cl}}[j]$. We may use this fact by expressing j as a function of ϕ_{cl} and by writing

$$W[\phi_{\text{cl}}] = \mathcal{A}[\phi_{\text{cl}}] + \phi_{\text{cl}} j[\phi_{\text{cl}}] + \Delta_1. \quad (22A.7)$$

We now insert (22.28) and re-expand everything around X rather than x_{cl} to find

$$\begin{aligned} \Gamma[\Phi] &= \mathcal{A}[\phi] - \hbar \mathcal{A}_\Phi[\Phi] \phi_1 - \hbar \phi_1 j[\Phi] + \hbar^2 \phi_1 j_\Phi[\Phi] \phi_1 + \frac{1}{2} \hbar^2 \phi_1 i \mathcal{G}^{-1}[\Phi] \phi_1 \\ &\quad + \hbar \Delta_1[\Phi] - \hbar^2 \Delta_{1\Phi}[\Phi] \phi_1 + \mathcal{O}(\hbar^3) \\ &= \mathcal{A}[\Phi] + \hbar \Delta_1[\Phi] + \hbar^2 \left\{ \frac{1}{2} \phi_1 i \mathcal{G}^{-1}[\Phi] \phi_1 + \phi_1 j_\Phi[\Phi] \phi_1 - \Delta_{1\Phi} \phi_1 \right\}. \end{aligned} \quad (22A.8)$$

From this we get the correction ϕ_1 to the classical vacuum expectation value ϕ_{cl} . Considering $W[j]$ in (22A.5) again as a functional in j , we see that

$$\Phi = \delta W[j] / \delta j = \phi_{\text{cl}} + \hbar \Delta_{1\phi_{\text{cl}}}[\phi_{\text{cl}}] \delta \phi_{\text{cl}} / \delta j, \quad (22A.9)$$

implying that

$$\phi_1 = \Delta_{1\phi_{\text{cl}}}[\phi_{\text{cl}}] \delta \phi_{\text{cl}} / \delta j. \quad (22A.10)$$

But the derivative $\delta \phi_{\text{cl}} / \delta j$ is known from

$$\delta j / \delta \phi_{\text{cl}} = -\mathcal{A}_{\phi\phi}[\phi_{\text{cl}}] = -i \hbar \mathcal{G}^{-1}[\phi_{\text{cl}}], \quad (22A.11)$$

so that

$$\phi_1 = \Delta_{1\phi_{\text{cl}}}[\phi_{\text{cl}}] i \mathcal{G}[\phi_{\text{cl}}]. \quad (22A.12)$$

Inserting this into (22A.8), the $\hbar^2$ -term becomes

$$-\frac{\hbar^2}{2} \phi_1 i \mathcal{G}^{-1}[\Phi] \phi_1 + \mathcal{O}(\hbar^3). \quad (22A.13)$$

In the derivative $\Delta_{1\phi}$, only the trace log term in (22A.6) has to be included, i.e.,

$$\mathcal{D}[X] = \frac{i}{2} \text{Tr} \left(\mathcal{D}^{-1} \frac{\delta}{\delta X} \mathcal{D} \right). \quad (22A.14)$$

Hence the effective action becomes, to this order in $\hbar$,

$$\begin{aligned} \Gamma[\Phi] &= \mathcal{A}[\Phi] + \hbar \Gamma_1[\Phi] + \hbar^2 \Gamma_2[\Phi] \\ &= \mathcal{A}[\Phi] + \frac{i}{2} \text{Tr} \log i \mathcal{G}^{-1}[\Phi] + \hbar^2 W_2[\Phi] \\ &\quad - \frac{\hbar^2}{2} \frac{i}{2} \text{Tr} \left(\mathcal{G} \frac{\delta}{\delta \Phi} \mathcal{G}^{-1} \right) i \mathcal{G} \frac{i}{2} \text{Tr} \left(\mathcal{G} \frac{\delta}{\delta \Phi} \mathcal{G}^{-1} \right). \end{aligned} \quad (22A.15)$$

We now calculate $W_2[\Phi]$ to lowest order in $\hbar$. The remainder $\mathcal{R}$ in (22A.3) has the expansion

$$\mathcal{R}[\Phi; \phi] = \frac{1}{3!} \phi^3 \mathcal{A}_{\Phi\Phi\Phi}[\Phi] + \frac{1}{4!} \phi^4 \mathcal{A}_{\Phi\Phi\Phi\Phi}[\Phi],$$

where we have replaced ϕ_{cl} by $\Phi + \mathcal{O}(\hbar)$. In order to obtain W_2 , we have to calculate all connected vacuum diagrams for the interactions r with a ϕ -particle propagator $\hbar \mathcal{G}[\Phi](x, x')$. Since every

contraction brings in a factor $\hbar$, we can truncate the expansion (22A.16) after Φ^4 . Thus the only contribution to $W_2[\Phi]$ are the connected vacuum diagrams

$$\begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ \hbar^2 \qquad \hbar^2 \qquad \hbar^2 \end{array} . \quad (22A.16)$$

Here a line stands for $\mathcal{G}[\Phi]$, a four-vertex for

$$\mathcal{A}_{\Phi\Phi\Phi\Phi}[\Phi] = i\mathcal{G}^{-1}[\Phi]_{\Phi\Phi}, \quad (22A.17)$$

and a three-vertex for

$$\mathcal{A}_{\Phi\Phi\Phi}[\Phi] = i\mathcal{G}^{-1}[\Phi]_{\Phi}. \quad (22A.18)$$

Only the first two graphs are one-particle irreducible. It is now a pleasant feature to realize that the third graph cancels with the last term in (22A.15). In order to verify this, we write the diagram more explicitly as

$$-\frac{\hbar^2}{8}\mathcal{G}_{\Phi_1\Phi_2}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}\mathcal{G}_{\Phi_3\Phi_3'}\mathcal{A}_{\Phi_3'\Phi_1'\Phi_2'}\mathcal{G}_{\Phi_1'\Phi_2'} \quad (22A.19)$$

which is now part of iW_2 . Thus, only the one-particle irreducible vacuum graphs produce the $\hbar^2$ -correction to $\Gamma[\Phi]$:

$$i\hbar^2\Gamma_2[\Phi] = i\hbar^2\frac{3}{4!}\mathcal{G}_{12}\mathcal{A}_{\Phi_1\Phi_2\Phi_3\Phi_4}\mathcal{G}_{34} + i\hbar^2\frac{1}{4!^2}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}\mathcal{G}_{\Phi_1\Phi_1'}\mathcal{G}_{\Phi_2\Phi_2'}\mathcal{G}_{\Phi_3\Phi_3'}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}, \quad (22A.20)$$

whose graphical representation is

$$i\hbar^2\Gamma_2[\Phi] = \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ \hbar^2 \qquad \hbar^2 \end{array} . \quad (22A.21)$$

This topological property of the diagram is true for arbitrary orders in $\hbar$. To calculate Γ , we define fundamental vertices of n th order

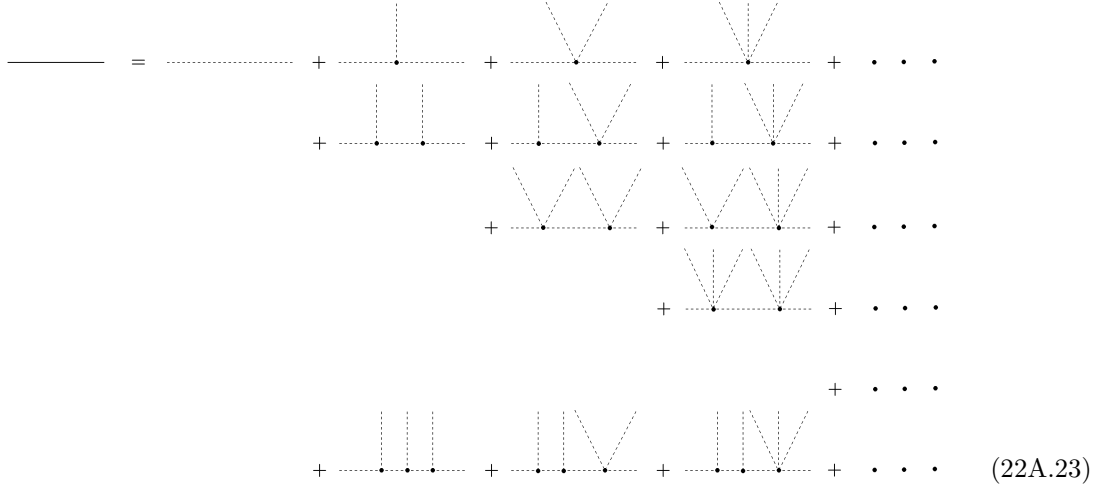
$$\mathcal{A}_{\Phi_1\dots\Phi_n}[\Phi],$$

and sum up all connected one particle irreducible vacuum graphs ²

$$\begin{array}{c} \sum_{n \geq 2} i\hbar^n \Gamma_n[\Phi] = \begin{array}{c} \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ \hbar^3 \qquad \hbar^3 \qquad \hbar^3 \\ + \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \\ \hbar^3 \qquad \hbar^3 \qquad \hbar^3 \end{array} . \quad (22A.22) \end{array}$$

²Note that each line carries a factor $\hbar$ from the propagator, the n -vertex contributes a factor $\hbar^{1-n}$.

Note the content of the lines $\mathcal{G}$ in terms of fundamental Feynman diagrams. The lines in these diagrams contain infinite sums of diagrams in the original perturbation expansion. If propagators of the original ϕ -theory are indicated by a dashed line, an expansion of $\mathcal{G}$ in powers of Φ reveals that every line corresponds to a sum



$$\begin{aligned}
 \text{---} &= \text{---} + \text{---} + \text{---} + \text{---} + \dots \\
 &+ \text{---} + \text{---} + \text{---} + \dots \\
 &+ \text{---} + \text{---} + \dots \\
 &+ \text{---} + \dots
 \end{aligned} \tag{22A.23}$$

of lines which emit 1, 2, 3... lines via vertices ϕ^n in arbitrary combinations. The expansion to order $\hbar^n$ is an expansion according to the number of loops.

The general structure of the series (22A.22) becomes rapidly involved and must be organized via a functional formalism. It is treated in the next section.

Appendix 22B Effective Action to All Orders in $\hbar$

In order to find the general loop expansion, let us expand Φ not around the classical solution ϕ_{cl} but around some other functional $\phi_0 = \phi_0[j]$ whose properties will be specified later. Then the generating functional is

$$Z[j] = e^{\frac{i}{\hbar}W[j]} = \mathcal{N}e^{\frac{i}{\hbar}\{\mathcal{A}[\phi_0] + \phi_0 j + \hbar\Gamma_1[\phi_0[j]]\}}, \tag{22B.1}$$

where

$$e^{i\Gamma_1[\phi_0]} \equiv \int \mathcal{G}\phi' e^{\frac{i}{\hbar}\{\mathcal{A}[\phi_0 + \phi'] - \mathcal{A}[\phi_0] + j[\phi_0]\phi'\}}. \tag{22B.2}$$

On the right-hand side we have inverted the relation $\phi_0[j]$ and expressed j as a functional of Φ_0 . The field Φ may be calculated as

$$\Phi = \frac{\delta W[j]}{\delta j} = \phi_0 + \left\{ \frac{\delta \mathcal{A}[\phi_0]}{\delta \phi_0} + j + \hbar \frac{\delta \Gamma_1[\phi_0]}{\delta \phi_0} \right\} \frac{\delta \phi_0}{\delta j}. \tag{22B.3}$$

Since ϕ_0 is not equal to ϕ_{cl} , the first two terms in the bracket do not cancel. Instead, we shall determine ϕ_0 by the requirement that the whole bracket vanishes for $j = j[\phi_0]$:

$$\frac{\delta \mathcal{A}[\phi_0]}{\delta \phi_0} + j[\phi_0] + \hbar \frac{\delta \Gamma_1[\phi_0]}{\delta \phi_0} = 0. \tag{22B.4}$$

This requirement makes ϕ_0 directly equal to Φ and

$$\Gamma[\Phi] = \mathcal{A}[\Phi] + \hbar\Gamma_1[\Phi]. \tag{22B.5}$$

Since $\Gamma_1[\phi_0]$ depends on ϕ_i also via $j[\phi_0]$, it looks impossible to solve equation (22B.4) for ϕ_0 . In fact, reinserting (22B.4) into (22B.2) we can find a pure equation for ϕ_0 :

$$e^{i\Gamma_1[\phi_0]} = \int \mathcal{G}\phi' e^{\frac{i}{\hbar}\{\mathcal{A}[\phi_0+\phi']-\mathcal{A}[\phi_0]-\phi'\mathcal{A}_{\phi_0}[\phi_0]-\hbar'\phi\Gamma_{1\phi_0}[\phi_0]\phi'\}}, \quad (22B.6)$$

which is a functional integro-differential equation. It is possible to extract from (22B.6) the desired result. Let us consider an auxiliary generating functional

$$e^{iW_{\text{aux}}[\phi_0, K]} \equiv \int \mathcal{G}\phi' e^{\frac{i}{\hbar}\{\mathcal{A}_{\text{aux}}[\phi_0, \phi'] + \int d^4x K\phi\}} \quad (22B.7)$$

with an action

$$\mathcal{A}_{\text{aux}}[\phi_0, \phi'] = \mathcal{A}[\phi_0 + \phi'] - \mathcal{A}[\phi_0] - \phi'\mathcal{A}_{\phi_0}[\phi_0]. \quad (22B.8)$$

For an arbitrary *fixed* function ϕ_0 , the exponent in Eq. (22B.7) defines an auxiliary field theory with an external source K . The expansion of $W_{\text{aux}}[\phi_0, K]$ in powers of K collects all connected diagrams for the action (22B.8). They are built from propagators

$$\text{————} = \mathcal{G}[\phi_0] \quad (22B.9)$$

and vertices

$$\begin{array}{c} \begin{array}{ccccc} & & & 6 & \\ & \cdot & \cdot & & \\ n & \diagdown & & \diagup & \\ 1 & \text{---} & \bullet & \text{---} & 5 \\ & \diagup & & \diagdown & \\ 2 & & & & 4 \\ & & 3 & & \end{array} & = & \frac{\delta^n \mathcal{A}[\phi_0]}{\delta\phi_0 \dots \delta\phi_0}. \end{array} \quad (22B.10)$$

Thus, if we succeed in enforcing $\phi_0 = \Phi$, we are dealing exactly with the field theory whose one-particle irreducible vacuum graphs are supposed to make up the corrections $\Gamma_1[\Phi]$. How can we show this? By comparing (22B.6) with (22B.2) we see that, for the special choice of the current

$$K \equiv K_0 - \hbar\Gamma_{1\phi_0}[\phi_0], \quad (22B.11)$$

the auxiliary functional $W_{\text{aux}}[\phi_0, K_0]$ becomes identical to the generating functional, that we are trying to calculate. The auxiliary functional also has an auxiliary Legendre transformed field

$$\Phi_{\text{aux}} = \frac{\delta W_{\text{aux}}[\phi_0, K]}{\delta K}. \quad (22B.12)$$

With the help of

$$\Phi_{\text{aux}} = \frac{\delta W_{\text{aux}}[\phi_0, K]}{\delta K} = \Phi_{\text{aux}}[\phi_0, K], \quad (22B.13)$$

we now define an auxiliary effective action

$$\Gamma_{\text{aux}}[\Phi_{\text{aux}}] \equiv W_{\text{aux}}[\phi_0, K] - \int d^4x K\Phi_{\text{aux}}, \quad (22B.14)$$

where $\Gamma_{\text{aux}}[\Phi_{\text{aux}}]$ is also a functional of ϕ_0 . There is one important property of $\Gamma_{\text{aux}}[\Phi_{\text{aux}}]$. If evaluated at $\Phi_{\text{aux}} = 0$, it collects all one-particle irreducible vacuum graphs of $\mathcal{A}_{\text{aux}}$ [see (11.45),

(11.46)]. But these are exactly the graphs we want. Hence the proof can be completed by showing that the condition $K = K_0 = -\Gamma_{1\phi_0}[\phi_0]$ leads to

$$\Phi_{\text{aux}} = 0. \quad (22\text{B.15})$$

But this is trivial to see: The condition $K = K_0$ was just made up to enforce $\Phi = \phi_0$. The fluctuating fields ϕ' are the difference between ϕ and ϕ_0 :

$$\phi' = \phi - \phi_0 = \phi - \Phi. \quad (22\text{B.16})$$

Now $\Phi \equiv \langle \phi \rangle$ implies $\langle \phi' \rangle = 0$. But in the auxiliary theory we have

$$\Phi_{\text{aux}} \equiv \langle \phi' \rangle. \quad (22\text{B.17})$$

Thus $\Phi_{\text{aux}} = 0$, and $W_{\text{aux}}[\phi_0, K]$ collects the one-particle irreducible vacuum graphs with propagators and vertices (22B.11) and (22B.13). This completes the proof.

Notes and References

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It is the nature of all greatness not to be exact.
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23

Exactly Solvable $O(N)$ -Symmetric Four-Fermion Theory in $2 + \epsilon$ Dimensions

As in the $O(N)$ -symmetric ϕ^4 -theory in Section 18.2, there exists also a class of fermionic field theories which can be solved exactly by introducing collective quantum fields of the type discussed in Section 18.1. In this chapter we shall investigate the properties of a model that contains a large number N of identical fermion fields, coupled by an $O(N)$ -symmetric four-field interaction.

23.1 Four-Fermion Self-Interaction

The Lagrange density reads at finite N :

$$\mathcal{L} = \bar{\psi}_a (i\partial\!\!\!/ - m_0) \psi_a + \frac{g_0}{2N} (\bar{\psi}_a \psi_a)^2, \quad (23.1)$$

where the index a runs from 1 to N . This model has first been studied in slightly different forms by Anselm, by Vaks and Larkin, and by Nambu and Jona-Lasinio to exhibit the phenomenon of spontaneous breakdown of chiral symmetry. In a so-called chiral version of the model, the latter authors were the first to point out the existence of Nambu-Goldston bosons as consequence of the spontaneous symmetry breakdown. Moreover, an extended version of the model proposed in 1976 [1] was capable of illustrating the properties of all low-energy phenomena in hadron physics.

However, some years later it was discovered that the approximations used in that model were too crude so that the approximate treatment used so far was not really reliable [2]. The chiral fluctuations are so strong that the spontaneously broken symmetry is restored. This will be discussed in Section 23.10.

The original inspiration for studying this model had come from the microscopic theory of superconductivity which had been found in 1957 by Bardeen, Cooper, and Schrieffer [3]. A satisfactory definition of the model is only possible in $D = 2 + \epsilon$ spacetime dimensions, where it is renormalizable and called the *Gross-Neveu model* [4]. At the mean-field level, the effective action becomes

$$\Gamma[\Psi, \bar{\Psi}] = \mathcal{A}[\Psi, \bar{\Psi}] = \int d^D x \left[\bar{\Psi} (i\partial\!\!\!/ - m_0) \Psi + \frac{g_0}{2N} (\bar{\Psi}_a \Psi_a)^2 \right]. \quad (23.2)$$

It yields an equation of motion

$$\left(i\cancel{\partial} - m_0 + \frac{g_0}{N}\bar{\Psi}_a\Psi_a\right)\Psi_b(x) = 0. \quad (23.3)$$

This equation differs in an important physical aspect from the Bose case. Unlike the Bose field expectation, the expectation value of a Fermi field $\psi_a(x)$,

$$\Psi_a \equiv \langle 0|\psi_a|0\rangle, \quad (23.4)$$

can never become non-zero, since Ψ_a is an anticommuting Grassmann field. Nevertheless, the model can exhibit a spontaneous symmetry breakdown. As before, we shall discuss the phenomenon in any dimension D .

The generating functional contains linear terms in which the fields $\psi_a(x)$ are coupled to fermionic, anticommuting sources $\eta_a(x)$ and $\bar{\eta}_a(x)$:

$$Z[\eta_a, \bar{\eta}_a] = e^{iW[\eta_a, \bar{\eta}_a]} = \prod_{a=1}^N \int \mathcal{D}\psi_a \mathcal{D}\bar{\psi}_a e^{i\mathcal{A}[\psi_a, \bar{\psi}_a] + i(\bar{\psi}_a\eta_a + \text{c.c.})}. \quad (23.5)$$

We introduce a collective field σ , that fluctuates on the average around $g\bar{\psi}_a\psi_a$, very similar to Eq. (18.4), and rewrite (23.5) as

$$Z[\eta, \bar{\eta}] = \prod_{a=1}^N \int \mathcal{D}\psi_a \mathcal{D}\bar{\psi}_a \mathcal{D}\sigma e^{i \int d^D x \left[\bar{\psi}_a(i\cancel{\partial} - m_0 - \sigma)\psi_a + (\bar{\psi}_a\eta_a + \text{c.c.}) - \frac{N}{2g_0}\sigma^2 \right]}. \quad (23.6)$$

If we integrate out the σ -field, one recovers the original partition function (23.5). Instead, if we integrate out the fields ψ_a according to the rule (14.98), we obtain the generating functional in a form that contains only the collective field σ :

$$Z[\eta, \bar{\eta}] = \int \mathcal{D}\sigma e^{i\mathcal{A}_{\text{coll}}[\sigma] - \bar{\eta}_a G_\sigma \eta_a}, \quad (23.7)$$

where $\mathcal{A}_{\text{coll}}[\sigma]$ is the collective action

$$\mathcal{A}_{\text{coll}}[\sigma] = N \left\{ -\frac{N}{2g_0} \int d^D x \sigma^2 - iN \text{Tr} \log [i\cancel{\partial} - m_0 - \sigma] \right\}, \quad (23.8)$$

and

$$G_\sigma(x, x') \equiv \frac{i}{i\cancel{\partial} - m_0 - \sigma}(x, x') \quad (23.9)$$

is the propagator of the fermi field $\psi_a(x)$ in the presence of the collective σ -field. This is analogous to Eq. (18.6).

In the limit $N \rightarrow \infty$, the field σ is squeezed into the extremum of the action and we obtain the effective action [compare (18.24)]

$$\begin{aligned} \frac{1}{N} \Gamma[\Sigma, \Psi_a, \bar{\Psi}_a] &= -\frac{1}{2g_0} \int d^D x \Sigma^2(x) - i \text{Tr} \log [i\cancel{\partial} - m_0 - \Sigma(x)] \\ &\quad + \frac{1}{N} \int d^D x \Psi_a(x) [i\cancel{\partial} - m_0 - \Sigma(x)] \Psi_a(x). \end{aligned} \quad (23.10)$$

The extremum of $\Gamma[\Sigma, \Psi_a, \bar{\Psi}_a]$ yields the equations of motion,

$$[i\not{\partial} - m_0 - \Sigma(x)] \Psi_a(x) = 0, \quad (23.11)$$

and

$$\Sigma(x) = g_0 \text{tr} \left(\frac{i}{i\not{\partial} - m_0 - \Sigma} \right) (x, x) - \frac{1}{N} g_0 \bar{\Psi}_a \Psi_a(x), \quad (23.12)$$

where tr indicates a trace over the Dirac indices. As argued above, the field expectation $\Psi_a(x)$ must vanish, so that the only equation to be solved is

$$\Sigma(x) = g_0 \text{tr} \left(\frac{i}{i\not{\partial} - m_0 - \Sigma} \right) (x, x). \quad (23.13)$$

It is called the *gap equation*. The name alludes to the first appearance of such an equation to explain the energy gap in the electron gas of superconductors.

Thus, as far as the extremum is concerned, we may study only the purely collective part of the exact action

$$\frac{1}{N} \Gamma[\Sigma] = -\frac{1}{2g_0} \int d^D x \Sigma^2 - i \text{Tr} \log (i\not{\partial} - m_0 - \Sigma). \quad (23.14)$$

Let us seek for an extremal constant solution Σ_0 . Then the gap equation reduces to

$$\begin{aligned} \Sigma_0 &= ig_0 \text{tr} \int \frac{d^D p}{(2\pi)^D} \frac{\not{p} + m_0 + \Sigma_0}{p^2 - (m_0 + \Sigma_0)^2} \\ &= \text{tr}(1) g_0 \int \frac{d^D p_E}{(2\pi)^D} \frac{m_0 + \Sigma_0}{p_E^2 + (m_0 + \Sigma_0)^2}. \end{aligned} \quad (23.15)$$

The Dirac matrices have disappeared, except for the unit matrix inside the trace. This makes it possible to use this equation in any desired number dimensions. We only need to know the dimension of the Dirac matrices, which is $2^{D/2}$ for even D . In this form, Eq. (23.15) may be extrapolated analytically to any non-integer value of D [10].

For a constant Σ , the effective action gives rise to an effective potential

$$\frac{1}{N} v(\Sigma) = -\frac{1}{NV} \Gamma[\Sigma] = \frac{1}{2g_0} \Sigma^2 - \text{tr}(1) \frac{1}{2} \int \frac{d^D p_E}{(2\pi)^D} \log [p_E^2 + (m_0 + \Sigma)^2], \quad (23.16)$$

where $V \equiv \int d^D x$ is the total volume of the system. The last term is obtained from the $\text{Tr} \log$ in (23.10) by the following calculation

$$\begin{aligned} \int \frac{d^D p}{(2\pi)^D} \log (\not{p} - m_0 - \Sigma) &= \frac{1}{2} \int \frac{d^D p}{(2\pi)^D} [\log (\not{p} - m_0 - \Sigma) + \log (-\not{p} - m_0 - \Sigma)] \\ &= \frac{1}{2} \int \frac{d^D p}{(2\pi)^D} \log [-p^2 + (m_0 + \Sigma)^2] \\ &= \frac{i}{2} \int \frac{d^D p_E}{(2\pi)^D} \log [p_E^2 + (m_0 + \Sigma)^2]. \end{aligned}$$

The integral is performed with the help of formula (11.134), leading to

$$\frac{1}{N}v(\Sigma) = \frac{1}{2g_0}\Sigma^2 - 2^{D/2-1}\mu^{D-2}\frac{1}{2}S_D\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}\left(\frac{m_0+\Sigma}{\mu}\right)^D\mu^2. \quad (23.17)$$

We have introduced, as usual, an arbitrary mass scale μ , which will enable us to study the theory in the limit $m_0 = 0$.

We now focus attention upon the spacetime dimensions in the neighborhood of $D = 2$, setting

$$D = 2 + \epsilon, \quad \text{with } \epsilon > 0. \quad (23.18)$$

Then the potential (23.17) can be written as

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{m_0+\Sigma}{\mu}\right)^{2+\epsilon}\mu^2\right], \quad (23.19)$$

where the constant b_ϵ stands for

$$\begin{aligned} b_\epsilon &= \frac{2}{D}2^{\epsilon/2}S_D\Gamma(D/2)\Gamma(1-D/2) = \frac{2}{D}\frac{1}{(2\pi)^{D/2}}\Gamma(1-D/2) \\ &= \frac{2}{2+\epsilon}\frac{1}{(2\pi)^{1+\epsilon/2}}\Gamma(-\epsilon/2). \end{aligned} \quad (23.20)$$

For small ϵ , the constant b_ϵ behaves like

$$b_\epsilon \sim -\frac{1}{\epsilon\pi}\left[1 - \frac{\epsilon}{2}\log(2\pi e^{-\gamma})\right] + \mathcal{O}(\epsilon). \quad (23.21)$$

Therefore, the bare parameters must somehow diverge if the theory is supposed to remain finite in the limit $\epsilon \rightarrow 0$.

For simplicity, consider first the case of a vanishing bare mass, i.e., $m_0 = 0$. Then a renormalized coupling constant can be defined via

$$\frac{1}{g_0\mu^\epsilon} - b_\epsilon = \frac{1}{g}. \quad (23.22)$$

The limit $\epsilon \rightarrow 0$ can now be taken at a finite g and we obtain the renormalized potential

$$\frac{1}{N}v(\Sigma) \rightarrow \frac{1}{2}\left[\frac{\Sigma^2}{g} + \frac{\Sigma^2}{\pi}\log\left(\frac{\Sigma}{\mu}\right)\right] = \frac{\Sigma^2}{2\pi}\log\left(\frac{\Sigma}{\mu e^{-\pi/g}}\right). \quad (23.23)$$

The minimum of this lies at $\Sigma = \Sigma_0$ which satisfies the equation

$$\frac{\Sigma_0}{\pi}\left[\log\left(\frac{\Sigma_0}{\mu e^{-\pi/g}}\right) + \frac{1}{2}\right] = \frac{\Sigma_0}{\pi}\left[\log\left(\frac{\Sigma_0}{\mu e^{-\pi/g-1/2}}\right)\right] = 0. \quad (23.24)$$

The nontrivial solution of this is

$$\Sigma_0 = M \equiv \mu e^{-c}, \quad (23.25)$$

where c is the constant $c = \pi/g + 1/2$.

Let us study the effect of a nonzero bare fermion mass m_0 by going through the same discussion once more starting from the potential (23.19). Setting $m_0 + \Sigma \equiv \Sigma_1$ the renormalized potential (23.23) becomes

$$\frac{1}{N}v(\Sigma) \rightarrow \frac{1}{2} \left[\frac{\Sigma^2}{g} + \frac{\Sigma_1^2}{\pi} \log \left(\frac{\Sigma_1}{\mu} \right) \right], \quad (23.26)$$

which is minimized at the modified version of (23.24)

$$-\frac{m_0}{g} + \frac{\Sigma_1}{\pi} \log \left(\frac{\Sigma_1}{\mu e^{-c}} \right) = \frac{\Sigma_1}{\pi} \log \left(\frac{\Sigma_1}{M e^{-m_0 \pi / \Sigma_1 g}} \right) = 0. \quad (23.27)$$

For small m_0 , this is solved by

$$\Sigma_1 = M \left(1 - \frac{m_0 \pi}{M g} + \dots \right). \quad (23.28)$$

Thus a small bare mass lowers the physical mass by a small amount.

For arbitrary $0 < \epsilon < 2$, we may define a renormalized potential $v(\Sigma)$ as

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2} \left\{ \frac{\Sigma^2}{g} + b_\epsilon \Sigma^2 \left[1 - \left(\frac{\Sigma}{\mu} \right)^\epsilon \right] \right\}. \quad (23.29)$$

It reduces to the expression (23.23) for $\epsilon \rightarrow 0$.

Let us also see that the potential minimum at $\Sigma = \Sigma_0$ of Eq. (23.25) solves the gap equation (23.13) for fermions with a vanishing bare mass $m_0 = 0$. In the renormalized version, Σ_0 at minimum of (23.29) satisfies

$$1 = g b_\epsilon \left[\left(1 + \frac{\epsilon}{2} \right) \left(\frac{\Sigma_0}{\mu} \right)^\epsilon - 1 \right]. \quad (23.30)$$

In the limit $\epsilon \rightarrow 0$, this becomes

$$1 = -\frac{1}{\pi} g \left(\frac{1}{2} + \log \frac{\Sigma_0}{\mu} \right), \quad (23.31)$$

yielding once more the energy gap (23.25).

The question arises whether this non-trivial solution corresponds to the true ground state of the problem. For this, we differentiate $v(\Sigma)$ once more, and find

$$\frac{1}{N}v''(\Sigma) = \frac{1}{g_0} - b_\epsilon (D - 1) \frac{D}{2} \Sigma^\epsilon. \quad (23.32)$$

Inserting (23.30), this becomes

$$\frac{1}{N}v''(\Sigma) = -\frac{1}{g_0}(D-2) = -\epsilon b_\epsilon (1 + \epsilon/2) \Sigma_0^\epsilon, \quad (23.33)$$

which is positive for $D > 2$ if

$$g_0 < 0. \quad (23.34)$$

What does this condition mean for the renormalized coupling g ? Using (23.22), we see that $g_0 < 0$ and $g_0 > 0$ amount to $g > g^*$ and $g < g^*$, respectively, with

$$g^* \equiv -b_\epsilon^{-1} = \epsilon\pi. \quad (23.35)$$

This is a critical coupling constant above which the model has a phase with a non-vanishing field expectation Σ_0 . If the renormalized coupling lies below g^* , the bare coupling constant is positive and only the trivial solution $\Sigma_0 = 0$ has a positive $v''(\Sigma_0)$ indicating stability.

What are the physical properties of the two solutions? Looking back at the effective action (23.110), we see that Σ_0 increased the fermion mass term to $M = m_0 + \Sigma_0$. In the present zero- m_0 case, we have

$$M = \Sigma_0. \quad (23.36)$$

We therefore conclude that, for $g < g^*$, the massless initial fermions remain massless. For $g > g^*$, on the other hand, the massless fermions acquire a mass $M = \Sigma_0$ from the fluctuations. We observe a *spontaneous generation of fermion mass*. The result may also be phrased differently: In the weak-coupling phase with $g < g^*$, the fermions keep their initial long-range correlations. In the strong-coupling phase with $g > g^*$, however, the spontaneously generated mass limits the range of the correlation functions to $1/M$.

23.2 Spontaneous Symmetry Breakdown

The spontaneous mass generation is closely related to the fact that the model displays, for zero initial mass, the phenomenon of spontaneous symmetry breakdown (recall Chapters 18, and see the later Chapter 25). Indeed, for $m_0 = 0$, the Lagrangian (23.1) possesses an additional symmetry called γ_5 -invariance. In two dimensions, we may choose the following γ -matrices

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma^1, \quad \gamma^1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma^2, \quad (23.37)$$

which satisfy

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} = 2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{\mu\nu}. \quad (23.38)$$

The Hermitian γ^5 -matrix is defined by analogy with the four-dimensional case in Eq. (4.544) as

$$\gamma^5 = \frac{1}{2!} \epsilon_{\mu\nu} \gamma^\mu \gamma^\nu = \gamma^0 \gamma^1, \quad (23.39)$$

where $\epsilon_{\mu\nu}$ is the completely antisymmetric tensor, with $\epsilon_{01} = 1$. In the representation (23.37), γ_5 is equal to the Pauli matrix σ_3 :

$$\gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (23.40)$$

We now introduce γ_5 -transformations T_{γ_5} as follows:

$$\psi \xrightarrow{T_{\gamma_5}} \gamma_5 \psi, \quad (23.41)$$

which satisfies $T_{\gamma_5}^2 = 1$. Under T_{γ_5} , we have

$$\bar{\psi} \xrightarrow{T_{\gamma_5}} \psi^\dagger \gamma_5 \gamma_0 = -\bar{\psi} \gamma_5. \quad (23.42)$$

Hence:

$$\begin{aligned} \bar{\psi} \psi &\xrightarrow{T_{\gamma_5}} -\bar{\psi} \psi, \\ \bar{\psi} \gamma^\mu \psi &\xrightarrow{T_{\gamma_5}} \bar{\psi} \gamma^\mu \psi. \end{aligned} \quad (23.43)$$

If the bare mass m_0 in (23.1) is zero, the Lagrangian is invariant under T_{γ_5} .

In addition, the actions in the exponents of (23.6) and (23.7) are invariant if we assign to $\sigma \sim g\bar{\psi}\psi$ the transformation

$$\sigma \xrightarrow{T_{\gamma_5}} -\sigma, \quad (23.44)$$

in accordance with (23.39) and (23.41).

Thus the $m_0 = 0$ collective action (23.8) is symmetric in σ . It is precisely this γ_5 -symmetry which is broken by the non-vanishing expectation value $\langle \sigma \rangle = \Sigma^0$. We may compare this result with the Bose discussion in Section 18.4. There we found that the continuous $O(N)$ -symmetry could not be broken in less or equal to two dimensions, due to fluctuations. This would imply that such a state would contain massless Nambu-Goldstone bosons in two dimensions, whose correlation functions diverge at any distance, which is unphysical. This is in contrast to a discrete symmetry that can be broken in two dimensions.

23.3 Dimensionally Transmuted Coupling Constant

It is worth pointing out an important structural property of the final result: The characteristic parameter of the two-dimensional system is the fermion mass which

is determined from the coupling strength and the arbitrary mass parameter μ via (23.25), (23.36) as

$$M = \mu e^{-(1/2 + \pi/g)}. \quad (23.45)$$

The original theory with $m_0 = 0$ had only a single free parameter, namely the coupling strength g_0 . The auxiliary mass parameter μ was only introduced for the purpose of renormalizing the theory in the massless case. The renormalized coupling g depends on the choice of μ , and (23.22) should more explicitly be written as

$$\frac{1}{g_0 \mu^\epsilon} - b_\epsilon = \frac{1}{g(\mu)}. \quad (23.46)$$

In this way, a system with a single parameter g_0 has been recharacterized by two parameters, μ and $g(\mu)$.

This increase of parameters is certainly an artifact. There must be a relation between μ and $g(\mu)$ such that different pairs $(\mu, g(\mu))$ correspond to the same set of Green's functions, i. e., to the same physical theory. Indeed, such a relation follows from (23.22). At a fixed g_0 , we can plot curves in the (μ, g) plane which correspond to one and the same theory. In the limit $\epsilon \rightarrow 0$, this relation between μ and g has a subtlety. It goes over into the mass relation (23.45).

The fermion mass is a physically observable finite quantity. There are infinitely many pairs of parameters μ and couplings $g(\mu)$, which lead to the same fermion mass, and this mass is the most economic single parameter by which all properties of the theory can be expressed. Let us illustrate this by reexpressing the potential (23.23) in terms of M . For this we write the renormalized gap equation in the form (with $\Sigma_0 = M$)

$$\frac{\pi}{g} + \frac{1}{2} + \log \frac{M}{\mu} = 0. \quad (23.47)$$

Multiplying this by $\Sigma^2/2$, and subtracting the result from the potential (23.23), we find

$$\frac{1}{N} v(\Sigma) = \frac{\Sigma^2}{2\pi} \left(\log \frac{\Sigma}{M} - \frac{1}{2} \right). \quad (23.48)$$

This has indeed the desired property that neither μ nor $g(\mu)$ appear but only the single parameter M . The same property can, of course, be verified in $D > 2$ dimensions. Here we may combine (23.30) with (23.29) and find

$$\begin{aligned} \frac{1}{N} v(\Sigma) &= \frac{\mu^\epsilon}{2} \left[\frac{\Sigma^2}{g_0 \mu^\epsilon} - b_\epsilon \left(\frac{\Sigma}{\mu} \right)^{2+\epsilon} \mu^2 \right] \\ &= \frac{M^\epsilon}{2} b_\epsilon \Sigma^2 \left[1 + \frac{\epsilon}{2} - \left(\frac{\Sigma}{M} \right)^\epsilon \right]. \end{aligned} \quad (23.49)$$

For $\epsilon \rightarrow 0$, this reduces to (23.48).

23.4 Scattering Amplitude for Fermions

We calculate the scattering amplitude for fermions. As we know from the discussion in the Bose case, this is given entirely by the exchange of Σ -propagators. These can be extracted from the effective action (23.10) with $m_0 = 0$ by forming the second functional derivative at Σ_0 [compare the discussion leading to (18.137) and (18.138)]. The quadratic piece in $\Sigma' \equiv \Sigma - \Sigma_0 = \Sigma - M$ is

$$\delta^2\Gamma = -\frac{N}{2} \left[\frac{1}{g_0} \int d^D x \Sigma'^2 + i \operatorname{Tr} \left(\frac{i}{i\cancel{\partial} - M} \Sigma' \frac{i}{i\cancel{\partial} - M} \Sigma' \right) \right]. \quad (23.50)$$

From this we extract the propagator of the σ' -fluctuations in momentum space

$$G_{\sigma'\sigma'}(q) = -\frac{1}{N} \frac{i}{g_0^{-1} + \Pi(q)}, \quad (23.51)$$

where the self-energy of the σ' -field is given by the integral

$$\begin{aligned} \Pi(q) &= i \operatorname{tr} \int \frac{d^D k}{(2\pi)^D} \frac{i}{\cancel{k} - M + i\eta} \frac{i}{(\cancel{k} - \cancel{q}) - M + i\eta} \\ &= -i \operatorname{tr} \int \frac{d^D k}{(2\pi)^D} \frac{[(\cancel{k} + M)(\cancel{k} - \cancel{q} + M)]}{(k^2 - M^2)[(k - q)^2 - M^2]}, \end{aligned} \quad (23.52)$$

with the momenta illustrated in the Feynman diagram shown in Fig. 23.1.

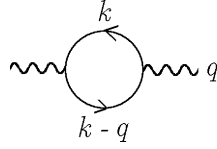


FIGURE 23.1 One-loop Feynman diagram in the inverse propagator of the σ' -field.

Forming the trace and going to euclidean momentum space yields

$$\Pi(q) = -2^{D/2} \int \frac{d^D k_E}{(2\pi)^D} \frac{k(k - q)_E - M^2}{(k_E^2 + M^2)[(k - q)_E^2 + M^2]}. \quad (23.53)$$

In the last line we have gone to the euclidean form. The denominator can be treated with the help of the Feynman formula (11.157), and we may write [compare (11.160)]

$$\Pi(q) = -2^{D/2} \int \frac{d^D k_E}{(2\pi)^D} \int_0^1 dx \frac{k(k - q)_E - M^2}{(k_E^2 - 2k_E q_E x + q_E^2 x + M^2)^2}. \quad (23.54)$$

The integrand can be rearranged to

$$\frac{(k - qx)_E^2 + (k - qx)_E q_E (2x - 1) - q_E^2 x(1 - x) - M^2}{[(k - qx)_E^2 + q_E^2 x(1 - x) + M^2]^2}. \quad (23.55)$$

Upon integration over the shifted momentum $k' \equiv k - qx$, the second term in the numerator will vanish since it is odd in k' . We therefore remain with the integral

$$\Pi(q) = -2^{D/2} \int_0^1 dx \int \frac{d^D k_E}{(2\pi)^D} \times \left\{ \frac{1}{k_E^2 + q_E^2 x(1-x) + M^2} - 2 \frac{M^2 + q_E^2 x(1-x)}{[k_E^2 + q_E^2 x(1-x) + M^2]^2} \right\}. \quad (23.56)$$

This can be integrated using formulas (11.123), leading to

$$\begin{aligned} \Pi(q) &= -2^{D/2} S_D \left[\frac{1}{2} \frac{\Gamma(D/2)\Gamma(1-D/2)}{\Gamma(1)} - 2 \frac{1}{2} \frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)} \right] \\ &\times \int_0^1 dx [q_E^2 x(1-x) + M^2]^{D/2-1} \end{aligned} \quad (23.57)$$

$$\begin{aligned} &= -2^{D/2-1} S_D (D-1) \Gamma(D/2) \Gamma(1-D/2) M^\epsilon \int_0^1 dx \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right]^{D/2-1} \\ &= -\frac{D(D-1)}{2} b_\epsilon M^\epsilon \int_0^1 dx \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right]^{-\epsilon/2}, \end{aligned} \quad (23.58)$$

where we have introduced the parameter b_ϵ of (23.20). Inserting this into (23.50), we obtain the propagator in terms of the renormalized coupling g :

$$\begin{aligned} G_{\sigma'\sigma'} &= -\frac{i}{N} \mu^{-\epsilon} \left\{ \frac{1}{g_0 \mu^\epsilon} - \frac{D(D-1)}{2} b_\epsilon \left(\frac{M}{\mu} \right)^\epsilon \int_0^1 dx \left[\frac{g_\epsilon^2}{M^2} x(1-x) + 1 \right]^{\epsilon/2} \right\}^{-1} \\ &= -\frac{i}{N} \mu^{-\epsilon} \left(\frac{1}{g} + b_\epsilon \left\{ 1 - \frac{D(D-1)}{2} \left(\frac{M}{\mu} \right)^\epsilon \int_0^1 dx \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right]^{\epsilon/2} \right\} \right)^{-1}. \end{aligned} \quad (23.59)$$

The expression in the last curly brackets behaves for small ϵ like

$$\begin{aligned} 1 - \left(1 + \frac{\epsilon}{2} \right) (1 + \epsilon) \left\{ 1 + \frac{\epsilon}{2} \int_0^1 dx \log \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right] + \epsilon \log \frac{M}{\mu} \right\} \\ = -\frac{\epsilon}{2} \left\{ \left[\int_0^1 dx \log \left(\frac{q_E^2}{M^2} x(1-x) + 1 \right) \right] + 3 + 2 \log \frac{M}{\mu} \right\}, \end{aligned} \quad (23.60)$$

so that the denominator in (23.51) becomes, in $D = 2$ dimensions,

$$\left(\frac{1}{g} + \frac{1}{2\pi} \left\{ \int_0^1 dx \log \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right] + 3 + 2 \log \frac{M}{\mu} \right\} \right). \quad (23.61)$$

This result can be expressed completely in terms of M . For this purpose, we subtract again the gap equation (23.31) and find

$$\frac{1}{2\pi} \int_0^1 dx \left\{ \log \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right] + 2 \right\}. \quad (23.62)$$

Then the σ' -propagator takes the form

$$\begin{aligned} G_{\sigma'\sigma'}(q) &= -\frac{i}{N} \frac{1}{g_0^{-1} + \Pi(q)} \\ &= -\frac{i}{N} \frac{2\pi}{\int_0^1 dx \log \left[\frac{q_E^2}{M^2} x(1-x) + 1 \right] + 2}. \end{aligned} \quad (23.63)$$

The integral in the denominator has been solved before in Eqs. (22.49)–(11.175)], where we found, with $z \equiv q_E^2/M^2$,

$$J(z) = \int_0^1 dx \log [zx(1-x) + 1] = -2 + 2\theta \coth \theta, \quad (23.64)$$

where

$$\theta = \operatorname{atanh} \sqrt{\frac{z}{z+4}} = \operatorname{atanh} \sqrt{\frac{q_E^2}{q_E^2 + 4M^2}}, \quad \sinh \theta = \sqrt{\frac{z}{4}} = \sqrt{\frac{q_E^2}{4M^2}}. \quad (23.65)$$

The function $J(z)$ is monotonously increasing in q_E^2 , with the minimum lying at the origin, as shown in Fig. 23.2. The propagator itself starts out, in momentum space, with the value

$$G_{\sigma'\sigma'}(q)|_{q_E^2=0} = -i \frac{\pi}{N}, \quad (23.66)$$

and has a monotonously decreasing size for growing euclidean momentum q_E .

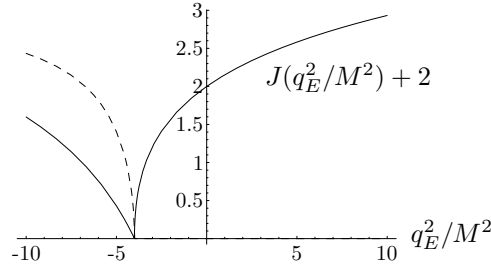


FIGURE 23.2 Function $J(z) + 2$ in the denominator of the σ' -propagator (23.63). For $z < -4$, the curve shows the real part, the dashed curve the imaginary part.

We may now ask whether there exists a scalar ground state in the fermion antifermion scattering amplitude, which is usually called σ -particle, by analogy with a resonance of $\pi^+\pi^-$ in the proton-proton scattering amplitude which is seen at roughly 700 MeV, and which was the origin of using the name σ for the collective field $\sigma \sim \bar{\psi}\psi$ from the beginning. This particle would have to manifest itself in a pole in the propagator $G_{\sigma'\sigma'}(q_E^2)$ at timelike q^2 , i.e., at a negative value of $q_E^2 = -s = -M_\sigma^2$. Indeed, the denominator (23.64) is seen to vanish for

$$s = 4M^2, \quad (23.67)$$

as can be verified by continuing (23.64) to $0 < s < 4M^2$ using

$$\theta \coth \theta = \bar{\theta} \coth \bar{\theta}. \quad (23.68)$$

In terms of s , the parameter θ is given by

$$\theta = \arctan \sqrt{\frac{s}{s - 4M^2}}, \quad \sin \theta = \sqrt{\frac{s}{4M^2}}. \quad (23.69)$$

Close to $4M^2$ the propagator behaves like

$$G_{\sigma'\sigma'} = -\frac{2i}{N} \sqrt{\frac{s}{s - 4M^2}}. \quad (23.70)$$

Thus we see that there is no proper particle pole at $s = 4M^2$, but only a branch cut which runs from $s = 4M^2$ to infinity. Such a cut is present in every scattering amplitude. It is commonly referred to as the *elastic cut*. This is an artifact of the leading large- N approximation investigated in the present discussion. For finite N , the Green function does have a proper bound-state pole before the cut starts.

As in the effective potential, there is only the fermion mass M which characterizes the theory, rather than the pair of parameters μ and bare coupling g_0 , thereby avoiding the problem that the latter becomes undefined for $\epsilon \rightarrow 0$. The fermion mass M is independent of the particular renormalization procedure. It may come as a surprise that a dimensionless quantity g_0 has been replaced by a quantity with the dimension of a mass. This process is often referred to as *dimensional transmutation*. It was first observed in the microscopic theory of superconductivity. There are many superconductors with different coupling strengths g and mass parameters μ , that characterized the energy scale of the pair interactions caused by phonon exchange (see Chapter 17). But there is only one quantity that governs the superconductivity properties, namely the critical temperature T_c . Theories with the same T_c are identical superconductors independent on what g or μ they were derived from.

Note that in the fundamental Lagrangian (23.1), the mass parameter μ and the associated $g(\mu)$ are not detectable separately by any physical experiment. Only their combination M is. If a superconductor is investigated at microscopic scales, both quantities are properties of the substructure. They can both be measured. The supercurrent properties, however, are completely described by the knowledge of the Lagrangian of type (23.1) and the parameters μ and $g(\mu)$.

This points at an important physical aspect of the renormalization procedure: Every theory that requires renormalization of the coupling constant has a redundancy in its parameterization with a mass parameter μ and a renormalized coupling constant $g(\mu)$. This redundancy cannot be resolved at the level of the theory itself. But there may be a more microscopic theory in which both parameters μ and $g(\mu)$ acquire a separate physical significance. Until now, theoretical physics has gone precisely this way. Every theory which was initially considered to be microscopic turned later out to be a phenomenological description of even more microscopic substructures.

The reader may wonder how this description applies to the phase in which the model is at small coupling constants $g < g^*$ or $g^0 > 0$, where the fermions remain massless and the correlations have a long range. The potential may still be parametrized in the form (23.19), (23.29), with $m_0 = 0$:

$$\begin{aligned} \frac{1}{N}v(\Sigma) &= \frac{\mu^\epsilon}{2} \left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon \left(\frac{\Sigma}{\mu} \right)^{2+\epsilon} \mu^2 \right] \\ &= \frac{\mu^2}{2} \left\{ \frac{\Sigma^2}{g} - b_\epsilon \Sigma^2 \left[\left(\frac{\Sigma}{\mu} \right)^\epsilon \mu^2 - 1 \right] \right\}. \end{aligned} \quad (23.71)$$

It contains the arbitrary mass parameter μ , and the renormalized coupling g depending on the choice of μ . There is no fermion mass in terms of which the result can be expressed in a renormalization-independent fashion. Nevertheless, it is still possible to substitute the pair of parameters $\mu, g(\mu)$ by a single parameter whose dimension is “mass”. For this we simply define M by the equation

$$1 \equiv -g_0\mu^\epsilon b_\epsilon \frac{D}{2} \left(\frac{M}{\mu} \right)^\epsilon. \quad (23.72)$$

Then $v(\Sigma)$ can be rewritten as

$$\frac{1}{N}v(\Sigma) = -\frac{M^\epsilon}{2} b_\epsilon \Sigma^2 \left[\frac{D}{2} + \left(\frac{\Sigma}{M} \right)^\epsilon \right]. \quad (23.73)$$

Note that this potential exists only if ϵ is truly larger than zero. For $\epsilon \rightarrow 0$, there is no finite limit. This is due to the fact that only for negative g_0 , $1/g_0\mu^\epsilon - b_\epsilon$ can be compensated to become a finite quantity $1/g$ in the limit $\epsilon \rightarrow 0$.

If we calculate (23.61) for a vanishing fermion mass, we obtain

$$\begin{aligned} G_{\sigma'\sigma'}(q) &= -\frac{i}{N}\mu^{-\epsilon} \left\{ \frac{1}{g_0\mu^\epsilon} - \frac{D(D-1)}{2} b_\epsilon \left(\frac{q_E^2}{\mu^2} \right)^{\epsilon/2} \int_0^1 dx [x(1-x)]^{\epsilon/2} \right\}^{-1} \\ &= -\frac{i}{N}\mu^{-\epsilon} \left\{ \frac{1}{g_0\mu^\epsilon} - \frac{D(D-1)}{2} b_\epsilon \frac{\Gamma^2(1+\epsilon/2)}{\Gamma(2+\epsilon)} \left(\frac{q_E^2}{\mu^2} \right)^{\epsilon/2} \right\}^{-1}. \end{aligned} \quad (23.74)$$

This may be expressed in terms of the auxiliary mass parameter (23.72) as

$$G_{\sigma'\sigma'}(q) = \frac{i}{N} \left(\frac{D}{2} b_\epsilon M^\epsilon \right)^{-1} \left[1 + \frac{\Gamma^2(1+\epsilon/2)}{\Gamma(1+\epsilon)} \left(\frac{q_E^2}{M^2} \right)^{\epsilon/2} \right]^{-1}. \quad (23.75)$$

The following should be pointed out here. If we had calculated the propagator $G_{\sigma'\sigma'}(q)$ by expanding the action around the wrong ground state solution, say $\Sigma_0 = 0$ for $g_0 < 0$, $g > g^*$, the resulting propagator would show the mistake of doing this.

The above Eq. (23.74) is an example for this. It is singular in euclidean momentum space by having an unphysical tachyon pole [9] at

$$q_E^2 = \left[\frac{1}{g_0 b_\epsilon} \frac{\Gamma(2 + \epsilon)}{\Gamma^2(1 + \epsilon/2)} \frac{2}{D(D-1)} \right]^{2/\epsilon}. \quad (23.76)$$

This may also be expressed in terms of renormalized quantities as

$$\frac{q_E^2}{\mu^2} = \left[\left(1 + \frac{1}{g b_\epsilon} \right) \frac{\Gamma(2 + \epsilon)}{\Gamma(1 + \epsilon/2)} \frac{2}{D(D-1)} \right]^{2/\epsilon}. \quad (23.77)$$

When going to Minkowski space, the propagator (23.75) has a particle pole at

$$q^2 = -q_E^2.$$

The situation is similar to that in the scalar ϕ^4 -theory in four dimensions. Also there we found such a particle with an imaginary mass, which in Minkowski space-time travels faster than light and is therefore unphysical. There it appeared for very large q^2 , here for very small q^2 . Since a tachyon can have states with arbitrary negative energy, there must be another ground state for the theory which lies lower than the zero-field configuration. Indeed, the potential $v(\Sigma)$ in Eq. (23.73) shows that a phase, in which there might possibly exist a tachyon, cannot really exist in nature. If it did, the energy could be lowered by going into another phase where the energy is lower. An unstable house will collapse until the ruins are stable. See the similar situation in ϕ^4 -theory discussed on p. 1134.

It can be argued that, for finite N , positive couplings g_0 correspond to another interesting physical phase for which the collective field $\sigma \sim (g_0/N) \bar{\psi}_a \psi_a$ is no longer appropriate. Instead, a collective field that is proportional to $\psi_a \psi_a$ would lead to a more appropriate description. This will become clearer after the next section.

There is one more observation that should be made for the massive phase. One may express the potential (23.29) also in terms of g^* , and find the form

$$\frac{1}{N} v(\Sigma) = \frac{\mu^\epsilon}{2} \frac{1}{g} \left[\left(1 - \frac{g}{g^*} \right) \Sigma^2 + \frac{g}{g^*} \left(\frac{\Sigma}{\mu} \right)^\epsilon \right] \epsilon^2. \quad (23.78)$$

This form exhibits very nicely the unstable origin for $g > g^*$ and the stabilization due to the term $\Sigma^{2+\epsilon}$. The potential looks very similar to the previously discussed ϕ^4 -theory. In fact, for $\epsilon \rightarrow 2$ ($D \rightarrow 4$) it takes exactly this form. The minimum lies at $\Sigma = \Sigma_0 = M$, where M is the fermion mass

$$\frac{M}{\mu} = \left[\frac{2}{D} \frac{g^*}{g} \left(\frac{g}{g^*} - 1 \right) \right]^{1/\epsilon}, \quad (23.79)$$

in terms of which the potential may be written in a natural parametrization

$$\frac{1}{N} v(\Sigma) = \frac{\mu^\epsilon}{2} M^2 \frac{1}{g} \left(\frac{g}{g^*} - 1 \right) \left[- \left(\frac{\Sigma}{M} \right)^2 + \frac{2}{D} \left(\frac{\Sigma}{M} \right)^D \right]. \quad (23.80)$$

The mass scale ν can be replaced by the physical mass at infinite g :

$$M_\infty = \left(\frac{2}{D}\right)^{1/\epsilon}. \quad (23.81)$$

Then (23.79) reads

$$\frac{M}{M_\infty} = \left(1 - \frac{g^*}{g} - 1\right)^{1/\epsilon}. \quad (23.82)$$

We argued before that g, g^* play the role of temperature T and critical temperature T_c in surface layers. There the mass goes with

$$\frac{M}{\mu} \propto \left(\frac{T}{T_c} - 1\right)^{1/\epsilon} \triangleq \left(\frac{g}{g^*} - 1\right)^{1/\epsilon}. \quad (23.83)$$

It vanishes at the critical point in which case v takes on a pure power behavior

$$\frac{1}{N}v(\Sigma) \underset{\Sigma \rightarrow 0}{\sim} \mu^D \left(\frac{\Sigma}{\mu}\right)^D. \quad (23.84)$$

This power can also be seen at arbitrary T , if Σ is increased to be much larger than the mass scale M [ultraviolet (UV) limit of the theory].

Note that in the opposite limit of small Σ [infrared (IR) limit], the power behavior is

$$\frac{1}{N}v(\Sigma) \underset{\Sigma \rightarrow 0}{\sim} \Sigma^2, \quad (23.85)$$

which corresponds to $g \rightarrow 0$, i.e., the free-field limit of the theory. One says that the theory behaves IR-free. Such UV- and IR-power behaviors are typical at a critical point. They have been the subject of extended experimental and theoretical investigation.

23.5 Nonzero Bare Fermion Mass

Before we come to that, let us briefly indicate what happens to the Gross-Neveu model if there is a fermion mass from the beginning, a possibility that we discarded so far for the sake of simplicity. We may assume m_0 to be positive, since otherwise its sign can be changed by a simple γ_5 transformation under which $m_0\bar{\psi}\psi \rightarrow -m_0\bar{\psi}\psi$. Differentiating (23.19), we obtain the gap equation

$$\frac{\Sigma_0}{g_0\mu^\epsilon} = \left(1 + \frac{\epsilon}{2}\right) b_\epsilon \left(\frac{m_0 + \Sigma_0}{\mu}\right)^{1+\epsilon} \mu \quad (23.86)$$

which has a solution $\Sigma_0 > 0$ for $g_0 < 0$, or a solution $-m_0 < \Sigma_0 < 0$ for $g_0 > 0$. In other words, for a repulsive interaction the mass becomes larger and for an attractive interaction it becomes smaller. The second derivative is

$$\frac{1}{N}v''(\Sigma) = \mu^\epsilon \left[\frac{1}{g_0\mu^\epsilon} - b_\epsilon \frac{D}{2}(D-1) \left(\frac{m_0 + \Sigma}{\mu} \right)^{D-2} \right], \quad (23.87)$$

and at the solution Σ_0 of the gap equation (23.86):

$$\begin{aligned} \frac{1}{N}v''(\Sigma_0) &= \mu^\epsilon \frac{1}{g_0\mu^\epsilon} \left[1 - (1+\epsilon) \frac{\Sigma_0}{m_0 + \Sigma} \right] \\ &= -\frac{1}{g_0} \frac{\epsilon(\Sigma + m_0) - (1+\epsilon)m_0}{m_0 + \Sigma}. \end{aligned} \quad (23.88)$$

From this we deduce the stability regions for negative and positive g_0 .

Let us renormalize the effective potential (23.19). Introducing the sum $\Sigma^{\text{tot}} \equiv m_0 + \Sigma$, whose equilibrium value $\Sigma_0^{\text{tot}} = m_0 + \Sigma_0$ is the total finite fermion mass M , we obtain

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2} \left[\frac{\Sigma^{\text{tot}2} - 2\Sigma^{\text{tot}}m_0 + m_0^2}{g_0\mu^\epsilon} - b_\epsilon \left(\frac{\Sigma^{\text{tot}}}{\mu} \right)^{2+\epsilon} \mu^2 \right]. \quad (23.89)$$

Here we renormalize the coupling again by using Eq. (23.22). The term $2\Sigma^{\text{tot}}m_0/g_0\mu^\epsilon$ is made finite by defining the renormalized mass as

$$\frac{m_0}{g_0\mu^\epsilon} = \frac{m}{g}, \quad (23.90)$$

i.e.,

$$\frac{m_0}{m} = \frac{g_0\mu^\epsilon}{g} = 1 - g_0\mu^\epsilon b_\epsilon = (1 + gb_\epsilon)^{-1}. \quad (23.91)$$

The term $m_0^2/g_0\mu^\epsilon$ in (23.89) is not finite for $\epsilon \rightarrow 0$. It needs a trivial additive renormalization of the vacuum energy. Assuming that this has been supplied, we find the renormalized potential [compare (23.29)]

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2} \left\{ \frac{(\Sigma^{\text{tot}} - m)^2}{g} - b_\epsilon \Sigma^{\text{tot}2} \left[\left(\frac{\Sigma^{\text{tot}}}{\mu} \right)^\epsilon - 1 \right] \right\}, \quad (23.92)$$

in which g and m depend on μ . The renormalized gap equation becomes

$$1 = gb_\epsilon \left[\left(1 + \frac{\epsilon}{2} \right) \left(\frac{M}{\mu} \right)^\epsilon - 1 \right] \frac{M}{M - m}, \quad (23.93)$$

where Σ_0^{tot} has been replaced by the fermion mass M . At $\Sigma_0^{\text{tot}} = M$, the effective potential has the value

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2} b_\epsilon \left[\frac{m(m - \Sigma^{\text{tot}})}{g} + b_\epsilon \Sigma^{\text{tot}2} \frac{\epsilon}{2 + \epsilon} \right]. \quad (23.94)$$

Note that the potentials (23.29) and (23.92) for the massless and the massive models differ by a term

$$\Delta v(\Sigma) = \frac{\mu^\epsilon}{2} \frac{(\Sigma^{\text{tot}} - m)^2}{g}. \quad (23.95)$$

23.6 Pairing Model and Dynamically Generated Goldstone Bosons

The model discussed in the last section is somewhat uninteresting, since the symmetry which is broken is discrete. It is instructive to consider a slightly modified situation in which there is a spontaneous breakdown of a continuous symmetry. From the Nambu-Goldstone theorem we then expect the appearance of a massless particle. For this purpose consider once more a theory of N fields ψ_a in $D = 2 + \epsilon$ dimensions, but now we take the Lagrangian to be

$$\mathcal{L} = \bar{\psi}_a (i\partial\!\!\!/ - m_0) \psi_a + \frac{g_0}{2N} (\bar{\psi}_a C \bar{\psi}_a^T) (\psi_b^T C \psi_b). \quad (23.96)$$

Here C is the matrix of charge conjugation which is defined by [recall (4.602)]

$$C\gamma^\mu C^{-1} = -\gamma^{\mu T}. \quad (23.97)$$

In two dimensions, where the γ -matrices have the explicit form (23.37), we may use $C = \gamma^1$:

$$C = \gamma^1 = -i\sigma^2. \quad (23.98)$$

It is the same matrix which was introduced in the four-dimensional discussion in Eq. (26.69) as the 2×2 -submatrix c of the 4×4 charge conjugation matrix C .

Due to the antisymmetry of C , we have

$$(\bar{\psi}_a C \bar{\psi}_a^T)^\dagger = \psi_a^T C \psi_a. \quad (23.99)$$

As a consequence, the interaction potential in (23.96) is negative for $g_0 < 0$, amounting to an attractive potential.

Now we introduce a collective field by adding to $\mathcal{L}$ the term

$$\frac{N}{2g_0} \left| \Delta - \frac{g_0}{N} \psi_a^T C \psi_a \right|^2,$$

leading to the partition function

$$\begin{aligned} Z[\eta, \bar{\eta}] &= \prod_{a=1}^N \int \mathcal{D}\psi_a \mathcal{D}\bar{\psi}_a \mathcal{D}\Delta \mathcal{D}\Delta^\dagger \\ &\times \exp \left\{ i \int d^D x \left[\bar{\psi}_a (i\partial\!\!\!/ - m_0) \psi_a + \frac{1}{2} (\Delta^\dagger \psi_a^T C \psi_a + \text{c.c.}) + \bar{\psi}_a \eta_a + \bar{\eta}_a \psi_a - \frac{N}{2g_0} |\Delta|^2 \right] \right\}. \end{aligned} \quad (23.100)$$

In order to integrate out the Fermi fields, we rewrite the free part of the Lagrangian in the matrix form

$$\frac{1}{2} (\psi^T C, \bar{\psi}) \begin{pmatrix} 0 & i\partial - m_0 \\ i\partial - m_0 & 0 \end{pmatrix} \begin{pmatrix} \psi \\ C\bar{\psi}^T \end{pmatrix}, \quad (23.101)$$

which is the same as $\bar{\psi} (i\partial - m_0) \psi$, since

$$\begin{aligned} \psi^T C C \bar{\psi}^T &= -\psi^T \bar{\psi}^T = \bar{\psi} \psi, \\ \psi^T C \overset{\leftrightarrow}{\partial} C \bar{\psi}^T &= \psi^T \overset{\leftrightarrow}{\partial} \bar{\psi}^T = \bar{\psi} \partial \psi. \end{aligned} \quad (23.102)$$

But then the interaction with Δ can be combined with (23.84) in the form

$$\frac{1}{2} \phi^T iG_{\Delta}^{-1} \phi, \quad (23.103)$$

where

$$\phi \equiv \begin{pmatrix} \psi \\ C\bar{\psi}^T \end{pmatrix}, \quad \phi^T \equiv (\psi^T, \bar{\psi} C^{-1}) \quad (23.104)$$

denotes the doubled fermion fields. The matrix G_{Δ}^{-1} is the inverse propagator of the doubled fermion fields:

$$iG_{\Delta}^{-1} = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} \Delta^{\dagger} & i\partial - m_0 \\ i\partial - m_0 & \Delta \end{pmatrix} \quad (23.105)$$

in the presence of the external field Δ . Observe that ϕ is a quasi-real field, since ϕ^* is related to ϕ by the similarity transformation

$$\phi^* = \begin{pmatrix} \psi^* \\ C\bar{\psi}^{T*} \end{pmatrix} = \begin{pmatrix} 0 & C\gamma^0 \\ C\gamma^0 & 0 \end{pmatrix} \begin{pmatrix} \psi \\ C\bar{\psi}^T \end{pmatrix} = \begin{pmatrix} 0 & C\gamma^0 \\ C\gamma^0 & 0 \end{pmatrix} \phi. \quad (23.106)$$

For a quasi-real field, G_{Δ}^{-1} must be an antisymmetric matrix in the combined spinor- and functional space, as can easily be verified:

$$\begin{aligned} \begin{pmatrix} C\Delta^{\dagger} & C(\partial - m_0) \\ C(\partial - m_0) & C\Delta \end{pmatrix}^T &= \begin{pmatrix} C^T \Delta^{\dagger} & (\partial^T - m_0) C^T \\ (\partial^T - m_0) C^T & C^T \Delta \end{pmatrix} \\ &= - \begin{pmatrix} C\Delta^{\dagger} & C(\partial - m_0) \\ C(\partial - m_0) & C\Delta \end{pmatrix}, \end{aligned} \quad (23.107)$$

using the identity $C\partial^T C^{-1} = \gamma^{\mu} \partial_{\mu}^T = -\partial$. The transposition applies to the combined space, and this is the origin of the negative sign in the relation $C\gamma^{\mu T} C^{-1} = -\gamma^{\mu}$ of Eq. (23.97). In spinor space, partial integration makes the derivative ∂ equivalent to the manifestly antisymmetric functional matrix $\frac{1}{2}(\vec{\partial} - \overleftarrow{\partial})$. In momentum space, the kinetic part of $iG_{\Delta}^{-1}(p', p) = \delta^{(2)}(p' + p) iG_{\Delta}^{-1}(p)$ is antidiagonal. This ensures

that $G_{\Delta}^T(p, p') = -G_{\Delta}(p, p')$, since $\delta^{(D)}(p' + p)p$ is an antisymmetric functional matrix. The minus sign is necessary to have a nonzero kinetic part in the fermionic Lagrangian, which reads in terms of the quasi-real field $\phi(p)$:

$$\int d^D p' d^D p \phi(p') iG_{\Delta}^{-1}(p', p) \phi(p) = \int d^D p \phi(-p) iG_{\Delta}^{-1}(p) \phi(p). \quad (23.108)$$

We can now perform the functional integral over the fermion fields, according to the rule (14.97), leading to

$$Z[j] = \int \mathcal{D}\Delta \mathcal{D}\Delta^{\dagger} e^{iN\mathcal{A}[\Delta] + \frac{1}{2}j_a^T G_{\Delta} j_a}, \quad (23.109)$$

where $\mathcal{A}[\Delta]$ is the collective action

$$\mathcal{A}[\Delta] = -\frac{1}{2g_0} \int d^D x |\Delta|^2 - \frac{i}{2} \text{Tr} \log iG_{\Delta}^{-1}, \quad (23.110)$$

and j_a is the doubled version of the external source, by analogy with (23.89),

$$j_a = \begin{pmatrix} \bar{\eta}_a^T \\ C^{-1} \eta_a \end{pmatrix}. \quad (23.111)$$

This is chosen to ensure that

$$\bar{\psi}\eta + \bar{\eta}\psi = \frac{1}{2} (j^T \phi - \phi^T j), \quad (23.112)$$

where we have omitted the subscript a , for brevity. A quadratic completion gives

$$\frac{1}{2} \phi^T iG_{\Delta}^{-1} \phi + \frac{1}{2} (j^T \phi - \phi^T j) = \frac{1}{2} (\phi^T + j^T iG_{\Delta}^T) iG_{\Delta}^{-1} (\phi + iG_{\Delta} j) - \frac{i}{2} j^T G_{\Delta} j. \quad (23.113)$$

Note the sign change in front of $\frac{1}{2} j^T G_{\Delta} j$ in Eq. (23.109), with respect to the Bose case, in accordance with the negative relative sign of the source term $\frac{1}{2} (j^T \phi - \phi^T j)$.

In the limit $N \rightarrow \infty$ we obtain, from (23.110), the effective action

$$\frac{1}{N} \Gamma[\Delta, \Psi] = \frac{1}{2g_0} |\Delta|^2 - \frac{i}{2} \text{Tr} \log iG_{\Delta}^{-1} + \frac{1}{2N} \Phi_a^T iG_{\Delta}^{-1} \Phi_a, \quad (23.114)$$

in the same way as in the last chapter for the simpler model with a real σ -field.

The ground state has $\Phi = 0$, whereas $\Delta = \Delta_0$ satisfies the gap equation

$$\frac{\Delta_0}{g_0} = -\frac{1}{2} \text{tr} G_{\Delta_0} \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix}, \quad (23.115)$$

where we may assume Δ_0 to be real, as we shall show later.

As before, we shall consider first the case of zero initial mass m_0 . Then the Green's function is inverted as follows

$$G_{\Delta_0}(x, y) = \int \frac{d^D p}{(2\pi)^D} e^{-ip(x-y)} \frac{i}{p^2 - \Delta_0} \begin{pmatrix} -\Delta_0 & \not{p} \\ \not{p} & -\Delta_0 \end{pmatrix} \begin{pmatrix} C^{-1} & 0 \\ 0 & C^{-1} \end{pmatrix}. \quad (23.116)$$

We can verify this by multiplying it with (23.105). Thus the gap equation (23.115) becomes simply

$$\frac{1}{g_0} = 2^{D/2} \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 + M^2}, \quad (23.117)$$

where we have introduced the notation

$$M \equiv \Delta_0 \quad (23.118)$$

to indicate the significance of Δ_0 as a spontaneously generated fermion mass. We have also taken the trace in Dirac space to be $2^{D/2}$ in D dimensions.

The integral in (23.116) can be performed just as before and we find

$$\frac{1}{g_0 \mu^\epsilon} = -b_\epsilon \frac{D}{\epsilon} \left(\frac{M}{\mu} \right)^\epsilon. \quad (23.119)$$

For $\Phi_a = 0$, the effective potential is now

$$\frac{1}{N} v(\Delta) = \frac{1}{2g_0} |\Delta|^2 + \frac{i}{2} \int \frac{d^D p}{(2\pi)^D} \log \begin{pmatrix} \Delta^\dagger & \not{p} \\ \not{p} & \Delta \end{pmatrix}, \quad (23.120)$$

such that we obtain, after a Wick rotation,

$$\frac{1}{N} v(\Delta) = \frac{1}{2g_0} |\Delta|^2 - \frac{1}{2} 2^{D/2} \int \frac{d^D p_E}{(2\pi)^D} \log(p_E^2 + |\Delta|^2).$$

Performing the integral gives

$$\begin{aligned} \frac{1}{N} v(\Delta) &= \frac{1}{2g_0} |\Delta|^2 - \frac{1}{2} 2^{D/2-1} S_D \Gamma(D/2) \Gamma\left(1 - \frac{D}{2}\right) \frac{2}{D} |\Delta|^D \\ &= \frac{\mu^\epsilon}{2} \left[\frac{|\Delta|^2}{g_0 \mu^\epsilon} - b_\epsilon \left(\frac{|\Delta|}{\mu} \right)^{2+\epsilon} \mu^2 \right], \end{aligned} \quad (23.121)$$

from which the gap equation (23.119) can again be recovered by differentiation. Stability is insured for $g_0 < 0$, i.e., for attractive interactions. For $\Delta_0 = 0$, only the trivial solution $\Delta_0 = 0$ is stable.

For $\Delta_0 \neq 0$, we may use (23.119) and express the potential in terms of M rather than the bare coupling constant g_0 as

$$\frac{1}{N} v(\Delta) = \frac{M^\epsilon}{2} b_\epsilon |\Delta|^2 \left[\frac{D}{2} - \left(\frac{|\Delta|}{M} \right)^\epsilon \right]. \quad (23.122)$$

As before in (23.22), $v(\Delta)$ can be expressed in terms of the renormalized coupling:

$$\frac{1}{g_0 \mu^\epsilon} - b_\epsilon = \frac{1}{g}, \quad (23.123)$$

which brings it to the alternative form

$$\frac{1}{N}v(\Delta) = \frac{\mu^\epsilon}{2} \left\{ \frac{|\Delta|^2}{g} + b_\epsilon \left[1 - \left(\frac{|\Delta|}{\mu} \right)^{D-2} \right] |\Delta|^2 \right\}. \quad (23.124)$$

From either expression, we find in the limit of $\epsilon \rightarrow 0$:

$$\begin{aligned} \frac{1}{N}v(\Delta) &= \frac{1}{2\pi} \left(\log \frac{|\Delta|}{M} - \frac{1}{2} \right) |\Delta|^2 \\ &= \frac{1}{2} \left[\frac{|\Delta|^2}{g} + \frac{1}{\pi} |\Delta|^2 \log \frac{|\Delta|}{\mu} \right], \end{aligned} \quad (23.125)$$

by analogy with (23.23) and (23.48).

Let us now study the propagator of the complete Δ -field. For small deviations $\Delta' \equiv \Delta - \Delta_0$ from the ground state value of Δ we find, from (23.114), the quadratic term

$$\frac{1}{N}\delta^2\Gamma = -\frac{1}{2} \left\{ \int d^Dx \frac{|\Delta|^2}{g_0} + \frac{i}{2} \text{Tr} \left[\begin{pmatrix} \Delta'^\dagger & \\ & \Delta' \end{pmatrix} G_M \begin{pmatrix} \Delta'^\dagger & \\ & \Delta' \end{pmatrix} G_M \right] \right\}. \quad (23.126)$$

In momentum space, the trace term may be written more explicitly as

$$\begin{aligned} &\frac{i}{2} \left\{ M^2 [\Delta'(q)\Delta'(-q) + \Delta'^*(q)\Delta'^*(-q)] 2^{D/2} \int \frac{d^Dk}{(2\pi)^D} \frac{i}{k^2 - M^2} \frac{i}{(k-q)^2 - M^2} \right. \\ &\quad \left. + [\Delta'(q)\Delta'^*(-q) + \Delta'(-q)\Delta'^*(q)] \int \frac{d^Dk}{(2\pi)^D} \frac{i}{k^2 - M^2} \frac{i}{(k-q)^2 - M^2} \text{tr}[k(k-q)] \right\}. \end{aligned}$$

In a Wick-rotated form, this becomes

$$\begin{aligned} &\frac{1}{2} \left\{ M^2 [\Delta'(q)\Delta'(-q) + \Delta'^*(q)\Delta'^*(-q)] \tilde{\Pi}(q_E^2/M^2) \right. \\ &\quad \left. + [\Delta'(q)\Delta'^*(-q) + \Delta'(-q)\Delta'^*(q)] [\Pi(q_E^2/M^2) - M^2 \tilde{\Pi}(q_E^2/M^2)] \right\}, \end{aligned} \quad (23.127)$$

where $\Pi(q_E^2/M^2)$ is the previous self-energy (23.52) calculated in (23.58). The slightly simpler quantity $\tilde{\Pi}(q_E^2/M^2)$ stands for

$$\tilde{\Pi}(q_E^2/M^2) = i 2^{D/2} \int \frac{d^Dk}{(2\pi)^D} \frac{i}{k^2 - M^2} \frac{i}{(k-q)^2 - M^2}.$$

It is calculated as follows:

$$\begin{aligned} \tilde{\Pi}(q_E^2/M^2) &= 2^{D/2} \int \frac{d^Dk_E}{(2\pi)^D} \int_0^1 dx \frac{1}{[k_E^2 + q_E^2 x(1-x) + M^2]^2} \\ &= 2^{D/2} S_D \frac{1}{2} \Gamma(D/2) \Gamma(2-D/2) \int_0^1 dx [q_E^2 x(1-x) + M^2]^{D/2-2} \\ &= -\frac{D}{2} b_\epsilon (1-D/2) \int_0^1 dx [q_E^2 x(1-x) + M^2]^{D/2-2}. \end{aligned}$$

As a result, the action for the quadratic deviations from Δ_0 can be written as

$$\begin{aligned} \frac{1}{N} \delta^2 \Gamma = & -\frac{V}{4} \int \frac{d^D q}{(2\pi)^D} \left\{ \left(\frac{1}{g_0} + A \right) [\Delta'(q) \Delta'^*(-q) + \Delta'(-q) \Delta'^*(q)] \right. \\ & \left. + B [\Delta'(q) \Delta'(-q) + \Delta'^*(q) \Delta'^*(-q)] \right\}, \end{aligned} \quad (23.128)$$

with the coefficients

$$\begin{aligned} A &= \Pi(q_E^2/M^2) - \tilde{\Pi}(q_E^2/M^2) \\ &= -\frac{D}{2} b_\epsilon M^\epsilon \left[(D-1) J_1^\epsilon(q_E^2/M^2) + (1-D/2) J_2^\epsilon(q_E^2/M^2) \right], \end{aligned} \quad (23.129)$$

$$\begin{aligned} B &= \tilde{\Pi}(q_E^2/M^2) \\ &= \frac{D}{2} b_\epsilon (1-D/2) M^\epsilon J_2^\epsilon(q_E^2/M^2), \end{aligned} \quad (23.130)$$

and the integrals

$$J_1^\epsilon(z) = \int_0^1 dx [zx(1-x) + 1]^{D/2-1}, \quad J_2^\epsilon(z) = \int_0^1 dx [zx(1-x) + 1]^{D/2-2}. \quad (23.131)$$

Thus the propagators of real and imaginary parts of the field Δ' are

$$G_{\Delta'_{\text{re}} \Delta'_{\text{re}}} = -\frac{i}{N} \frac{1}{g_0^{-1} + A + B}, \quad (23.132)$$

$$G_{\Delta'_{\text{im}} \Delta'_{\text{im}}} = -\frac{i}{N} \frac{1}{g_0^{-1} + A - B}, \quad (23.133)$$

and for the complex fields Δ' , $\Delta'^\dagger$:

$$G_{\Delta'^\dagger \Delta'} = -2 \frac{i}{N} \frac{1}{(g_0^{-1} + A)^2 - B^2} (-B), \quad (23.134)$$

$$G_{\Delta' \Delta'^\dagger} = -2 \frac{i}{N} \frac{1}{(g_0^{-1} + A)^2 - B^2} (g_0^{-1} + A). \quad (23.135)$$

The expressions (23.132)–(23.135) can be made finite by using the gap equation (23.119). The term involving $1/g_0$,

$$\frac{1}{g_0} + A = \frac{D}{2} b_\epsilon M^\epsilon \left\{ \left[1 - (D-1) J_1^\epsilon(q_E^2/M^2) \right] - (1-D/2) J_2^\epsilon(q_E^2/M^2) \right\}, \quad (23.136)$$

depends only on the parameter M . It remains finite for $\epsilon \rightarrow 0$, where it becomes

$$\frac{1}{g_0} + A \rightarrow \frac{1}{2\pi} \left\{ \left[J(q_E^2/M^2) + 2 \right] - J_2^0(q_E^2/M^2) \right\}, \quad (23.137)$$

with $J(z) = 2dJ_2^\epsilon(z)/d\epsilon|_{\epsilon=0}$ being the function (23.64). The second function, B , in (23.134) and (23.135) needs no renormalization. It has the $\epsilon \rightarrow 0$ -limit

$$B \xrightarrow{\epsilon \rightarrow 0} \frac{1}{2\pi} J_2^0(q_E^2/M^2). \quad (23.138)$$

We now observe that there is a zero mass excitation in the imaginary part of the Δ' -field, that describes the component of Δ pointing orthogonally to the real ground state value $\Delta_0 = M$ in complex field space. To show this we consider the denominator of the propagator (23.133):

$$\frac{1}{g_0} + A - B = \frac{D}{2} b_\epsilon M^\epsilon \left\{ \left[1 - (D-1) J_1^\epsilon(q_E^2/M^2) \right] - (2-D) J_2^\epsilon(q_E^2/M^2) \right\}. \quad (23.139)$$

By expanding in powers of $z \equiv q_E^2/M^2$,

$$\begin{aligned} J_1^\epsilon &\sim 1 + \frac{D-2}{12} z + \mathcal{O}(z^2), \\ J_2^\epsilon &\sim 1 + \frac{D-4}{12} z + \mathcal{O}(z^2), \end{aligned} \quad (23.140)$$

we find, for small momenta,

$$\begin{aligned} \frac{1}{g_0} + A - B &= \frac{D}{2} b_\epsilon M^\epsilon \left\{ \left[1 - (D-1) \left(1 + \frac{D-2}{12} z \right) \right] - (2-D) \left(1 + \frac{D-4}{12} z \right) \right\} + \mathcal{O}(z^2) \\ &= -\frac{D}{2} b_\epsilon M^\epsilon \frac{D-2}{4} z + \mathcal{O}(z^2), \end{aligned} \quad (23.141)$$

such that the propagator of (23.133) becomes, expressed in terms of the Minkowski square momentum $q^2 = -q_E^2$,

$$G_{\Delta'_{\text{im}} \Delta'_{\text{im}}} = -\frac{1}{N} \frac{2}{D(D-2)b_\epsilon} 4M^{2-\epsilon} \frac{i}{q^2} + \text{regular part at } q^2 = 0. \quad (23.142)$$

Since $b_\epsilon < 0$ for $D > 2$, the residue is positive

$$\text{Res } G_{\Delta'_{\text{im}} \Delta'_{\text{im}}} \approx -\frac{1}{N} \frac{2}{D(D-2)b_\epsilon} 4M^{2-\epsilon} \rightarrow \frac{4\pi}{N} M^2, \quad (23.143)$$

such that the propagator exhibits a proper particle pole at $q^2 = 0$. The positive sign is necessary for a positive norm of the corresponding particle state in the Hilbert space.

In the limit $\epsilon \rightarrow 0$, expression (23.139) becomes

$$\frac{1}{g_0} + A - B \xrightarrow{\epsilon \rightarrow 0} \frac{1}{2\pi} [J(z) + 2 - 2J_2^0(z)]. \quad (23.144)$$

The integral $J(z)$ was calculated in Eq. (23.64). For the integral $J_2^0(z)$ we find, by a similar calculation,

$$J_2^0(z) = \frac{2\theta}{\sinh 2\theta} = \frac{\theta \coth \theta}{\cosh^2 \theta} = \frac{2}{z+4} [J(z) + 2], \quad (23.145)$$

such that we obtain, in Minkowski space, using the notation with $z \equiv q_E^2/M^2 = -q^2/M^2$:

$$\begin{aligned} G_{\Delta'_{\text{im}} \Delta'_{\text{im}}} &= \frac{i}{N} 2\pi \frac{1}{2\theta \tanh \theta} \\ &= \frac{i}{N} 2\pi \frac{4M^2 - q^2}{q^2} \frac{1}{J(-q^2/M^2) + 2}. \end{aligned} \quad (23.146)$$

The real part of the fluctuating field $\Delta' = \Delta - \Delta_0$ has, for $\epsilon \rightarrow 0$, the propagator

$$G_{\Delta'_{\text{re}} \Delta'_{\text{re}}} = -\frac{i}{N} 2\pi \frac{1}{J(-q^2/M^2) + 2}. \quad (23.147)$$

23.7 Spontaneously Broken Symmetry

We have identified the pole at $q^2 = 0$ as a Nambu-Goldstone boson of a spontaneously broken symmetry. To justify this identification, we have to exhibit the continuous symmetry which has been spontaneously broken by the ground state solution. Looking back at the original Lagrangian (23.96), we see that it is invariant under global gauge transformations

$$\begin{aligned} \psi &\rightarrow e^{i\alpha} \psi, & \alpha = \text{const.}, \\ \bar{\psi} &\rightarrow e^{-i\alpha} \bar{\psi}. \end{aligned} \quad (23.148)$$

By the same token, the collective action (23.100) remains invariant, if the collective pair field Δ , that is on the average equal to two ψ -fields, is transformed with twice the phase angle:

$$\Delta \rightarrow e^{2i\alpha} \Delta. \quad (23.149)$$

This invariance has been used before when we chose a real ground state expectation Δ_0 . Any other phase would have given the same physical result. Of course, once this phase is chosen, the invariance (23.148) is destroyed. Thus the zero-mass particle is indeed a Nambu-Goldstone particle. It corresponds to an excitation whose long-wavelength limit reduces to a pure global gauge transformation.

Strictly speaking, this zero mass boson can only exist in dimensions $D > 2$, as follows from a very general theorem of Mermin, Wagner, and Coleman (see Ref. 5 in Chapter 18). Indeed, we have seen before, in the Bose case, that fluctuations prevent the spontaneous breakdown of a continuous symmetry, which might be present at the mean-field level. Thus we may conclude that, if fluctuations are included in the

collective field, the theory will also exhibit this general feature in two space-time dimensions. In the limit $N \rightarrow \infty$ there are no fluctuations in Δ . Thus Coleman's theorem should be satisfied after including all $1/N$ -corrections. In two dimensions, however, things are more subtle. There is a critical coupling strength where a quasi-ordered state does exist. This will be discussed in Subsection 23.8.

The physical interpretation of the field Δ is the following: Due to the attraction for $g_0 < 0$, the fermions form bound-states of a particle and an antiparticle, the analogs of the *Cooper pairs* in a superconductor. These are bosons which can form a condensate, just as before the bosonic ϕ -fields in ϕ^4 -theory (recall in Chapter 18). In fact, the effective potential for the Δ -field looks qualitatively very similar to that of the bosonic potential $v(\Delta)$ of the $O(N)$ -symmetric theory for negative m^2 . The origin of this potential is unstable and there is a new minimum at $\Delta_0 \neq 0$ with an arbitrary phase [see (23.103) with $m_0 = 0$]. Just as in the previous model with an interaction $(g_0/2N) (\bar{\psi}_a \psi_a)^2$, the opposite sign $g_0 > 0$ does not lead to a spontaneous symmetry breakdown, and massless fermions remain massless.

Finally we must justify why we have called the vacuum expectation $\Delta_0 = M$ the spontaneously generated fermion mass. Looking back at the collective effective action (23.114), we see that $M0$ appears in the combinations

$$\bar{\Psi} i \not{\partial} \Psi + \frac{1}{2} M (\Psi^T C \Psi + \bar{\Psi} C \bar{\Psi}^T) = \frac{1}{2} (\Psi^T C, \bar{\Psi}) \begin{pmatrix} M & i \not{\partial} \\ i \not{\partial} & M \end{pmatrix} \begin{pmatrix} \Psi \\ C \bar{\Psi}^T \end{pmatrix}. \quad (23.150)$$

There is a simple transformation which brings this to the canonical Dirac form. With the two-dimensional γ^5 -matrix (23.39), we see that

$$\Psi' = \frac{1 - \gamma_5}{2} \Psi + \frac{1 + \gamma_5}{2} C \bar{\Psi}^T, \quad \bar{\Psi}' = \bar{\Psi} \frac{1 + \gamma_5}{2} + \Psi^T C \frac{1 - \gamma_5}{2}, \quad (23.151)$$

and hence

$$\bar{\Psi}' \Psi' = \frac{1}{2} (\Psi^T C \Psi + \bar{\Psi} C \bar{\Psi}^T) - \frac{1}{2} (\Psi^T C \gamma_5 \Psi - \bar{\Psi} \gamma_5 C \bar{\Psi}^T). \quad (23.152)$$

We have used the projection property

$$P_{\pm}^2 = P_{\pm} \quad (23.153)$$

of the chiral projection matrix

$$P_{\pm} \equiv \frac{1 \pm \gamma_5}{2}, \quad (23.154)$$

and the fact that

$$\gamma_{\mu} P_{\pm} = P_{\mp} \gamma_{\mu}, \quad (23.155)$$

which implies that

$$P_{\pm} \gamma_0 P_{\pm} = 0, \quad P_{\pm} \gamma_0 P_{\mp} = \gamma_0. \quad (23.156)$$

The γ_5 -terms in (23.152) vanish due to the relations

$$C\gamma_5^T C^{-1} = C(\gamma^0\gamma^1)^T C^{-1} = -\gamma^0\gamma^1 = -\gamma_5. \quad (23.157)$$

This brings the mass term in Eq. (23.150) to the simple form $M\bar{\Psi}'\Psi'$.

The gradient term in (23.150) is invariant under the transformation (23.151):

$$\bar{\Psi}' i \not{\partial} \Psi' = \bar{\Psi} i \not{\partial} \Psi. \quad (23.158)$$

This follows again from (23.155), which here implies that

$$P_{\pm} \gamma_0 \gamma_{\mu} P_{\pm} = \gamma_0 \gamma_{\mu}, \quad P_{\pm} \gamma_0 \gamma_{\mu} P_{\mp} = 0. \quad (23.159)$$

In this context it should be mentioned that the entire model could have been written from the outset using Ψ' -fields, which are defined in terms of Ψ -fields as in (23.151). If we supplement the relation (23.152) by

$$\bar{\Psi}' \gamma_5 \Psi' = -\frac{1}{2} (\Psi^T C \Psi - \bar{\Psi} C \bar{\Psi}^T) + \frac{1}{2} (\Psi^T C \gamma_5 \Psi + \bar{\Psi} \gamma_5 C \bar{\Psi}^T), \quad (23.160)$$

where the second parenthesis is again zero, we see that the fermion field part in the effective action (23.100) can be written for zero sources and mass as

$$\begin{aligned} \bar{\Psi}_a i \not{\partial} \Psi_a + \frac{1}{2} \Delta_{\text{re}} (\Psi_a^T C \Psi_a + \bar{\Psi}_a C \bar{\Psi}_a^T) - \frac{i}{2} \Delta_{\text{im}} (\Psi_a^T C \Psi_a - \bar{\Psi}_a C \bar{\Psi}_a^T) \\ = \bar{\Psi}'_a (i \not{\partial} - \sigma - i\pi\gamma_5) \Psi'_a - \frac{N}{2g_0} (\sigma^2 + \pi^2), \end{aligned} \quad (23.161)$$

where we have identified

$$\sigma \equiv -\Delta_{\text{re}}, \quad \pi = -\Delta_{\text{im}}. \quad (23.162)$$

The invariance under global gauge transformation (23.148) becomes, in terms of Ψ' -fields, an invariance under the transformation

$$\Psi' \equiv \begin{pmatrix} -\Psi_1^* \\ \Psi_2 \end{pmatrix} \rightarrow \begin{pmatrix} -e^{i\alpha} \Psi_1^* \\ e^{-i\alpha} \Psi_2 \end{pmatrix}, \quad (23.163)$$

$$= \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \Psi' = e^{i\alpha\gamma_5} \Psi'. \quad (23.164)$$

Such transformations involving γ_5 are referred to as *chiral transformations*. They play an important role in theories of weak interactions (see Chapter 27). Under the chiral transformation, $\bar{\Psi}'\Psi'$ and $\bar{\Psi}' i \gamma_5 \Psi$ behave like a vector in a plane

$$\begin{aligned} \bar{\Psi}'\Psi' &\rightarrow \bar{\Psi}' e^{2i\alpha\gamma_5} \Psi' = \cos 2\alpha \bar{\Psi}'\Psi' + \sin 2\alpha \bar{\Psi}' i \gamma_5 \Psi' \\ \bar{\Psi}' i \gamma_5 \Psi' &\rightarrow \bar{\Psi}' e^{i\alpha\gamma_5} \gamma_5 e^{i\alpha\gamma_5} \Psi' = -\sin 2\alpha \bar{\Psi}'\Psi' + \cos 2\alpha \bar{\Psi}' i \gamma_5 \Psi'. \end{aligned} \quad (23.165)$$

Thus the transformation (23.149) becomes, with (23.152) and (23.160),

$$\begin{pmatrix} \sigma \\ \pi \end{pmatrix} \rightarrow \begin{pmatrix} \sigma' \\ \pi' \end{pmatrix} = \begin{pmatrix} \cos 2\alpha & \sin 2\alpha \\ -\sin 2\alpha & \cos 2\alpha \end{pmatrix} \begin{pmatrix} \sigma \\ \pi \end{pmatrix}. \quad (23.166)$$

This leaves the transformed effective action (23.161) chirally invariant.

The ground state breaks chiral invariance since σ acquires an expectation value $\sigma_0 = M$. The Nambu-Goldstone boson generated by this phase transition is the massless field π . It is for this reason that chiral invariance is believed to be an important principle of strong interactions among elementary particles. There is a particle in nature, the pion, whose electrically neutral version has a mass roughly equal to $135 \text{ MeV}/c^2$, and lies much lower than any other strongly interacting particle. One therefore interprets the pion as an almost Nambu-Goldstone particle of the underlying Lagrangian. It was in this context that Nambu initiated the study of chiral symmetry in particle physics.

Finally, let us remark that the inclusion of an initial fermion mass $m_0 \neq 0$ is possible but will not be done here, since it merely makes the discussion more involved but adds little to the understanding of the model.

In $D = 2 + \epsilon$ dimensions, the model with the chirally invariant Lagrangian

$$\mathcal{L} = \bar{\psi}_a (i\partial\!\!\!/ - m_0 - \sigma - i\pi\gamma_5) \psi_a + \frac{g_0}{2N} \left[(\bar{\psi}_a \psi_a)^2 + (\bar{\psi}_a i\gamma_5 \psi_a)^2 \right] \quad (23.167)$$

can be treated by introducing the collective fields σ and π as in Eq. (23.6), which leads to a Lagrangian

$$\mathcal{L} = \bar{\psi}_a (i\partial\!\!\!/ - m_0 - \sigma - i\pi\gamma_5) \psi_a + \frac{N}{2g_0} (\sigma^2 + \pi^2). \quad (23.168)$$

This is called the *chiral Gross-Neveu model* [4]. At the mean-field level, it has an effective action (23.161).

23.8 Relation between Pairing and Gross-Neveu Model

Both versions of the fermionic $O(N)$ -model discussed so far in this chapter, the Gross-Neveu-model with the Lagrangian (23.1) and the pairing model with the Lagrangian (23.96), showed a spontaneous mass generation in the limit of $N \rightarrow \infty$. This happened only for one sign of the bare coupling constant. In the Gross-Neveu model with the interaction

$$\frac{g_0}{N} (\bar{\psi}_a \psi_a)^2, \quad \text{for } g_0 < 0, \quad (23.169)$$

and in the pairing model (23.100) with the interaction

$$\frac{g_0}{N} \psi_a^T C \psi_a \bar{\psi}_b C \bar{\psi}_b^T, \quad \text{for } g_0 < 0. \quad (23.170)$$

The forces between the fermions described by the fields are in the latter case attractive, in the former repulsive. In either case, the opposite sign of g_0 leaves the fermions massless for $N \rightarrow \infty$.

These exactly soluble models may provide us with idealized approximations of two phases of the not exactly solvable $N = 1$ model for $D > 2$ [5]:

$$\mathcal{L} = \bar{\psi} i \not{\partial} \psi + \frac{g_0}{2} (\bar{\psi} \psi)^2. \quad (23.171)$$

As before, we can certainly introduce a collective field σ as in the partition function (23.6). For $N = 1$, the field σ will fluctuate so violently, that the phase properties of the model cannot be derived in this way. Suppose now that fluctuations do not completely destroy the fact that, for $g_0 < 0$, there is a solution in which a mass is generated spontaneously, i.e., we suppose for a moment that the $N \rightarrow \infty$ limit gives at least a qualitatively correct description of the system for $g_0 < 0$. Then we might tend to believe that also the $N = 1$ version of the pairing model

$$\mathcal{L} = \bar{\psi} i \not{\partial} \psi + \frac{g_0}{2} \psi^T C \psi \bar{\psi} C \bar{\psi}^T \quad (23.172)$$

should have a solution for $g_0 < 0$ which resembles that of the $N \rightarrow \infty$ limit, i.e., a phase with massive fermions. The associated Cooper pair fields would then describe bound states which carry massless Nambu-Goldstone bosons.

The interesting observation is now that these solutions of the two large- N models are two different phases of one and the same system. The point is that the interactions in the Lagrangians (23.171) and (23.172) are identical, apart from an opposite sign of the coupling constant, and a factor two. This follows directly by rewriting the interactions in terms of spin up and spin down components of the field $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$. For the interaction in (23.171), we obtain

$$(\bar{\psi} \psi)^2 = (\psi_2^* \psi_1 + \psi_1^* \psi_2)^2 = 2\psi_2^* \psi_1 \psi_1^* \psi_2. \quad (23.173)$$

We have omitted terms containing squares of the fields $\psi_1^2 = \psi_2^2$ and their conjugates, since these vanish for Grassmann variables. Proceeding similarly with the interaction in (23.172), we obtain

$$\begin{aligned} |\psi^T C \psi|^2 &= |-\psi_1 \psi_2 + \psi_2 \psi_1|^2 = |2\psi_2 \psi_1|^2 \\ &= 4(\psi_2 \psi_1)^* \psi_2 \psi_1 = 4\psi_1^* \psi_2^* \psi_2 \psi_1 = -4\psi_2^* \psi_1 \psi_1^* \psi_2, \end{aligned} \quad (23.174)$$

such that, indeed,

$$(\bar{\psi} \psi)^2 = -\frac{1}{2} |\psi^T C \psi|^2. \quad (23.175)$$

Thus we expect the following two phases for the $N = 1$ -model: for $g_0 < 0$ or $g > g^*$, a phase with massive fermions and a spontaneously broken γ_5 -invariance. Here the system is symmetric under global gauge transformations. The other phase

for $g_0 > 0, g < g^*$ has again massive fermions but, in addition, massless Nambu-Goldstone modes due to a spontaneously broken global gauge symmetry. Physically, the second phase is distinguished from the first by strong long-range fluctuations which do not exist in the first phase.

For $N \rightarrow \infty$, either of the two phases becomes an exact solution of one of the two models. They differ by the arrangement of the indices over the four fermion fields in (23.169) and (23.170).

We pointed out before the analogy between the coupling constant in the model and the temperature in the euclidean formulation of the model. With this interpretation of g , the behavior of the model looks very similar to that found experimentally in thin films of ^4He . It has a phase transition at a certain temperature T_c . Above T_c , there are only short-range correlations, the system is *normal*. Below T_c , there are long-range correlations, the system is *super-fluid* and there are Goldstone excitations of the condensate. By the Mermin-Wagner theorem discussed in Ref. [5] of Chapter 18), there can be no Nambu-Goldstone bosons in exactly two dimensions, but there do exist quasi-long-range fluctuations with power-like correlation functions of the type (18.99).

23.9 Comparison with the $O(N)$ -Symmetric ϕ^4 -Theory

After having observed the possibility of spontaneously generating a mass in a massless theory via fluctuations, we may look once more back to the scalar ϕ^4 -version of the $O(N)$ model in $D = 4 - \varepsilon$ dimensions, that was discussed in Chapter 18. Note the different notation of ε in $D = 4 - \varepsilon$, in contrast to $D = 2 + \epsilon$ in the previous discussions. In the massless case the potential is

$$v(\Phi, \lambda) = \frac{1}{2} \lambda \Phi_a^2 - \frac{N}{4g_0} \lambda^2 + \frac{1}{2} N S_D \frac{1}{2} \Gamma(D/2) \Gamma(1 - D/2) \frac{2}{D} \lambda^{D/2}, \quad (23.176)$$

which may be written as

$$\frac{1}{N} v(\Phi, \lambda) = \frac{1}{2N} \lambda \Phi_a^2 - \frac{1}{4g_0} \lambda^2 - \frac{b'_\varepsilon}{4} \lambda^{D/2} \quad (23.177)$$

with

$$b'_\varepsilon \equiv -\frac{2}{D} S_D \Gamma(D/2) \Gamma(1 - D/2) = \frac{4}{D} S_D \frac{1}{\varepsilon} \approx \frac{1}{8\pi^2} \frac{1}{\varepsilon}. \quad (23.178)$$

Note the opposite sign of the last term (23.176), in comparison with the fermionic equation (23.17), and the absence in b'_ε of a factor $2^{D/2-1}$ with respect to the fermionic b_ε in Eq. (23.20). The latter is caused by the Dirac trace in D dimensions, and a factor $1/2$ caused by the linearity of the Dirac operator in p . The bosonic b'_ε is related by $b'_\varepsilon = 4c_\varepsilon/D$ to the bosonic constant introduced in the discussion of

the nonlinear σ -model in Eq. (19.37) by $b'_\epsilon = 4c_\epsilon/D = b'_\epsilon$. Extremization of (23.176) yields the two gap equations:

$$\lambda\Phi_a = 0, \quad (23.179)$$

to be solved with $\lambda = 0$ or $\Phi_a = 0$, and

$$\frac{1}{N}\Phi_a^2 - \frac{1}{g_0}\lambda - b'_\epsilon \frac{D}{4}\lambda^{D/2-1} = 0. \quad (23.180)$$

A renormalized coupling constant may be introduced by setting

$$\frac{1}{g_0\mu^{-\epsilon}} + b'_\epsilon = \frac{1}{g}. \quad (23.181)$$

Then $v(\Phi, \lambda)$ becomes

$$\frac{1}{N}v(\Phi, \lambda) = \frac{1}{2N}\lambda\Phi_a^2 - \frac{\mu^{-\epsilon}}{4}\left\{\frac{\lambda^2}{g} + b'_\epsilon\left[\left(\frac{\lambda}{\mu^2}\right)^{-\epsilon/2} - 1\right]\lambda^2\right\}. \quad (23.182)$$

In the renormalized form, the different signs of the bare coupling $g_0 >$ or $g_0 < 0$ correspond to $g < g^*$ or $g > g^*$ with $g^* = b'^{-1}_\epsilon \approx 8\pi^2\epsilon$.

There is a $O(N)$ -symmetric phase with $\Phi_a = 0$ and $\lambda_0 \neq 0$ for $g_0 < 0$, where the bosons acquire a mass. For $g_0 < 0$ there is only the solution $\Phi_a = 0$, $\lambda_0 = 0$, which is again a symmetric phase. But contrary to the previous one, this phase is massless.

Both phases are stable, since the determinant of the matrix of second-derivatives $v_{ab}(\Phi_a, \lambda(\Phi_a^2))$ is nonnegative, whereas the subscripts ab abbreviate the derivatives $\partial^2/\partial\Phi_a\partial\Phi_b$, and $\lambda(\Phi_a^2)$ is the solution of the gap equation (23.180).

Consider now the excitations, setting $\Sigma' \equiv \Sigma - \Sigma_0$. In the massless phase with $g < g^*$, we calculate the propagator $G_{\Sigma'\Sigma'}$ of Σ' -fluctuations from the quadratic variation

$$\delta^2\Gamma[\Phi, \Sigma] = \delta^2\Gamma[\Phi, \Sigma_0 + \Sigma'] = \frac{1}{2}\Sigma' \Gamma^{(2)} \Sigma', \quad (23.183)$$

where in euclidean space

$$\Gamma^{(2)} = -\frac{N}{2}\left[\frac{1}{g_0} + I(q)\right] \quad (23.184)$$

with [see (11.155), (11.164), and (11.168)]

$$\begin{aligned} I(q) &= \int \frac{d^D k}{(2\pi)^D} \frac{1}{k_E^2(k+q)_E^2} = -\left(1 - \frac{D}{2}\right) \frac{D}{4} b'_\epsilon \mu^{-\epsilon} \left(\frac{q_E^2}{\mu^2}\right)^{-\epsilon/2} \\ &\times \frac{\Gamma^2(1 - \epsilon/2)}{\Gamma(2 - \epsilon)} = c_\epsilon \mu^{-\epsilon} \left(\frac{q_E^2}{\mu^2}\right)^{\epsilon/2}. \end{aligned} \quad (23.185)$$

Here we have replaced b'_ε by its small- ε -limit

$$c_\varepsilon \equiv - \left(1 - \frac{D}{2}\right) \frac{D}{4} b'_\varepsilon \approx \frac{1}{8\pi^2\varepsilon}. \quad (23.186)$$

In this way, we obtain a propagator for the collective field Σ' :

$$G_{\Sigma'\Sigma'} = -\frac{2i}{N}\mu^\varepsilon \frac{1}{1/g_0\mu^{-\varepsilon} + c_\varepsilon (q_E^2/\mu^2)^{-\varepsilon/2}}. \quad (23.187)$$

For $g_0 > 0$ with $g < g^*$, this is a physically acceptable quantity. For $g_0 < 0$ with $g > g^*$, however, there is a tachyon pole at

$$\frac{q_E^2}{\mu^2} = \left(\frac{-1}{g_0\mu^{-\varepsilon}c_\varepsilon} \right)^{-2/\varepsilon}, \quad (23.188)$$

indicating that we have expanded around the wrong vacuum value $\lambda_0 = 0$. This has led to an unphysical solution.

We must insert the vacuum expectation for the field that minimizes the energy. Then there will be no tachyon since any unstable system will undergo a phase transition until the collapsed field configuration is stable. Recall the discussion on pages 1134 and 1294.

Alternatively, we can see that in the gap equation near four dimensions

$$\frac{1}{g_0\mu^{-\varepsilon}} = \frac{1}{g} - S_4 \frac{1}{\varepsilon}, \quad (23.189)$$

a finite renormalized coupling g can only be achieved in the limit $\varepsilon \rightarrow 0$ for negative $g_0 < 0$, in which case the ϕ^4 -potential turns the wrong way around. In this case the only consistent solution for $\varepsilon \rightarrow 0$ is the free one with $g = 0$. We now realize the difference with the $N \rightarrow \infty$ Fermi case. There were two possible consistent phases. One had a mass that was spontaneously generated. That happened for $g > g^*, g_0 < 0$. In the other phase with $g < g^*$, the fermions remained massless. Only the latter phase is physically acceptable.

The four-dimensional theory has no consistent ground state with $\lambda = 0$, except for $g = 0$. In contrast, the three-dimensional theory does have one for $g < g^* \sim 8\pi^2\varepsilon$.

In the Gross-Neveu model we pointed out the existence of certain power laws in the massive phase. One deals with the physical mass as a function of $g - g^*$ or $T - T^c$ [see (23.80)]. The other is a power law for $v(\Sigma) \sim \Sigma$ at the critical point $g = g^*$, i.e., at $T = T_c$. For $T \neq T_c$, this power was valid up to the UV limit $\Sigma \gg M$. The opposite limit $\Sigma \ll M$, on the other hand, was shown to follow the IR-free power law $v(\Sigma) \sim \Sigma^2$.

We now demonstrate that the $O(N)$ -symmetric ϕ^4 -theory displays quite a similar power behavior which, however, is opposite as far as IR and UV limits are concerned. For this the mass parameter m_0^2 has to be set proportional to $T/T_c - 1$, and the

critical theory will be obtained in the limit $m_0 \rightarrow 0$. In order to see this, consider the potential (23.176):

$$\frac{1}{N}v(\Phi, \lambda(\Phi_a^2)) = \frac{1}{2N}\lambda\Phi_a^2 + \frac{m_0^2}{2g_0}\lambda - \frac{1}{4g_0}\lambda^2 - \frac{b'_\epsilon}{4}\lambda^{D/2} - \frac{m_0^4}{4g_0}, \quad (23.190)$$

where $\lambda(\Phi_a^2)$ is the function of Φ_a^2 , for which $v_\lambda(\Phi, \lambda) = 0$:

$$\frac{1}{N}\Phi_a^2 = \frac{1}{g_0}\lambda - \frac{m_0^2}{g_0} + \frac{b'_\epsilon}{2}\frac{D}{2}\lambda^{1-\epsilon/2}. \quad (23.191)$$

Suppose we are in the normal phase with $\Phi_a = 0$ and $\lambda_0 \neq 0$. Consider the critical regime with very small m_0^2 . From (23.170) we see that λ behaves as a function of $m_0^2 \rightarrow 0$ as

$$\lambda \sim (m_0^2)^{1/(1-\epsilon/2)}. \quad (23.192)$$

Inserting this into (23.190) we obtain, for the minimal value of $v(\Phi, \lambda(\Phi_a^2))$, the power behavior

$$v_{\min} \sim (m_0^2)^{1+1/(1-\epsilon/2)}. \quad (23.193)$$

At the critical point with $m_0 = 0$, we have

$$\frac{1}{N}\Phi_a^2 = \frac{1}{g_0}\lambda + b'_\epsilon\frac{D}{4}\lambda^{1-\epsilon/2}. \quad (23.194)$$

Contrary to the Gross-Neveu model there is no pure power behavior. Only if also $g_0 = 0$, $g = 0$ (free theory) or $g_0 = \infty$ ($g = g^*$), a pure power behavior is obtained:

$$\begin{aligned} \Phi_a^2 &\sim \lambda, & g_0 = 0 & \quad g = 0 & \quad (\text{or } \lambda \rightarrow \infty), \\ \Phi_a^2 &\sim \lambda^{1-\epsilon/2}, & g_0 = \infty & \quad g = g^* & \quad (\text{or } \lambda \rightarrow 0). \end{aligned} \quad (23.195)$$

The same behavior is found at any coupling strength for $\lambda \rightarrow 0$ (ultraviolet limit) or $\lambda \rightarrow \infty$ (infrared limit), respectively. In the renormalized form of (23.195)

$$\frac{1}{N}\Phi_a^2 = \mu^\epsilon \left\{ \frac{1}{g} - b'_\epsilon \left[1 - \frac{D}{4} \left(\frac{\lambda}{\mu^2} \right)^{-\epsilon/2} \right] \right\} \lambda, \quad (23.196)$$

the two limits are separated by the scale parameter μ . For small λ , the potential itself behaves like

$$v(\Phi) \sim (\Phi^2)^{1+1/(1-\epsilon/2)}, \quad (23.197)$$

as determined by the first and last term in (23.176). The small- λ behavior can be collected in the single formula valid for m_0^2

$$v(\Phi) \sim \left[m_0^2 \left(\frac{\Phi^2}{m_0^2} + \frac{N}{g_0} \right) \right]^{1+1/(1-\epsilon/2)}, \quad (23.198)$$

which follows from writing (23.191) as

$$\frac{1}{N}\Phi_a^2 + \frac{m_0^2}{g_0} \sim b'_\varepsilon \frac{D}{4} \lambda^{1-\varepsilon/2}, \quad (23.199)$$

valid for small λ , and reinserting this into (23.190).

If Φ is interpreted as magnetization M , and $m_0^2 \approx (T/T_c - 1)$ is the relative distance of the temperature from the critical value, this corresponds to a general power law

$$v(M) \sim M^{\delta+1} f\left(\frac{T/T_c - 1}{M^{1/\beta}}\right), \quad (23.200)$$

which was first observed experimentally by Widom in magnetic systems. The present model has

$$\beta = \frac{1}{2}, \quad \frac{\delta + 1}{2} = \frac{2 - \varepsilon/2}{1 - \varepsilon/2}. \quad (23.201)$$

For large λ (UV-limit), there is again a free field behavior with

$$\frac{1}{N}\Phi_a^2 + \frac{m_0^2}{g_0} \sim \lambda \quad (23.202)$$

and

$$v \sim \left(\frac{\Phi_a^2}{N} + \frac{m_0^2}{g}\right)^2. \quad (23.203)$$

Note that there is great similarity with the Gross-Neveu model, as far as power behaviors are concerned. But the scaling limits are opposite to each other. In the Gross-Neveu model, there is only one scale, the fermion mass M . Its size depends on the relative distance of g from g^* (or of T from T_c). If g hits g^* (or T hits T_c) then M vanishes. At such a critical point, the behavior is power-like in the fields. Near such a critical point, the powers are different in the UV- and IR-limits. Moreover, the energy is extremal at a field strength that varies like a power of the relative distance of g from g^* (or of T from T_c).

23.10 Two Phase Transitions in the Chiral Gross-Neveu Model

We shall now demonstrate that the chiral Gross-Neveu model in $2 + \epsilon$ dimensions has, for a small number N of fermions, two phase transitions, one corresponding to *pair formation*, the other to *pair condensation* [6]. In a first transition, fermions and antifermions acquire a mass spontaneously and form bound states in a chirally symmetric state, consisting of pairs which behave like a Bose liquid. In a second transition, the Bose liquid condenses into a coherent state that breaks chiral symmetry. This suggests the possibility that, in particle physics, the generation of quark masses may also happen separately from the breakdown of chiral symmetry [2].

Starting point of our discussion is Eq. (23.142) for the propagator of the massless Goldstone modes of the pair field in $D = 2 + \epsilon$ dimensions:

$$G_{\Delta'_{\text{im}}\Delta'_{\text{im}}} = \frac{1}{N} \frac{4}{\epsilon} \left(\frac{1}{g^*} - \frac{1}{g} \right)^{-1} M^{2-\epsilon} \frac{i}{q^2} + \text{regular part at } q^2 = 0. \quad (23.204)$$

The sign of the pole term guarantees a positive norm of the corresponding particle state in the Hilbert space.

The residue of the pole term will allow us to conclude that the chiral model has two phase transitions. Consider first the case $\epsilon = 0$ where the collective field theory consists of a complex field Δ with the $O(2)$ -symmetry $\Delta \rightarrow e^{i\phi} \Delta$. From the discussion of the Kosterlitz-Thouless transition [7, 8] we know that a complex field system possesses macroscopic excitations of the form of vortices and antivortices. These attract each other by a logarithmic Coulomb potential, just like a gas of electrons and positrons in two dimensions. At low temperatures, the vortices and antivortices form bound pairs. The grand-canonical ensemble of pairs exhibits quasi-long-range correlations. At some temperature T_c , the vortex pairs break up, and the correlations become short-range. The phase transition is of infinite order.

We have shown in the textbook on *Gauge Fields in Condensed Matter* [7] that this transition is most easily understood in a model field theory involving a pure phase field $\theta(x)$, with a Lagrange density

$$\mathcal{L} = \frac{\beta}{2} [\partial\theta(x)]^2, \quad (23.205)$$

where β is the stiffness of the θ -fluctuations. The important feature of the phase field θ is that it is a cyclic field with $\theta = \theta + 2\pi$. In order to ensure that such jumps by 2π carry no energy, the gradient in the Lagrange density needs a modification which allows the existence of vortices and antivortices. After including vortices and antivortices at positions x_i, x_j , their partition function can be written as

$$Z = \sum_{\text{gas}} \exp \left\{ 4\pi^2 \beta \sum_{i < j} q_i q_j \frac{1}{2\pi} \log(|x_i - x_j|/r_0) \right\}, \quad (23.206)$$

where r_0 characterizes the size of the vortices. For a single vortex-antivortex pair, the average square distance r^2 diverges as the stiffness falls below the critical value¹

$$\beta_{\text{KT}} = 1/T_{\text{KT}} = 2/\pi \approx 0.63662. \quad (23.207)$$

The large-stiffness state with bound vortex pairs has a coherent phase field $\theta(x)$, the low-stiffness state with separated vortex pairs exhibits incoherent phase fluctuations. The same situation is found in three dimensions, only that the excitations are vortex lines. These become infinitely long and prolific in a continuous phase transition at a critical point $\beta_c \approx 0.33$.

¹Recall Section 11.10 in the textbook [7].

The result (23.204) for $\epsilon = 0$ can now be used to estimate a critical value of the number of field components $N = N_c$, below which the phase fluctuations of the complex field Δ' become so violent that the system has a phase transition. For this we write $\Delta'_{\text{im}} = M\theta$ and find from (23.204) a propagator of the θ -field:

$$G_{\theta\theta} \approx \frac{i}{N} \frac{4\pi}{q^2} + \text{regular terms.} \quad (23.208)$$

Comparing this with the propagator for the model Lagrange density (23.205),

$$G_{\theta\theta} = \frac{1}{\beta} \frac{i}{q^2}, \quad (23.209)$$

we identify the stiffness $\beta = N/4\pi$. The pair version of the chiral Gross-Neveu model has therefore a vortex-antivortex pair breaking transition, if N falls below the critical value $N_c = 8$.

Consider now the model in $2 + \epsilon$ dimensions where pairs form at $g = g^* \approx \pi\epsilon$. A comparison between the propagator (23.204) and (23.209) yields a stiffness of phase fluctuations

$$\beta = \frac{N}{4\pi} M^\epsilon \left(1 - \frac{g^*}{g}\right). \quad (23.210)$$

The linear vanishing of the stiffness as a function of the distance of the coupling constant g from the critical value g^* is in agreement with a general scaling relation, according to which the critical exponent of bending rigidity should be equal to $(D - 2)\nu$.

The propagator for the real part of the pair field has, by (23.141), a correlation length

$$\xi = \left(\frac{D-1}{12M^2}\right)^{1/2}. \quad (23.211)$$

Inserting the g -dependence of M from (23.82), we see that

$$\xi = \frac{1}{M_\infty} \left(\frac{D-1}{12}\right)^{1/2} \left(1 - \frac{g^*}{g}\right)^{-1/\epsilon}, \quad (23.212)$$

so that the coherence length diverges for $g \rightarrow g^*$ with a critical exponent $\nu = 1/\epsilon$. The stiffness (23.210) implies the existence of a phase transition in the neighborhood of two and three dimensions at roughly

$$N_c \approx 8 \left(1 - \frac{g^*}{g}\right)^{-1}, \quad D \approx 2, \quad N_c \approx 4.19 \left(1 - \frac{g^*}{g}\right)^{-1}, \quad D = 3. \quad (23.213)$$

As N is lowered below these critical values, the phase fluctuations of the pair field Δ become incoherent and the pair condensate dissolves. The different phases are indicated in Fig. 23.3. In the chiral formulation of the same model, the intermediate phase has chiral symmetry in spite of a nonzero spontaneously generated “quark

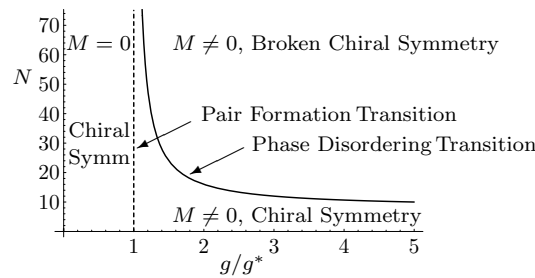


FIGURE 23.3 Two transition lines in the N - g -plane of the chiral Gross-Neveu model in $2 + \epsilon$ dimensions. For $\epsilon = 0$, the vertical transition line coincides with the N -axis, and the solid hyperbola degenerates into a horizontal line at $N_c = 8$. The quark masses and chiral properties are indicated.

mass" $M \neq 0$. The reason why this is possible is that the "quark mass" depends only on $|\Delta_0|$, thus allowing for arbitrary phase fluctuations preserving chiral symmetry.

The skeptical reader may wonder whether the solid hyperbola in Fig. 23.3 is not simply the proper (albeit approximate) continuation of the vertical line for smaller N . There are two simple counterarguments. One is formal: For infinitesimal ϵ the first transition lies precisely at $g = g^* = \pi\epsilon$ for *all* N , so that the horizontal transition line is clearly distinguished from it. The other argument is physical. If N is lowered at some very large g , the binding energy of the pairs *increases* with $1/N$. Observe that in two dimensions, the exact binding energy is $4M \sin^2[\pi/2(N-1)]$. It is then impossible that the phase fluctuations on the horizontal branch of the transition line, which are low-energy excitations, unbind the strongly bound pairs. This will only happen in the limit $N \rightarrow \infty$ where the binding energy becomes zero and the two transition curves merge into a single curve. This is the situation in the theory of superconductivity, where Cooper pair binding and pair condensation coincide.

In the ordinary Gross-Neveu model, the analog of the phase disordering transition is an Ising transition, in which the vacuum expectation value of σ jumps between $-\Sigma_0$ and Σ_0 in a disorderly fashion. In two dimensions, this occurs at some critical value N_c . In $2 + \epsilon$ dimensions, this transition should again exist independently of the transition at which the system enters into a state of nonzero Σ_0 . It will be interesting to see these two transitions confirmed by Monte-Carlo simulations.

There exists a four-dimensional version of this discussion in which it is shown that, very probably, a pion condensate cannot form in the Nambu-Jona-Lasinio model, due to directional fluctuations of the pion field [2].

23.11 Finite-Temperature Properties

It is useful to study also the behavior of the Gross-Neveu model at a finite temperature. The thermal properties of this model will closely resemble those of a

superconductor. For this we confine the imaginary-time variable τ to the interval $\tau \in (0, \hbar\beta)$ with $\beta = 1/k_B T$, and take the fields to be antiperiodic under $\tau \rightarrow \tau + \hbar\beta$. Equivalently, we may think of this model as a nonlinear σ -model on an infinitely long spatial strip with antiperiodic boundary conditions, whose width along the τ -axis is β . In the limit $N \rightarrow \infty$, we can study the effects of temperature exactly. For simplicity, we consider the model only for a vanishing initial bare mass m_0 . The corresponding effective potential of the Σ -field in Eq. (23.16),

$$\frac{1}{N}v(\Sigma) = -\frac{1}{N}\Gamma[\Sigma] = \frac{1}{2g_0}\Sigma^2 - \text{tr}(1)\frac{1}{2}\int \frac{d^D p_E}{(2\pi)^D} \log[p_E^2 + \Sigma^2], \quad (23.214)$$

is generalized to finite temperatures T by exchanging the momentum integral by a sum over Matsubara frequencies $\omega_m = \pi(2m+1)T/\hbar$, $m = 0, \pm 1, \pm 2, \dots$:

$$\int \frac{d^D p_E}{(2\pi)^D} \rightarrow \frac{d^{D-1}p}{(2\pi)^{D-1}} \frac{1}{\hbar\beta} \sum_{\omega_m=-\infty}^{\infty}, \quad (23.215)$$

thus becoming (in natural units with $k_B = 1$ and $\hbar = 1$)

$$\frac{1}{N}v(\Sigma) = \frac{1}{2g_0}\Sigma^2 - 2^{D/2}\frac{1}{2}\int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} T \sum_{m=-\infty}^{\infty} \log(\omega_m^2 + p_E^2 + \Sigma^2). \quad (23.216)$$

The gap equation is obtained by minimizing this potential. It reads [compare (23.15)]

$$\frac{1}{g_0} = 2^{D/2} \int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + p_E^2 + \Sigma^2}. \quad (23.217)$$

Using the well-known summation formula

$$T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega^2} = \frac{1}{2\Omega} \tanh\left(\frac{\Omega}{2T}\right), \quad (23.218)$$

the gap equation becomes an integral

$$\frac{1}{g_0} = 2^{D/2} \int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} \frac{1}{2\Omega} \tanh \frac{\Omega}{2T}. \quad (23.219)$$

We shall renormalize this by adding and subtracting, on the right-hand side, its zero-temperature limit:

$$\frac{1}{g_0} = 2^{D/2} \int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} \frac{1}{p_E^2 + \Sigma^2} + 2^{D/2} \int \frac{d^D p_E}{(2\pi)^D} \frac{1}{2\Omega} \left(\tanh \frac{\Omega}{2T} - 1 \right). \quad (23.220)$$

Near two dimensions, the first integral in this expression can be written as

$$2^{D/2-1} S_D \Gamma(D/2) \Gamma(1 - D/2) (\Sigma^2)^{D/2-1} = b_\epsilon \frac{D}{2} \Sigma^\epsilon \approx b_\epsilon \mu^\epsilon - \frac{\mu^\epsilon}{\pi} \left(\log \frac{\Sigma}{\mu} + \frac{1}{2} \right) + \mathcal{O}(\epsilon), \quad (23.221)$$

where we have used Eqs. (23.17) and (23.20). This leads to the renormalized gap equation at $\epsilon = 0$:

$$\frac{1}{g_R(\mu^2)} = \frac{1}{\pi} \log \frac{\Sigma}{\mu} + \frac{1}{2} + \frac{1}{\pi} \int_0^\infty \frac{dp}{\Omega} \left(\tanh \frac{\Omega}{2T} - 1 \right). \quad (23.222)$$

It is convenient to express the zero-temperature part of this equation without the arbitrary scale parameter μ , using the renormalization group invariant mass

$$M = \mu \exp \left[-\frac{\pi}{g_R(\mu)} - \frac{1}{2} \right], \quad (23.223)$$

which is the solution of the zero-temperature gap equation. Then we arrive at the finite-temperature equation

$$\log \frac{\Sigma}{\Sigma_0} = S_1 \left(\frac{\Sigma}{2\pi T} \right), \quad (23.224)$$

with the function [compare with the bosonic version of this in Eq. (19.112)]

$$S_1 \left(\frac{\Sigma}{2\pi T} \right) = \int_0^\infty \frac{dp}{\Omega} \left(\tanh \frac{\Omega}{2T} - 1 \right) = -2 \int_0^\infty dp \frac{1}{\Omega} \left(e^{\Omega/T} + 1 \right)^{-1}. \quad (23.225)$$

This determines the dimensionless ratio $\Sigma/2\pi T$ as a function of T . The dimensionless ratio $\Sigma/2\pi T$ will in the following be denoted by $\hat{\Sigma}$ for later convenience, i.e.,

$$\hat{\Sigma} = \frac{\Sigma}{2\pi T}. \quad (23.226)$$

The solution $\Sigma(T) \equiv M(T)$ of (23.224) is now the temperature-dependent fermion mass. For $T = 0$, the function $S_1(\hat{\Sigma})$ vanishes and $\Sigma(0) = \Sigma_0 = M$. As the temperature rises, the fermion mass $M(T)$ decreases, until it vanishes at a certain critical temperature T_c . The value of T_c is found by assuming $\Sigma(T)$ to be small, and by approximating the right-hand side of (23.225) as

$$2 \int_0^\infty \frac{dp}{2\pi} \left[\frac{1}{p} \tanh \left(\frac{p}{2T} \right) - \frac{1}{\sqrt{p^2 + \Sigma^2}} \right]. \quad (23.227)$$

Integrating the first term by parts gives

$$\frac{1}{\pi} \left\{ \log \left(\frac{p}{2T} \right) \tanh \left(\frac{p}{2T} \right) \Big|_0^\infty - \int_0^\infty dx \log x \cosh^{-2} x \right\}. \quad (23.228)$$

The integral is convergent and equal to $-\log(4e^\gamma/\pi)$, where $\gamma = 0.577\dots$ is the Euler number. This follows at once from the formula

$$\int_0^\infty dx x^{\mu-1} \cosh^{-2} ax = \frac{4}{(2a)^\mu} \left(1 - 2^{2-\mu} \right), \Gamma(\mu) \zeta(\mu - 1) \quad (23.229)$$

in the limit $\mu \rightarrow 1$, where

$$\zeta(z) \equiv \sum_{k=0}^{\infty} \frac{1}{k^z} \quad (23.230)$$

is Riemann's zeta function. Using the property $\zeta(0) = -1/2$ and $\zeta'(0) = -\frac{1}{2} \log(2\pi)\Gamma'(1) = -\gamma$, the second term in (23.227) can be integrated directly with the result $\operatorname{asinh}(p/\Sigma) = \log[p/\Sigma + \sqrt{p^2/\Sigma^2 + 1}]$. Hence (23.227) becomes

$$\frac{1}{\pi} \left\{ \left[\log\left(\frac{p}{2T}\right) \tanh\left(\frac{p}{2T}\right) - \log\left(\frac{p}{\Sigma} + \sqrt{\frac{p^2}{\Sigma^2} + 1}\right) \right]_0^{\infty} + \log\left(\frac{4e^{\gamma}}{\pi}\right) \right\} = \frac{1}{\pi} \log\left(\Sigma \frac{2e^{\gamma}}{\pi T}\right), \quad (23.231)$$

and (23.224) determines the critical temperature by the equation

$$\log\left(\frac{\Sigma}{\Sigma_0}\right) = \log\left(\Sigma \frac{e^{\gamma}}{\pi T_c}\right), \quad (23.232)$$

or

$$T_c = \Sigma_0 \frac{e^{\gamma}}{\pi} = M \frac{e^{\gamma}}{\pi}. \quad (23.233)$$

At this temperature, the fermion mass $M(T)$ vanishes.

In order to study the full temperature behavior of $M(T)$, the right-hand side of the gap equation (23.224) has to be evaluated numerically. For this purpose, we shall derive a more useful form of the gap equation. Let us once more go back to the original form (23.217), and rewrite it for $\epsilon \sim 0$ as [compare (23.47)]

$$\begin{aligned} \frac{1}{g_0} - 2^{D/2} \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 + \Sigma^2} &= \frac{1}{g_0} - b_{\epsilon} \mu^{\epsilon} + \frac{1}{2\pi} \left(\log \frac{\Sigma^2}{\mu^2} + 1 \right) \\ &= \frac{1}{\pi} S_1(\hat{\Sigma}) = T \sum_{m=0}^{\infty} \frac{1}{\sqrt{\omega_m^2 + \Sigma^2}} - \int_0^{\infty} \frac{d\omega_m}{2\pi} \frac{1}{\sqrt{\omega_m^2 + \Sigma^2}}. \end{aligned} \quad (23.234)$$

This can again be written as in (23.224):

$$\log \frac{\Sigma}{\Sigma_0} = S_1(\hat{\Sigma}), \quad (23.235)$$

where S_1 is given by the sum-minus-integral expression

$$S_1(\hat{\Sigma}) = \left(\sum_{m=0}^{\infty} - \int_{-1/2}^{\infty} dm \right) \frac{1}{\sqrt{\left(m + \frac{1}{2}\right)^2 + \Sigma_T^2}}. \quad (23.236)$$

It is useful to reorganize the sum as follows:

$$\begin{aligned} S_1(\hat{\Sigma}) &= \sum_{m=0}^{\infty} \left(\frac{1}{\sqrt{\left(m + \frac{1}{2}\right)^2 + \Sigma_T^2}} - \frac{1}{m + \frac{1}{2}} \right) \\ &\quad + \sum_{m=0}^{\infty} \frac{1}{m + \frac{1}{2}} - \int_{-1/2}^{\infty} dm \frac{1}{\sqrt{\left(m + \frac{1}{2}\right)^2 + \hat{\Sigma}^2}}. \end{aligned} \quad (23.237)$$

The integral up to some large number $m = \bar{m}$ gives $\text{asinh}(\bar{m}/\hat{\Sigma}) \rightarrow \log(2\bar{m}/\hat{\Sigma})$. The sum over $1/(m + \frac{1}{2})$ is equal to

$$\gamma + \log 4 + \psi(\bar{m} + 3/2) = \gamma + \log 4 + \psi(\bar{m} + 1/2) + 1/(\bar{m} + 1/2).$$

Using the large- z behavior $\psi(z) = \log z - 1/(2z) - 1/(12z^2) + \dots$, we find for $S_1(\hat{\Sigma})$ the convergent sum

$$\begin{aligned} S_1(\hat{\Sigma}) &= \sum_{m=0}^{\infty} \left[\frac{1}{\sqrt{(m + \frac{1}{2})^2 + \hat{\Sigma}^2}} - \frac{1}{m + \frac{1}{2}} \right] + \log(2e^\gamma \hat{\Sigma}) \\ &\equiv \tilde{S}_1(\hat{\Sigma}) + \log(2e^\gamma \hat{\Sigma}). \end{aligned} \quad (23.238)$$

The logarithm of $\hat{\Sigma}$ cancels a similar term on the left-hand side of the gap equation (23.224). Using now the relation (23.233) between Σ_0 and the critical temperature, we express Σ_0 in terms of M , and derive the gap equation in a form most suitable for a numerical evaluation:

$$\log \frac{T}{T_c} = \tilde{S}_1(\hat{\Sigma}). \quad (23.239)$$

This can be used to calculate T/T_c as a function of $\hat{\Sigma}$, and from this $M(T) = \Sigma = 2\pi T \hat{\Sigma}$. The resulting function $M(T)$ is plotted in Fig. 23.4.

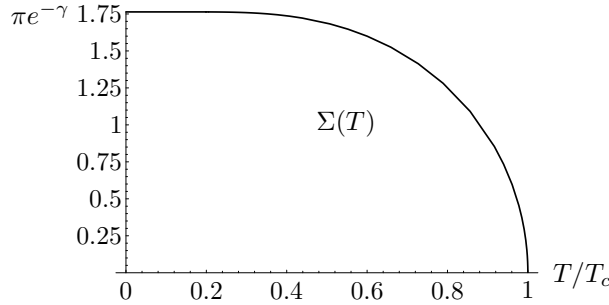


FIGURE 23.4 Solution of the temperature-dependent gap equation, showing the decrease of the fermion mass $M(T) = \Sigma(T)$ with increasing temperature T/T_c .

It is quite easy to calculate the way in which $M(T)$ vanishes as T approaches the critical temperature T_c . We simply expand

$$\begin{aligned} \tilde{S}_1(\hat{\Sigma}) &= \sum_{k=1}^{\infty} \binom{-1/2}{k} \hat{\Sigma}^{2k} \sum_{m=0}^{\infty} \frac{1}{(m + \frac{1}{2})^{2k+1}} \\ &= -\frac{1}{2} \hat{\Sigma}^2 \sum_{m=0}^{\infty} \frac{1}{(m + \frac{1}{2})^3} + \frac{3}{8} \hat{\Sigma}^4 \sum_{m=0}^{\infty} \frac{1}{(m + \frac{1}{2})^5} - \dots \end{aligned} \quad (23.240)$$

Expanding the logarithm near T_c as $\log(T/T_c) \sim T/T_c - 1$, we find in a first approximation

$$M(T) = \Sigma \approx \pi T_c \sqrt{\frac{8}{7\zeta(3)}} \sqrt{1 - \frac{T}{T_c}}. \quad (23.241)$$

In the opposite limit of low temperatures, the series (23.240) converges very slowly. It is, however, easy to find out how Σ behaves near $T = 0$ by expanding in (23.225)

$$\tanh \frac{\Omega}{2T} - 1 = 2 \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} e^{-\tilde{m}\Omega/T}. \quad (23.242)$$

Using the integral

$$\int_{-\infty}^{\infty} dp \frac{e^{-\tilde{m}\sqrt{p^2+\Sigma^2}/T}}{\sqrt{p^2+\Sigma^2}} = 2K_0(\tilde{m}\Sigma/T), \quad (23.243)$$

where $K_0(z)$ is the associated Bessel function, we find the alternative expression

$$\log \frac{\Sigma}{\Sigma_0} = S_1(\hat{\Sigma}) = 2 \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} K_0(2\pi\tilde{m}\hat{\Sigma}). \quad (23.244)$$

For small T , $K_0(\tilde{m}\Sigma/T)$ has the asymptotic behavior

$$K_0\left(\frac{\tilde{m}\Sigma}{T}\right) \sim \sqrt{\frac{\pi}{2\tilde{m}\Sigma/T}} e^{-\tilde{m}\Sigma/T}, \quad (23.245)$$

so that we can expand

$$\Sigma = \Sigma_0 \left(1 - \sqrt{\frac{2\pi}{\Sigma_0/T}} e^{-\Sigma/T}\right) + \mathcal{O}(e^{-2\Sigma/T}) \quad (23.246)$$

and see that Σ approaches its $T = 0$ -value Σ_0 exponentially fast from below (see Fig. 23.4).

Note that the properties of the gap equation (23.224) are quite similar to those of the corresponding equation (19.110) in the nonlinear σ -model.

It is instructive to go through the same discussion once more in D dimensions. For this it is convenient to rewrite the gap equation (23.234) in accordance with the general procedure of dimensional regularization in Section 11.5 as

$$\frac{1}{g_0} - 2^{D/2} \int_0^{\infty} d\tau \int \frac{d^D p}{(2\pi)^D} e^{-\tau(p^2+\Sigma^2)} = \frac{\Sigma^{D-2}}{\pi} 2^{1-D/2} \pi^{(1-D)/2} \Gamma(3/2 - D/2) S_1(\hat{\Sigma}). \quad (23.247)$$

The left-hand side corresponds to the zero-temperature gap equation and is integrated directly to

$$\frac{1}{g_0} - b_{\epsilon} \frac{D}{2} \Sigma^{\epsilon} = \frac{\mu^{\epsilon}}{g(\mu)} - b_{\epsilon} \left(\frac{D}{2} \Sigma^{\epsilon} - \mu^{\epsilon} \right), \quad (23.248)$$

while

$$\begin{aligned} S_1(\hat{\Sigma}) &= \pi \Sigma^{2-D} 2^{D-1} \pi^{(D-1)/2} \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \right]^{-1} \\ &\times \int_0^{\infty} d\tau \int \frac{d^{D-1} p}{(2\pi)^{D-1}} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \exp \left[-\tau (\omega_m^2 + p^2 + \Sigma^2) \right]. \end{aligned} \quad (23.249)$$

The momentum integrations can now be done, with the result

$$\frac{1}{g_0} - 2^{D/2} \frac{1}{2^D} \pi^{-D/2} \int_0^\infty \frac{d\tau}{\tau^{D/2}} e^{-\tau \Sigma^2} = \Sigma^{D-2} 2^{1-D/2} \pi^{-1/2 - \frac{D}{2}} \Gamma\left(\frac{3}{2} - \frac{D}{2}\right) S_1(\hat{\Sigma}), \quad (23.250)$$

where

$$S_1(\hat{\Sigma}) = 2\pi \Sigma^{2-D} \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \right]^{-1} \int_0^\infty \frac{d\tau}{\tau^{D/2-1}} \left(T \sum_{m=0}^\infty - \int_0^\infty \frac{d\omega_m}{2\pi} \right) e^{-\tau(\omega_m^2 + \Sigma^2)}. \quad (23.251)$$

By performing the τ -integral on the right-hand side, we find

$$\begin{aligned} S_1(\hat{\Sigma}) &= 2\pi \Sigma^{2-D} \left(T \sum_{m=0}^\infty - \int_0^\infty \frac{d\omega_m}{2\pi} \right) (\omega_m^2 + \Sigma^2)^{(D-3)/2} \\ &= \hat{\Sigma}^{2-D} \left(\sum_{m=0}^\infty - \int_{-1/2}^\infty dm \right) \left[\left(m + \frac{1}{2} \right)^2 + \hat{\Sigma}^2 \right]^{(D-3)/2}. \end{aligned} \quad (23.252)$$

Let us expand the sum over m formally in a power series of $\hat{\Sigma}$. Its contributions to $S_1(\hat{\Sigma})$ are

$$S_1(\hat{\Sigma}) \Big|_{\text{sum part}} = \hat{\Sigma}^{2-D} \sum_{k=0}^\infty \binom{(D-3)/2}{k} \hat{\Sigma}^{2k} \zeta(2k+3-D, 1/2), \quad (23.253)$$

where

$$\zeta(z, a) \equiv \sum_{k=0}^\infty \frac{1}{(k+n)^z} \quad (23.254)$$

is Riemann's zeta function, with $\zeta(z, 1) = \zeta(z)$ of Eq. (23.230). The integral over ω_m in (23.252) subtracts from this the $T = 0$ -limit of (23.253):

$$2^{D/2-1} \pi^{(D-1)/2} \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \right]^{-1} b_\epsilon \frac{D}{2} \pi = \frac{\sqrt{\pi}}{2} \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \right]^{-1} \Gamma\left(1 - \frac{D}{2}\right). \quad (23.255)$$

For D near an even dimension $\bar{D}$, say $D = \bar{D} + \epsilon$, the k th term with $k = \bar{D}/2 - 1$ has a $1/\epsilon$ -singularity coming from the zeta function

$$\zeta\left(1 + \bar{D} - D, 1/2\right) \sim \frac{1}{\epsilon} [1 + \epsilon \psi(1/2)]. \quad (23.256)$$

This is canceled by a singularity of opposite sign in b_ϵ . We now expand up to first order in ϵ :

$$\begin{aligned} \hat{\Sigma}^{2-D} \binom{(D-3)/2}{k} \Big|_{k=\bar{D}/2} \hat{\Sigma}^{\bar{D}-2} \zeta(1-\epsilon, 1/2) &= \frac{\Gamma((D-1)/2)}{\Gamma(\bar{D}/2) \Gamma(1/2 + \epsilon/2)} \hat{\Sigma}^{-\epsilon} \zeta(1-\epsilon, 1/2) \\ &\approx \frac{1}{\Gamma(3/2 - D/2) \Gamma(\bar{D}/2) \Gamma(1/2)} \frac{\pi}{\cos \pi(\bar{D}/2 - 1)} \frac{-1}{\epsilon} \left\{ 1 + \frac{\epsilon}{2} (-2 \log \hat{\Sigma} + \psi(1/2)) \right\} \\ &\approx -\frac{(-1)^{\bar{D}/2}}{\Gamma(3/2 - D/2) \Gamma(\bar{D}/2)} \frac{\sqrt{\pi}}{\epsilon} \left\{ 1 + \frac{\epsilon}{2} [-2 \log \hat{\Sigma} + \psi(1/2) + \psi(3/2 - \bar{D}/2)] \right\}. \end{aligned}$$

Here $\psi(x)$ is the *Digamma function* $\Gamma'(z)/\Gamma(z)$. Similarly we expand the $T = 0$ -term (23.255) as:

$$\begin{aligned} & \frac{\sqrt{\pi}}{2} \left[\Gamma \left(\frac{3}{2} - \frac{D}{2} \right) \right]^{-1} \Gamma \left(1 - \frac{D}{2} \right) \\ &= \frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2 - \bar{D}/2)} \frac{\sqrt{\pi}}{\epsilon} \left\{ 1 - \frac{\epsilon}{2} [\psi(\bar{D}/2) - \psi(3/2 - \bar{D}/2)] \right\}. \end{aligned} \quad (23.257)$$

Subtracting the two terms from each other yields

$$\begin{aligned} & -\frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2 - \bar{D}/2)} \frac{\sqrt{\pi}}{2} [2 \log \hat{\Sigma} - \psi(1/2) - \psi(\bar{D}/2)] \\ &= -\frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2 - \bar{D}/2)} \frac{\sqrt{\pi}}{2} [2 \log(2e^\gamma \hat{\Sigma}) - \psi(\bar{D}/2) - \gamma]. \end{aligned} \quad (23.258)$$

On the right-hand side we may replace the Digamma function $\psi(\bar{D}/2)$ for $\bar{D} = 2$ by $\psi(\bar{D}/2) = -\gamma$, and for $\bar{D} > 2$, $\psi(\bar{D}/2) = -\gamma + 2/\bar{D} + \dots + 2/(\bar{D} - 2)$. Going now to the limit $\epsilon \rightarrow 0$, we obtain for even $D = \bar{D}$:

$$\begin{aligned} S_1(\hat{\Sigma}) &= -\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(3/2 - D/2)} \frac{\sqrt{\pi}}{2} [2 \log(2e^\gamma \hat{\Sigma}) - \psi(D/2) - \gamma] \\ &+ \sum_{k=0, k \neq D/2-1}^{\infty} \binom{(D-3)/2}{k} \hat{\Sigma}^{2k+2-D} \zeta(2k+3-D, 1/2). \end{aligned} \quad (23.259)$$

By taking the negative powers of $\hat{\Sigma}^2$ out of the sum, we split

$$\begin{aligned} S_1(\hat{\Sigma}) &= -\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(9/2 - D/2)} \frac{\sqrt{\pi}}{2} [2 \log(2e^\gamma \hat{\Sigma}) - \psi(D/2) - \gamma] \\ &+ \sum_k^{D/2-2} \binom{(D-3)/2}{k} \hat{\Sigma}^{2k+2-D} \zeta(2k+3-D, 1/2) + \tilde{S}_1(\hat{\Sigma}), \end{aligned} \quad (23.260)$$

where

$$\tilde{S}_1(\hat{\Sigma}) \equiv \sum_{k=D/2}^{\infty} \binom{(D-3)/2}{k} \hat{\Sigma}^{2k+2-D} \zeta(2k+3-D, 1/2). \quad (23.261)$$

The sum $\tilde{S}_1(\hat{\Sigma})$ can also be calculated from the sum part in (23.252) by performing $D/2$ subtractions:

$$\begin{aligned} \tilde{S}_1(\hat{\Sigma}) &= \hat{\Sigma}^{2-D} \sum_{m=0}^{\infty} \left\{ \left[\left(m + \frac{1}{2} \right)^2 + \hat{\Sigma}^2 \right]^{(D-3)/2} \right. \\ &\quad \left. - \left(m + \frac{1}{2} \right)^{D-3} - \frac{D-3}{2} \hat{\Sigma}^2 \left(m + \frac{1}{2} \right)^{D-5} + \dots \right\}. \end{aligned} \quad (23.262)$$

This sum is convergent and starts out with $\tilde{S}_1(0) = 0$. It is the generalization of $\tilde{S}_1(\hat{\Sigma})$ in Eq. (23.238) to arbitrary even D .

Let us also generalize to arbitrary D the other expressions for $S_1(\hat{\Sigma})$ in Eqs. (23.225) and (23.244). It gives the finite-temperature correction to the gap equation

$$\begin{aligned} \Sigma^{-1} i \Delta_T \text{tr} \frac{1}{i \not{\partial} - \Sigma}(0) &= \left[2^{D/2} \int \frac{d^{D-1} p_E}{(2\pi)^{D-1}} T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + p_E^2 + \Sigma^2} \right] - \left[\dots \right]_{T \rightarrow 0} \\ &= \frac{\Sigma^{D-2}}{\pi} 2^{1-D/2} \pi^{(1-D)/2} \Gamma\left(\frac{3}{2} - \frac{D}{2}\right) S_1(\hat{\Sigma}). \end{aligned} \quad (23.263)$$

The symbol

$$\Delta_T X(T) \equiv X(T) - X(0) \quad (23.264)$$

denotes the finite-temperature correction to any quantity $X(T)$. By comparison with (23.249), we can identify

$$\begin{aligned} S_1(\hat{\Sigma}) &= 2^{D-2} \pi^{(D+1)/2} \Sigma^{2-D} \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \right]^{-1} \int \frac{d^{D-1} p}{(2\pi)^{D-1}} \frac{1}{\Omega} \left(\tanh \frac{\Omega}{2T} - 1 \right) \\ &= \pi \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \Gamma\left(\frac{D}{2} - \frac{1}{2}\right) \right]^{-1} \Sigma^{2-D} \int_0^\infty dp p^{D-2} \frac{1}{\Omega} \left(\tanh \frac{\Omega}{2T} - 1 \right). \end{aligned} \quad (23.265)$$

Writing $\tanh(\Omega/2T) - 1$ as $-2(1 + e^{\Omega/T})^{-1}$, and expanding this in powers of $e^{-\Omega/T}$, we have the alternative expression

$$S_1(\hat{\Sigma}) = 2\pi \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \Gamma\left(\frac{D}{2} - \frac{1}{2}\right) \right]^{-1} \Sigma^{2-D} \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} \int_0^\infty dp p^{D-2} \Omega^{-1} e^{-\tilde{m}\Omega/T}. \quad (23.266)$$

Using the integral representation for the modified Bessel function

$$K_\nu(z) = \left(\frac{z}{2}\right)^\nu \frac{\Gamma(1/2)}{\Gamma(\nu + 1/2)} \int_0^\infty ds s^{2\nu} (s^2 + 1)^{-1/2} e^{-z\sqrt{s^2+1}}, \quad (23.267)$$

we arrive at the expansion

$$S_1(\hat{\Sigma}) = \pi \left[\Gamma\left(\frac{3}{2} - \frac{D}{2}\right) \Gamma\left(\frac{1}{2}\right) \right]^{-1} 2^{D/2} \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} \left(2\pi\tilde{m}\hat{\Sigma}\right)^{1-D/2} K_{D/2-1}(2\pi\tilde{m}\hat{\Sigma}), \quad (23.268)$$

which, for $D = 2$, reduces properly to (23.244).

Let us also calculate the finite-temperature correction to the free energy for all dimensions D . By integrating the gap equation (23.247) in Σ , using (23.248) and (23.249), we obtain

$$\frac{1}{N} v(\Sigma) = \frac{\Sigma^2}{2g} + i \text{Tr} \log(i \not{\partial} - \Sigma) + i \Delta_T \log(i \not{\partial} - \Sigma), \quad (23.269)$$

with

$$\begin{aligned} i\Delta_T \text{Tr} \log(i\hat{\phi} - \Sigma) &= -2^{D/2} \int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} \frac{1}{2} \left(T \sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 - \Omega^2) \\ &= -2^{D/2} T \int \frac{d^{D-1}p_E}{(2\pi)^{D-1}} \log(1 + e^{-\Omega/T}). \end{aligned} \quad (23.270)$$

We now introduce a function $S_0(\hat{\Sigma})$, so that

$$i\Delta_T \text{Tr} \log(i\hat{\phi} - \Sigma) \equiv \frac{1}{N} \Delta_T v(\Sigma) = -\frac{\Sigma^D}{\pi} 2^{-D/2} \pi^{1/2-D/2} \Gamma\left(\frac{1}{2} - \frac{D}{2}\right) S_0(\hat{\Sigma}), \quad (23.271)$$

and find for $S_0(\hat{\Sigma})$ the following expression

$$S_0(\hat{\Sigma}) = 4\pi \Sigma^{-D} \left[\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \Gamma\left(\frac{D}{2} - \frac{1}{2}\right) \right]^{-1} T \int_0^\infty dp p^{D-2} \log(1 + e^{-\Omega/T}), \quad (23.272)$$

or, alternatively,

$$S^0(\hat{\Sigma}) = \hat{\Sigma}^{-D} \left(\sum_{m=0}^{\infty} - \int_{-1/2}^{\infty} dm \right) \left[\left(m + \frac{1}{2}\right)^2 + \hat{\Sigma}^2 \right]^{(D-1)/2}. \quad (23.273)$$

The new function $S_0(\hat{\Sigma})$ is related to $S_1(\hat{\Sigma})$ by an integration:

$$S_0(\hat{\Sigma}) = \frac{D-1}{2} \hat{\Sigma}^{-D} \int_0^{\hat{\Sigma}^2} d\Sigma_T^2 \left[\Sigma_T^{D-2} S_1(\hat{\Sigma}) \right]. \quad (23.274)$$

We can now integrate (23.259)-(23.262), and see that the latter expression is separated into a convergent sum

$$\begin{aligned} \tilde{S}_0(\hat{\Sigma}) &= \hat{\Sigma}^{-D} \sum_{m=0}^{\infty} \left\{ \left[\left(m + \frac{1}{2}\right)^2 + \Sigma_T^2 \right]^{(D-1)/2} \right. \\ &\quad \left. - \left(m + \frac{1}{2}\right)^{(D-1)/2} - \frac{D-1}{2} \hat{\Sigma}^2 \left(m + \frac{1}{2}\right)^{D-3} + \dots \right\}, \end{aligned} \quad (23.275)$$

with $D/2 + 1$ subtractions, an additional logarithmic term

$$\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(1/2-D/2)} \frac{\sqrt{\pi}}{2} \left[2 \log(2^\gamma \hat{\Sigma}) - \psi(D/2 + 1/2) - \gamma \right], \quad (23.276)$$

and a sum over negative powers of $\hat{\Sigma}$ from the integral over the second term in (23.260).

Alternatively, we find from the integral (23.274) over the expansion (23.268):

$$S_0(\hat{\Sigma}) = 2\pi 2^{D/2} \left[\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \Gamma\left(\frac{1}{2}\right) \right]^{-1} \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} (2\pi \tilde{m} \hat{\Sigma})^{-D/2} K_{D/2}(2\pi \tilde{m} \hat{\Sigma}). \quad (23.277)$$

According to Eq. (23.274), this has to satisfy

$$\frac{d\hat{\Sigma}^D S_0}{d\hat{\Sigma}^2} = -\frac{1-D}{2}\hat{\Sigma}^{D-2}S_1, \quad (23.278)$$

and a comparison with (23.268) shows that it does, since

$$\left[z^{D/2}K_{D/2}(z)\right]' = -z^{D/2}K_{D/2-1}(z). \quad (23.279)$$

In the high-temperature limit, we use the small- z behavior

$$K_{D/2}(z) \approx \frac{1}{2}\Gamma\left(\frac{D}{2}\right)\left(\frac{z}{2}\right)^{-D/2}, \quad (23.280)$$

to find

$$S_0(\hat{\Sigma}) \approx \pi^{1-D}\hat{\Sigma}^{-D}\frac{\Gamma(D/2)}{\Gamma(1/2-D/2)}\Gamma\left(\frac{1}{2}\right)\sum_{\tilde{m}=1}^{\infty}(-1)^{\tilde{m}}(\tilde{m})^{-D}. \quad (23.281)$$

The sum can be expressed in terms of Riemann's zeta function (23.230) as

$$\sum_{\tilde{m}=1}^{\infty}(-1)^{\tilde{m}}(\tilde{m})^{-D} = -\left(1-2^{1-D}\right)\zeta(D). \quad (23.282)$$

For $D = 2$, we thus obtain

$$S_0(\hat{\Sigma}) \rightarrow \pi\frac{T^2}{\Sigma^2}\zeta(2). \quad (23.283)$$

Recalling (23.271), this yields the low-temperature behavior of the effective potential in two dimensions:

$$\frac{1}{N}\Delta_T v(\Sigma) \rightarrow \frac{1}{\pi}T^2\zeta(2) = \frac{T^2\pi}{6}. \quad (23.284)$$

This is the well-known free energy of a hot or massless Fermi Gas in two dimensions. It could have been obtained directly by dimensional regularization from the $\Sigma = 0$ -expression

$$\begin{aligned} \frac{1}{N}\Delta_T v(\Sigma) &= -\int \frac{dp}{2\pi} \left(T \sum_{m=-\infty}^{\infty} - \int \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2) \\ &= -T \sum_{m=-\infty}^{\infty} \sqrt{\omega_m^2} = -4\pi T^2 \zeta(-1, 1/2) = -T^2 \frac{\pi}{6}, \end{aligned} \quad (23.285)$$

the last equation following from $\zeta(-1, 1/2) = (2^{-1} - 1)\zeta(-1) = 1/24$.

In $D = 4$ dimensions, the result is

$$\begin{aligned} S_0(\hat{\Sigma}) &= \frac{1}{\pi^3}\hat{\Sigma}^{-4} \left[\Gamma(-3/2) \sqrt{\pi} \right]^{-1} \sum_{\tilde{m}=1}^{\infty} (-)^{\tilde{m}} \tilde{m}^{-4} \\ &= \Sigma^{-4} 2^4 \pi T^4 \left[\Gamma(-3/2) \sqrt{\pi} \right]^{-1} \frac{7}{8} \zeta(4), \end{aligned} \quad (23.286)$$

and for the potential:

$$\frac{1}{N}\Delta_T v(\Sigma) \rightarrow -4T^4 \frac{7}{8} \frac{\pi^2}{g^D}. \quad (23.287)$$

The latter follows directly from

$$\begin{aligned} \frac{1}{N}\Delta_T v(\Sigma) &= -2 \int \frac{d^3 p}{(2\pi)^3} \left(T \sum_{m=-\infty}^{\infty} - \int \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2) \\ &= 2 \int_0^\infty \frac{d\tau}{\tau} \int \frac{d^3 p}{(2\pi)^3} T \sum_{m=-\infty}^{\infty} e^{-\tau(\omega_m^2 + p^2)} \\ &= (4\pi^{3/2})^{-1} \Gamma(-\tfrac{3}{2}) T \sum_{m=-\infty}^{\infty} (\omega_m^2)^{3/2} = T^4 4\pi^{3/2} \Gamma(-\tfrac{3}{2}) \zeta(-3, \tfrac{1}{2}). \end{aligned} \quad (23.288)$$

It is the fermion equivalent to the *Stefan-Boltzmann law* for the free energy density f of hot or massless fermions. Compare the discussion for the bosonic model in the paragraph below Eq. (19.169), where we show that, for a pure power behavior of T^n of f , the entropy density $s = -\partial f / \partial T$ is related to f by a factor $-4/T$. On the other hand, the internal energy density $u \equiv E/V = f + TS$ and the specific heat at constant volume $c_V = \partial u / \partial T|_V$ carry the relative factors $1 - n$ and $(1 - n)n/T$ with respect to f , respectively.

Thus, Eq. (23.288) yields for these three thermodynamic quantities

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -4 \frac{2}{3} \frac{\pi^2}{60} \frac{7}{8} T^4. \quad (23.289)$$

In proper physical units, this reads

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -4 \frac{2}{3} \frac{\sigma}{c} \frac{7}{8} T^4, \quad (23.290)$$

where σ is the Stefan-Boltzmann constant (19.172). The prefactor 4 accounts for the two polarization degrees of freedom of both particles and antiparticles, while the factor $7/8$ is typical for fermions.

Recall that the black-body radiation of photons has a free energy

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -2 \frac{\pi^2}{90} T^4 = -2 \frac{2}{3} \frac{\sigma}{c} T^4, \quad (23.291)$$

where the prefactor 2 on the right-hand side accounts now for the two polarization degrees of photons. In contrast to the fermion case, particles and antiparticles coincide.

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*In science one tries to tell people something
that no one ever knew before.
But in poetry, it's the exact opposite.*
PAUL DIRAC (1902–1984)

24

Internal Symmetries of Strong Interactions

If we open up a standard table of the presently known elementary particles, we see a confusing variety of them with many different properties. Before trying to develop a more detailed theory of their interactions it is useful to find certain organizing principles which correlate their quantum numbers and mass spectra [1].

24.1 Classification of Elementary Particles

The most fundamental distinction concerns their statistical properties. They can be of the Fermi-Dirac or Bose-Einstein type, in which case the particles are called fermions or bosons, respectively. Historically, the fermions were subdivided into light and heavy fermions. The former are called leptons (named after the Greek $\lambda\epsilon\pi\tau\acute{o}\varsigma$ = “fine, small, thin”), which were historically electrons, muons, and neutrinos. Recently, also heavier particles were found which should be considered as leptons. This is due to the similarity of their interactions with those of the traditional, truly light leptons. In fact, the characteristic property of leptons is now that they are fermions with no strong interactions. The distinction according to mass is no longer significant.

The most important of the traditional heavy fermions are those particles which provide most of the mass of to atomic nuclei. These are the so-called nucleons, which can be protons or neutrons. These particles have strong interactions. They can be excited in nuclear collisions, thereby producing short-lived resonances. Also these are classified as elementary heavy fermions. The set of all heavy fermions with strong interactions are called baryons (particles named after the Greek $\beta\alpha\rho\acute{\upsilon}\varsigma$ = “heavy”). All baryons can be produced in collision or decay processes, sometimes in the form of antiparticles which, according to the spin-statistics theorem of Section 7.10, have exactly the same mass and spin as the corresponding particles, except for some quantum numbers such as the charge. They carry an opposite sign.

The particles with Bose-Einstein statistics are separated into those that don't and those that do possess strong interactions. The former play an important role in the theoretical description of gravitational, electromagnetic, and weak interactions.

They are called gravitons, photons, and intermediate vector bosons W and Z . The bosons with strong interactions are called mesons (middle-heavy particles after the Greek $\mu\acute{\epsilon}\sigma\acute{o}\varsigma$). The set of all particles with strong interactions, baryons and mesons, are called *hadrons* (after the Greek $\alpha\delta\rho\acute{o}\varsigma$ = “stout”).

Only few of all these particles are completely stable. The most prominent ones make up the stable matter of the universe. These are the protons, electrons, photons, neutrinos, and gravitons. The proton is the only stable baryon. The other important nuclear constituents, the neutrons, live on the average only 898 ± 16 seconds. After this, a neutron decays into a proton, an electron, and an antineutrino.

Among the leptons, only electrons and neutrinos are stable particles. The muons are particles very similar to the electrons, but much heavier. They decay in about 10^{-6} seconds into an electron, a neutrino, and an antineutrino.

The proton is not only the only stable heavy fermion, it is the only stable strongly interacting particle. All mesons are unstable. The decays proceeding over a “long” time, as in the case of the neutron, are called *weak*. Even lifetimes of 10^{-13} seconds are still considered as “long” in elementary particle physics, and the decay is called weak. A particle with such a lifetime down to 10^{-11} sec leaves an observable trace in a bubble chamber.

Most of the hadrons which decay via strong interaction processes live only for a much shorter time than that, so short that they do travel any visible distance in a bubble chamber. They are observable only as resonances in scattering cross sections. The most prominent example is the first resonance in pion nucleon scattering shown in Figs. 24.1 and 24.2. The resonance is called $\Delta(1232)$. It is found at a pion beam momentum

$$p_\pi = 0.34 \text{ GeV}/c. \quad (24.1)$$

In the center of mass coordinate frame, the energy is equal to the mass of the resonance M ,

$$E_{\text{CM}} = M = \sqrt{(E_\pi + m_p)^2 - p_\pi^2} = \sqrt{m_\pi^2 + m_p^2 + 2m_p E_\pi} \quad (24.2)$$

where $E_\pi = \sqrt{p_\pi^2 + m_\pi^2}$ is beam energy and m_π, m_p are the masses of pion and proton. From $p_\pi = 0.34 \text{ GeV}/c$ one finds $M = 1232 \text{ MeV}/c^2$ which is the number given in the parenthesis of $\Delta(1232)$. The large width in the total cross section shows the rather short lifetime. The peak is of the Lorentz shape and can be parametrized as

$$\sigma_{\text{tot}} \propto 2\pi\lambda^2 \frac{\Gamma^2}{(E_{\text{CM}} - M)^2 + (\Gamma/2)^2}, \quad (24.3)$$

where $\lambda \equiv \hbar/p_\pi$ is the Compton wavelength of the incoming pion beam. At the energies $E_{\text{CM}} = M \pm \Gamma/2$, the cross section has fallen to half its peak value. The parameter Γ is therefore identified with the *width* of the resonance. From the experimental curve we extract the width

$$\Gamma \approx 115 \text{ MeV}. \quad (24.4)$$

In the quantum mechanical theory of resonance scattering it is known that such a cross section indicates an exponentially decaying wave function of the form

$$\Psi \propto e^{-i(M-i\Gamma/2)t/\hbar}. \quad (24.5)$$

Indeed, such a wave function leads to a scattering amplitude which contains a pole in the energy plane below the real axis, proportional to

$$\frac{1}{E_{\text{CM}} - M + i\Gamma/2}. \quad (24.6)$$

Its absolute square gives the above Lorentzian cross section. The lifetime of such a wave function is

$$\tau = 2\hbar/\Gamma. \quad (24.7)$$

This is why the inverse width is sometimes called *half-life*. In physical units, the right-hand side has to be multiplied with $\hbar$ if Γ is measured in MeV and τ in seconds. The $\Delta(1231)$ -resonance has therefore a lifetime of

$$\begin{aligned} \tau &= 2\hbar/\Gamma = 0.6583 \times 10^{-21} \frac{\text{MeV}}{\Gamma} \text{sec} \\ &\approx 5.72 \times 10^{-24} \text{ sec.} \end{aligned} \quad (24.8)$$

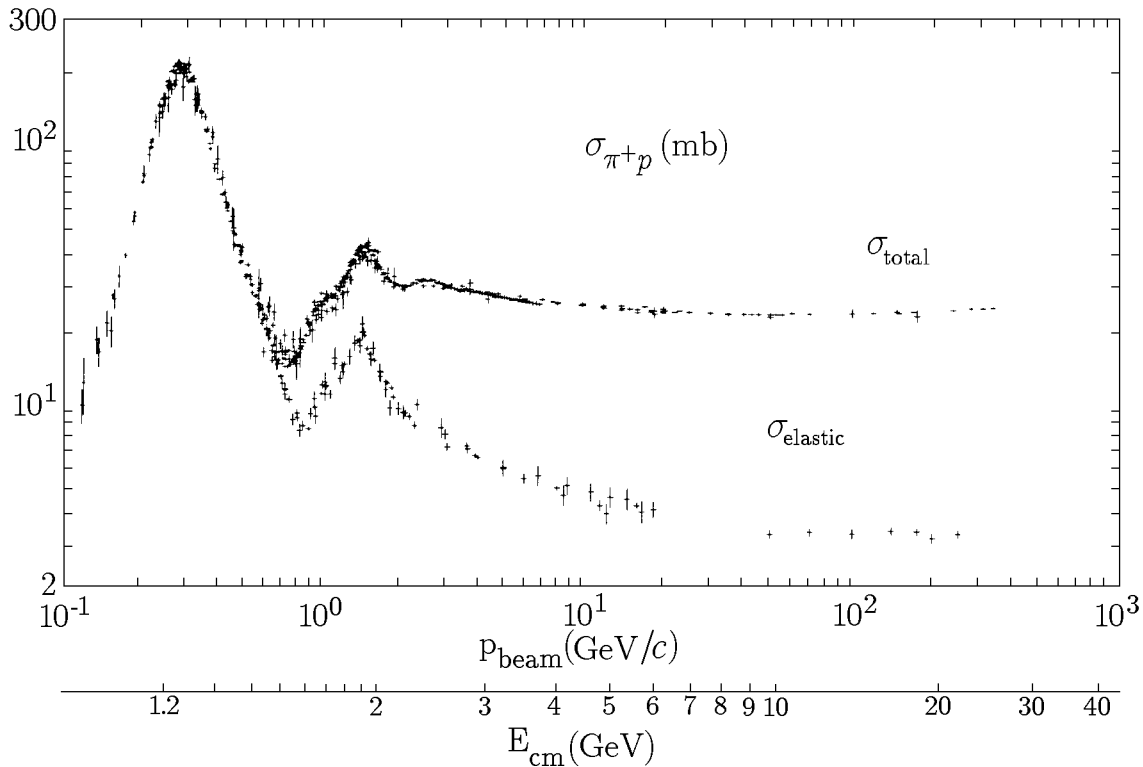


FIGURE 24.1 Total and elastic π^+ -proton cross section showing clearly the first nucleon resonance called $\Delta(1232)$.

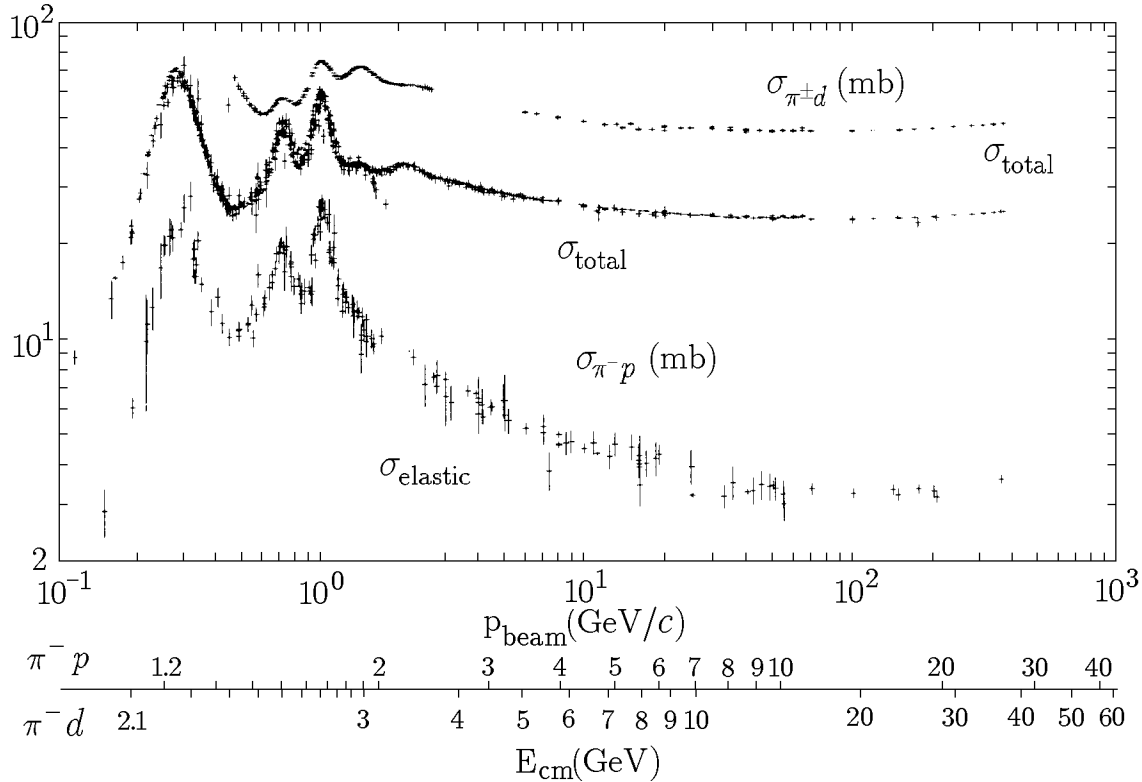


FIGURE 24.2 Total and elastic π^- -proton cross section of the proton in a beam of negatively charged pions π^- . It shows once more the first nucleon resonance called $\Delta(1232)$ as in the previous Figure 24.1, but with only a third of the height. This agrees with the isospin-3/2 assignment and the amplitude relations (24.44) if one invokes the optical theorem (9.36), according to which the total cross section is proportional to the imaginary part of the forward scattering amplitude.

It decays mostly into a pion and a nucleon. Such a short-lived decay is called *strong decay*.

A small fraction, however, about 0.6% of the decays, goes into a nucleon and a photon. This is called the *radiative decay* channel.

Since the $\Delta(1232)$ -resonance can decay into a nucleon and a photon, we should expect that it can also be produced in a collision taking place from the final states, i.e., when a photon hits a nucleon. Indeed, the cross sections in Fig. 24.3 clearly show this resonance.

In the past twenty years, various simple organizing principles have been found according to which the variety of particles and resonances can be classified and remembered and their interactions be related. These principles are based on symmetry groups associated with certain characteristic invariances of the different interactions.

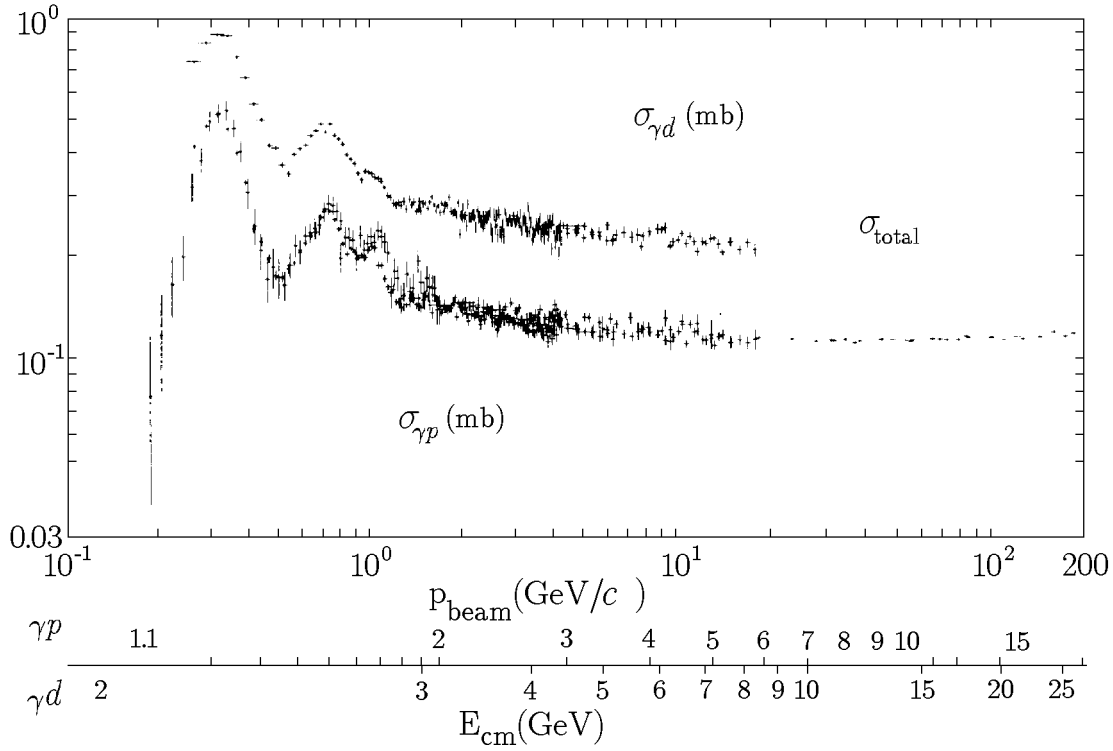


FIGURE 24.3 Photon-proton and photon-deuteron total cross sections showing clearly the first nucleon resonance $\Delta(1232)$ as well as a second resonance called $N(1520)$.

They have helped in understanding the quantum numbers, the energy spectra, the various decay channels, and the different scattering cross sections.

24.2 Isospin in Nuclear Physics

If one compares binding energies of so-called mirror nuclei (which are obtained from each other by the interchange of protons and neutrons), one finds that the difference may be attributed entirely to the different electromagnetic interactions of protons and neutrons. For instance, ${}^3\text{H} = nnp$ and ${}^3\text{He} = ppn$ have binding energies $B_{{}^3\text{H}} = 8.452 \text{ MeV}$ and $B_{{}^3\text{He}} = 7.728 \text{ MeV}$, respectively, with the difference being caused by the proton-neutron mass difference $m_n - m_p = 1.293323 \pm .000016 \text{ MeV}$ and by the different Coulomb field energy around the nuclei. Indeed, if the Coulomb energy is approximated by that of a uniformly charged sphere of charge Z and radius R , the field energy is

$$E_{\text{Coul}} = (1/2)(Z-1)\frac{6}{5}\frac{e^2}{4\pi R} = (1/2)Z(Z-1)\frac{6}{5}\frac{\alpha\hbar c}{R}m, \quad (24.9)$$

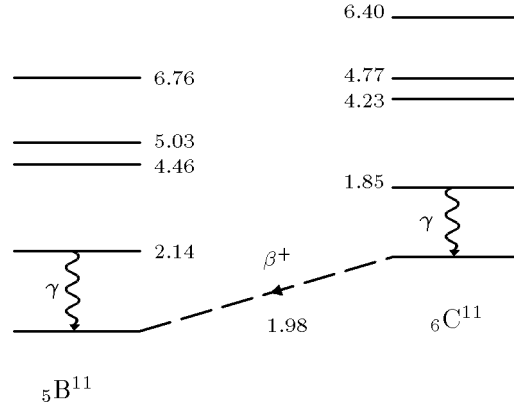


FIGURE 24.4 Mirror nuclei ${}^5\text{B}^{11}$ and ${}^6\text{C}^{11}$ with their excited states (the numbers are the excitation energies in MeV). The ground state of ${}^6\text{C}^{11}$ decays into that of ${}^5\text{B}^{11}$ by a positive β -decay (i.e., emission of a positron and a neutrino) as indicated by the arrow. An estimate of the Coulomb energy via formula (24.9) explains roughly the energy difference of 1.98 MeV between the two level schemes.

with $\alpha = e^2/4\pi\hbar c \approx 1/137$ being the fine-structure constant. Using the estimate $R \approx 1.45 A^{1/3} \times 10^{-13}$ cm for the nuclear radius, where A is the atomic number, we can write

$$E_{\text{Coul}} \approx Z(Z-1) \frac{6}{5} \cdot A^{-1/3} \text{ MeV}. \quad (24.10)$$

For $A = 3, Z = 2$ we estimate $E_{\text{Coul}} \approx 0.57$ MeV, and find the difference of the binding energies to be

$$B_{\text{H}^3} - B_{\text{He}^3} \approx 1.29 \text{ MeV} - 0.57 \text{ MeV} \approx 0.72 \text{ MeV}, \quad (24.11)$$

in rough agreement with the observed 0.76 MeV.

Not only the binding energies, but also the excitation spectra of mirror nuclei differ merely by a common electromagnetic shift, as seen in the example in Fig. 24.4. This property of mirror nuclei has led nuclear theorists to postulate that, if it were possible to switch off the electromagnetic interactions, the potentials V_{pp} and V_{nn} would turn out to be exactly equal. This symmetry is called *charge symmetry*.

The charge symmetry possesses a natural extension. When analyzing the data of nucleon-nucleon scattering at low energy, it was found that also $V_{pp} \approx V_{pn}$. This led Heisenberg to postulate that within purely nuclear interactions, protons and neutrons should be two indistinguishable states of the same particle, the nucleon N . He described the two states in analogy with the two spin states of a spin $1/2$ object by a two-component object

$$N = \begin{pmatrix} p \\ n \end{pmatrix}, \quad (24.12)$$

and he called this object an *isospinor* state. Heisenberg considered the states as a representation of a rotation group in a fictitious space, the space of *isotopic spin*. Its generators are denoted by I_i . They obey the commutation rules of the rotation group

$$[I_i, I_j] = i\epsilon_{abc}I_k. \quad (24.13)$$

The two-component isospinors are rotated by the 2×2 representation of I_i , given by $I_i = \sigma^i/2$. Proton and neutron are eigenstates of the third component $I_3 = \sigma^3/2$, with eigenvalue $1/2$ and $-1/2$.

The exchange of protons and neutrons corresponds to a rotation around the 2 axes of isospin by 180° :

$$e^{i\pi I_2} \begin{pmatrix} p \\ n \end{pmatrix} = e^{i\pi\sigma^2/2} \begin{pmatrix} p \\ n \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} p \\ n \end{pmatrix} = \begin{pmatrix} n \\ -p \end{pmatrix}. \quad (24.14)$$

The postulate of indistinguishability of protons and neutrons can then be formulated mathematically as the commutativity of the generators of isospin I_i with the Hamiltonian of strong interactions

$$[I_i, H_{\text{strong}}] = 0. \quad (24.15)$$

This is called *isotopic spin symmetry* or *isospin invariance* of strong interactions. If $|A\rangle$ is a nuclear n body wave function, then the isospin acts additively on each nucleon, just as ordinary angular momentum (compare Appendix 3B)

$$I_i|A\rangle = (I_i \times 1 \times \dots \times 1 + \dots + 1 \times 1 \times 1 \times \dots \times I_i)|A\rangle. \quad (24.16)$$

Nuclei, which possess a large difference in their number of protons n_p and neutrons n_n , have a third component of isospin

$$I_3|A\rangle = \frac{1}{2}(n_p - n_n)|A\rangle. \quad (24.17)$$

Their total isospin I must be at least equal to I_3 . The ground state has $I = I_3$, the excited states have a higher I . If the Coulomb energies are taken into account, they can be seen to be members of isospin multiplets formed together with neighboring nuclei of equal total number of nucleons and different $n_p - n_n$ (see Fig. 24.5). With the help of isospin rotations, the charge symmetry operation may be represented as a rotation around the second axis by an angle π , namely as $\exp(i\pi I_2)$.

The postulate of isospin symmetry leads immediately to interesting selection rules for decay processes by nuclear interactions, such as α decay or emission of deuterons. Consider a nucleus $|A\rangle$ that has an equal number of protons and neutrons, i.e. a nucleus that is charge symmetric to itself, a so-called *self-conjugate nucleus*. Since it consists of an even number of isospin $1/2$ nucleons, its total isospin is necessarily integer, and the third component of its isospin is zero. The operation $\exp(i\pi I_2)$ must therefore produce the same state, except for a phase factor η :

$$\exp(i\pi I_2)|A\rangle = \eta|A\rangle. \quad (24.18)$$

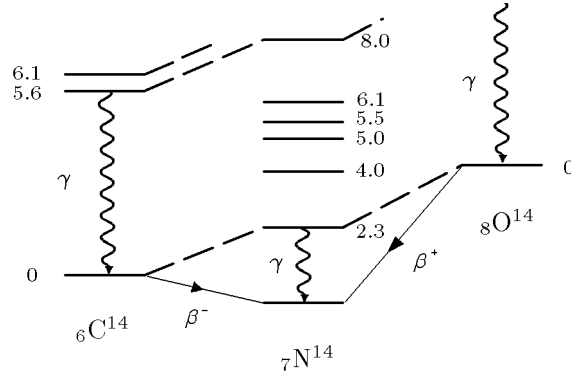


FIGURE 24.5 Singlets and triplets of isospin in the nuclei ${}^6\text{C}^{14}$, ${}^7\text{N}^{14}$, ${}^8\text{O}^{14}$ (with the excitation energies in MeV). The dotted lines connect levels that are roughly degenerate after subtracting the Coulomb energy according to the estimate (24.9).

Applying this operation twice must lead back to the original state. Hence the phase factor η can only be ± 1 . It is called the intrinsic *charge parity* of the nucleus. Every charge-symmetric nucleus has a definite charge parity.

The charge parity η is calculable uniquely as a function of the total isospin. We use the property of the eigenfunctions of angular momentum $Y_{lm}(\Theta, \varphi)$ with $m = 0$ to pick up a phase $(-)^l$, when rotated around the y -axis by an angle π [see the matrix elements of the rotation matrix (4.883)]. This is also obvious from the representation $[(I + I_3)!(I - I_3)!]^{1/2} a_p^\dagger(I + I_3) a_n^\dagger(I - I_3) |0\rangle$ of an isospin I, I_3 -state in terms of creation operators $a_p^\dagger, a_n^\dagger$ of isospin up and down, as constructed in Eq. (4.871). Under an isospin rotation around the 2-axis by an angle π , the operators $a_p^\dagger$ and $a_n^\dagger$ go over into $a_n^\dagger$ and $-a_p^\dagger$, respectively. A charge symmetric state with $I_3 = 0$ has therefore the charge parity

$$\eta = (-)^I. \quad (24.19)$$

The charge parity gives rise to interesting selection rules for decay processes via nuclear interactions. If the Hamiltonian commutes with all generators of isospin, the initial and final states must have equal charge parities. Typical forbidden processes are

$${}^5\text{B}^{*10} \begin{cases} \nearrow {}^3\text{Li}^6 + \alpha, \\ \searrow {}^4\text{Be}^8 + d, \end{cases} \quad (24.20)$$

where ${}^5\text{B}^{*10}$ can be the 4.5 MeV or the 6.5 MeV resonance of ${}^5\text{B}^{10}$. Now, the excited nucleus ${}^5\text{B}^{*10}$ of excitation energy 4.5 MeV is a member of an isospin triplet formed together with ground states of the isotopes ${}^4\text{Be}^{10}$ and ${}^6\text{C}^{10}$. It therefore has a charge parity $\eta = -1$. On the other hand, the nuclei ${}^3\text{Li}^6$ and ${}^4\text{Be}^8$ have isospin 0 and therefore a positive charge parity $\eta = +1$. The two processes (24.20) are thus forbidden processes, which have indeed never been observed in the laboratory.

Let us now study the consequences of the larger isotopic spin symmetry in nuclear reactions. A deuteron in its ground state has the orbit in a symmetric s -wave, and the spin states are given by the three symmetric triplet states

$$|\uparrow\downarrow\rangle, \quad \frac{1}{\sqrt{2}}|\uparrow\downarrow + \downarrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle. \quad (24.21)$$

The antisymmetry of the wave function requires the isotopic wave function to be antisymmetric, i.e., it must be

$$\frac{1}{\sqrt{2}}|pn - np\rangle. \quad (24.22)$$

This is an $I = 0$ -state of isospin.

If a deuteron collides with ${}_4\text{Be}^9$, which has $I = \frac{1}{2}, I_3 = -\frac{1}{2}$, the isospin of the two-particle system is necessarily $I = \frac{1}{2}, I_3 = -\frac{1}{2}$. We can now compare two possible final states, namely

$${}_5\text{B}_{1.7\text{MeV}}^{*10} + n \quad (24.23)$$

and

$${}_4\text{Be}^{10} + p. \quad (24.24)$$

If we denote the isospins of the two particles by $I^{(1)}, I^{(2)}$, the isospin states are in the first case

$$|I^{(1)}, I_3^{(1)}; I^{(2)}, I_3^{(2)}\rangle = |1, 0; \frac{1}{2}, -\frac{1}{2}\rangle, \quad (24.25)$$

and in the second

$$|I^{(1)}, I_3^{(1)}; I^{(2)}, I_3^{(2)}\rangle = |1, -1; 1, \frac{1}{2}\rangle. \quad (24.26)$$

The strengths, with which these two final states are coupled to the initial state $|\frac{1}{2}, -\frac{1}{2}\rangle$, are proportional to the Clebsch-Gordan coefficients

$$\langle \frac{1}{2}, -\frac{1}{2} | 1, 0; \frac{1}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}}, \quad (24.27)$$

$$\langle \frac{1}{2}, -\frac{1}{2} | 1, -1; 1, \frac{1}{2} \rangle = -\sqrt{\frac{2}{3}}, \quad (24.28)$$

respectively (recall Table 4.2). Hence the first reaction cross section should be half as big as the second, a fact borne out by experiment.

24.3 Isospin in Pion Physics

In 1935, Hideki Yukawa [2] postulated the existence of a Bose particle which should mediate the strong interactions between nucleons in a similar way as the photons do between charges. Since the size of nuclei are of the order of 10^{13}cm , Yukawa concluded that instead of a Coulomb potential

$$v(\mathbf{x}) = \frac{1}{4\pi r}, \quad (24.29)$$

which solves the field equation

$$-\partial_{\mathbf{x}}^2 v(\mathbf{x}) = \delta^{(3)}(\mathbf{x}), \quad (24.30)$$

the potential between nucleons should have a finite range and read

$$v^Y(\mathbf{x}) = \frac{e^{-\mu r}}{4\pi r}. \quad (24.31)$$

This solves the differential equation

$$(-\partial_{\mathbf{x}}^2 + \mu^2)v^Y(\mathbf{x}) = \delta^{(3)}(\mathbf{x}). \quad (24.32)$$

He identified the inverse range μ with the mass of the particle. This particle was discovered experimentally around 1946, and is now called the *pion*. It exists in three charge states π^+, π^0, π^- . The neutral pion has a mass

$$m_{\pi^0} = 134.9642 \pm .0038 \text{ MeV}, \quad (24.33)$$

from which the masses of the charged pions differ by

$$m_{\pi^\pm} - m_{\pi^0} = 4.6043 \pm .00037 \text{ MeV}. \quad (24.34)$$

The π -mesons exist only for a small time. The neutral π^0 meson decays mainly into two photons, with a lifetime

$$\tau_{\pi^0} \approx (0.87 \pm .04) \times 10^{-16} \text{ sec}. \quad (24.35)$$

This relatively fast decay is caused purely by electromagnetic interactions. The charged $\pi^\pm$ -states decay mainly into μ, ν_μ with a lifetime of

$$\tau_{\pi^\pm} \approx (2.6030 \pm 0.0023) \times 10^{-8} \text{ sec}. \quad (24.36)$$

This decay is so slow that it proceeds via weak interactions.

Since nuclear forces are supposed to arise mainly from pion interactions, the isosymmetry of nuclear forces implies that the pion-nucleon coupling should be symmetric under isospin rotations. The pion itself is obviously an isospin 1 object. If it interacts with a nucleon of isospin $1/2$, the total isospin can be either $\frac{3}{2}$ or $\frac{1}{2}$. The Clebsch-Gordan coefficients for the different channels of total isospin $|I, I_3\rangle$ are the following (see Table 4.2)

$$\begin{aligned} |\pi^+ p\rangle &= |1, 1; \frac{1}{2}, \frac{1}{2}\rangle &= |\frac{3}{2}, \frac{3}{2}\rangle, \\ |\pi^+ n\rangle &= |1, 1; \frac{1}{2}, -\frac{1}{2}\rangle &= \frac{1}{\sqrt{3}}|\frac{3}{2}, \frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|\frac{1}{2}, \frac{1}{2}\rangle, \\ |\pi^0 p\rangle &= |1, 0; \frac{1}{2}, \frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}|\frac{3}{2}, \frac{1}{2}\rangle - \frac{1}{\sqrt{3}}|\frac{1}{2}, \frac{1}{2}\rangle, \\ |\pi^0 n\rangle &= |1, 0; \frac{1}{2}, -\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}|\frac{3}{2}, -\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|\frac{1}{2}, -\frac{1}{2}\rangle, \\ |\pi^- p\rangle &= |1, -1; \frac{1}{2}, \frac{1}{2}\rangle &= \frac{1}{\sqrt{3}}|\frac{3}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}|\frac{1}{2}, -\frac{1}{2}\rangle, \\ |\pi^- n\rangle &= |1, -1; \frac{1}{2}, -\frac{1}{2}\rangle &= |\frac{3}{2}, -\frac{3}{2}\rangle. \end{aligned} \quad (24.37)$$

From these we find the amplitudes for scattering processes to be all given in terms of two amplitudes, one for total isospin $I = \frac{3}{2}$ and one for total isospin $I = \frac{1}{2}$. The amplitudes are given by the so-called scattering matrix, whose matrix elements are obtained by evaluating the scattering operator S between incoming and outgoing states. The detailed theory of the scattering matrix has been given in Chapter 9. From that theory it follows that if all generators I_i of isospin rotations commute with the Hamiltonian operator of strong interactions H_{strong} , they also commute with the scattering operator S . Then the amplitudes do not depend on the I_3 components of the total isospin:

$$[I_i, S] = 0. \quad (24.38)$$

We therefore can use I_+ inside the matrix elements $\langle I, I_3 | S | I, I_3 \rangle$ to change I_3 to any allowed value $|I_3| \leq I$. From

$$\langle I, I_3 | I_+ S | I, I_3 - 1 \rangle = \langle I, I_3 | S I_+ | I, I_3 - 1 \rangle \quad (24.39)$$

it follows that

$$\begin{aligned} \langle I, I_3 - 1 | S | I, I_3 - 1 \rangle \sqrt{(I + I_3)(I - I_3 + 1)} \\ = \langle I, I_3 | S | I, I_3 \rangle \sqrt{(I + I_3)(I - I_3 + 1)} \end{aligned} \quad (24.40)$$

[see Eqs. (4.370), (4.374)]. Thus the diagonal matrix elements $\langle I, I_3 | S | I, I_3 \rangle$ are independent of I_3 . Similarly one sees that the non-diagonal elements vanish. We therefore define the reduced scattering amplitude S^I of a given isospin I by the equation

$$\langle I, I_3 | S | I, I_3 \rangle \equiv \delta_{I_3 I_3} S^I. \quad (24.41)$$

This statement is a special case of the Wigner-Eckart theorem (4.899) for the matrix elements of an arbitrary spherical tensor operator T_{I, I_3} of isospin I . Such a tensor operator is defined by the transformation law [compare (4.895)]

$$[I_i, T_{I, I_3}] = T_{I, I'_3} D^I(I_i)^{I'_3}_{I_3}, \quad (24.42)$$

where $D^I(I_i)^{I'_3}_{I_3}$ are the representation matrices of the generators I_i of the isospin rotation group. According to the Wigner-Eckart theorem, the matrix elements of a tensor operator between the representation states $|I, I_3\rangle$ are related by Clebsch-Gordan coefficients:

$$\langle I'', I''_3 | T_{I', I'_3} | I, I_3 \rangle = \langle I'', I''_3 | I', I'_3; I, I_3 \rangle \langle I'' || T || I \rangle. \quad (24.43)$$

These account for the dependence on the quantum numbers I_3, I'_3, I''_3 . The matrix elements depend only on a few *reduced matrix elements* $\langle I'' || T || I \rangle$ which are nonzero if the isospins I and I' can be coupled to I'' . Within this definition, the scattering operator is a trivial tensor operator of isospin zero, in which (24.43) reduces to (24.41).

Note that (24.41) is also a manifestation of Schur's Lemma, according to which a matrix commuting with an irreducible set of matrices must be proportional to the unit matrix.

As an application of (24.41), the scattering amplitudes for various pion-nucleon scattering processes are given by the following combinations of only two amplitudes, $S^{3/2}$ and $S^{1/2}$:

$$\begin{aligned}
 S_{\pi^+p \rightarrow \pi^+p} &= S^{3/2}, \\
 S_{\pi^+n \rightarrow \pi^+n} &= (1/3)S^{3/2} + (2/3)S^{1/2}, \\
 S_{\pi^0p \rightarrow \pi^0p} &= (2/3)S^{3/2} + (1/3)S^{1/2}, \\
 S_{\pi^+n \leftrightarrow \pi^0p} &= (\sqrt{2}/3)S^{3/2} - (\sqrt{2}/3)S^{1/2}, \\
 S_{\pi^0n \rightarrow \pi^0n} &= (2/3)S^{3/2} + (1/3)S^{1/2}, \\
 S_{\pi^-p \rightarrow \pi^-p} &= (1/3)S^{3/2} + (2/3)S^{1/2}, \\
 S_{\pi^0n \leftrightarrow \pi^-p} &= (\sqrt{2}/3)S^{3/2} - (\sqrt{2}/3)S^{1/2}, \\
 S_{\pi^-n \rightarrow \pi^-n} &= S^{3/2}.
 \end{aligned} \tag{24.44}$$

The $\leftrightarrow$ symbols in the charge-exchange reactions exhibit time-reversal invariance. By taking the absolute squares of the amplitudes, we see that the cross sections must satisfy

$$2\sigma_{\pi^0p \rightarrow \pi^0p} = \sigma_{\pi^+p \rightarrow \pi^+p} + \sigma_{\pi^-p \rightarrow \pi^-p}. \tag{24.45}$$

This is borne out by experiment.

24.4 $SU(3)$ -Symmetry

In 1944, the set of fundamental particles was enriched by a particle which was a heavy neutral meson of mass ≈ 500 MeV [3], with a lifetime of $\tau \approx 10^{-10}$ sec. It became known as a *strange particle* [4] under the name K^0 . It is observed to decay mainly into π^+, π^- and has a mass and a lifetime

$$\begin{aligned}
 m_{K^0} &\approx 497.72 \pm 0.07 \text{ MeV}, \\
 \tau_{K^0} &\approx (0.8323 \pm 0.0022) \times 10^{-10} \text{ sec}.
 \end{aligned} \tag{24.46}$$

In 1951, a charged partner of this particle was discovered which decays mostly into a μ^+ and a neutrino of the meson type, namely the K^+ meson. It has a mass and a lifetime

$$\begin{aligned}
 m_{K^+} &\approx 493.667 \pm 0.014 \text{ MeV}, \\
 \tau_{K^+} &\approx (1.2371 \pm 0.0026) \times 10^{-8} \text{ sec}.
 \end{aligned} \tag{24.47}$$

Later also a K^- meson was found, that decays into a negatively charged meson and a neutrino with the same lifetime. In 1955 one discovered, moreover, that there

are actually two K^0 -mesons, now called K^0 and $\bar{K}^0$. These mesons could soon be produced abundantly in particle accelerators and it became possible to study their interactions with nucleons. In the course of this it was found that not only the mesons but also the nucleons possess strange partners. Moreover, if one assigned to the strange mesons a quantum number $S = 1$, called *strangeness*, and to the strange partner of the baryons in the associate production a quantum number $S = -1$, then strangeness is a conserved quantum number in a nuclear scattering process. If an ordinary non-strange meson such as a pion hits a nucleon, the result is either a pion and a nucleon, both of strangeness zero, or a strange meson with $S = 1$ together with a strange partner of the nucleon with $S = -1$. For example

$$\pi^- p \rightarrow \pi^- p \quad (24.48)$$

or

$$\pi^- p \begin{array}{l} \nearrow \\ \searrow \end{array} \begin{array}{l} K^0 \Lambda^0, \\ K^+ \Sigma^- \end{array}. \quad (24.49)$$

There are also associate production processes where two K 's are produced in addition to a nucleon:

$$\pi^- p \rightarrow K^- K^0 p, \quad (24.50)$$

$$\pi^+ p \rightarrow K^+ \bar{K}^0 p. \quad (24.51)$$

These allow to deduce that the strangeness of K^+ , K^- is $S = 1, -1$, respectively. By scattering further a strange meson K^- on a proton,

$$K^- p \rightarrow K^+ \Xi^-, \quad (24.52)$$

one is able to produce a new particle Ξ^- of strangeness $S = -2$. This particle is called *cascade* since it decays in a cascade-like process with the first step

$$\Xi^- \rightarrow \Lambda^0 \pi^- \quad (24.53)$$

and the second steps

$$\Lambda^0 \rightarrow p \pi^-, \quad (24.54)$$

$$\pi^- \rightarrow \mu^- \bar{\nu}_\mu. \quad (24.55)$$

Note that in contrast to the production process, the decay of the strange particles violates strangeness. For instance:

$$\begin{array}{ccc} \Sigma^- & \rightarrow & \pi^- \quad n \\ S : & -1 & \quad 0 \quad 0. \end{array} \quad (24.56)$$

However, this violation can be blamed on another interaction, the weak interaction, since the decay proceeds quite slowly, with a lifetime of roughly 10^{-10} sec.

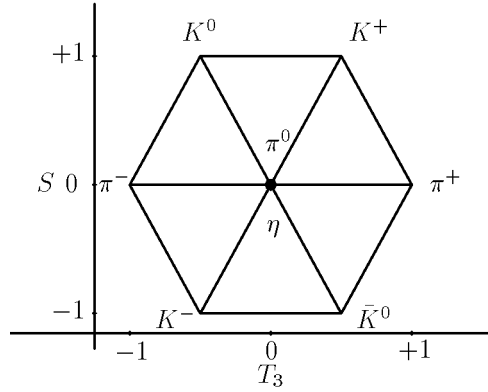


FIGURE 24.6 Pseudoscalar meson octet states associated with the triplet of pions. The same picture holds for the vector meson octet states with the replacement (24.62).

While non-strange particles have a charge

$$Q = N/2 + I_3, \quad (24.57)$$

where N is the total nucleon-number, the charge of strange particles is given by

$$Q = Y/2 + I_3, \quad (24.58)$$

with Y being defined as a convenient combination of N , and S , called hypercharge

$$Y \equiv N + S. \quad (24.59)$$

Murray Gell-Mann plotted the known ordinary and strange pseudoscalar meson states in the I_3, Y plane and found the multiplet of eight particles shown in Fig. 24.6 (there and in subsequent similar plots the ket symbols $|\dots\rangle$ of the states are omitted). The center contains, beside the π^0 -meson, another pseudoscalar neutral meson called the η meson. Its mass is

$$m_\eta = 548.8 \pm 0.6 \text{ MeV} \quad (24.60)$$

and it decays with a width of

$$\Gamma \approx 1.05 \pm 0.15 \text{ keV}, \quad (24.61)$$

principally into $\gamma\gamma$ and $3\pi^0$. A ninth much heavier pseudoscalar meson $\eta'(958)$ of width 8.5 MeV , known at that time, did not fit into the scheme by having a larger mass, and no partners.

Gell-Mann applied the same extension to the spin 1 meson resonances of negative parity to nine pseudoscalar particles, replacing

$$\begin{aligned} K &\rightarrow K^*(892), \\ \pi &\rightarrow \rho(770), \\ \eta &\rightarrow \phi(1020), \\ \eta' &\rightarrow \omega(783). \end{aligned} \quad (24.62)$$

He continued to organize the nucleons and their strange partners in this way and found again an octet, shown in Fig. 24.7, with the masses and lifetimes given in Table 24.1.

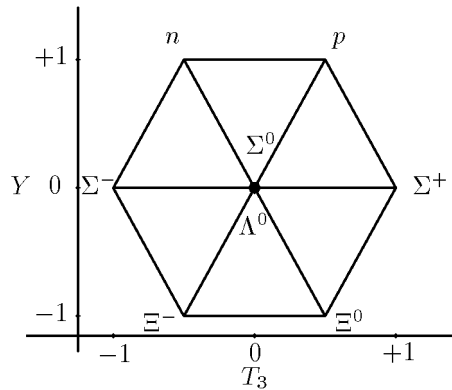


FIGURE 24.7 Baryon octet states associated with isodoublet of nucleons.

TABLE 24.1 Masses and lifetimes of the octet states associated with the isodoublet of nucleons.

	$m(\text{ MeV})$	$\tau (10^{-10} \text{ sec})$
p	938.2796 ± 0.0027	stable
n	939.5731 ± 0.0027	$(898 \pm 16) \times 10^{-10}$
Σ^+	1189.37 ± 0.06	0.8 ± 0.004
Σ^-	1197.34 ± 0.05	1.482 ± 0.011
Σ^0	1192 ± 0.08	$(5.8 \pm 1.3) \times 10^{-10}$
Λ^0	1115.60 ± 0.05	2.632 ± 0.020
Ξ^0	1314.9 ± 0.6	1.642 ± 0.015
Ξ^-	1321.32 ± 0.13	1.642 ± 0.015

Gell-Mann further noticed that there exists no similar regularity for the most prominent excited states of the nucleon, the resonance $\Delta(1232)$ of mass 1232 MeV and width 115 ± 5 MeV. They exist with charges $-, 0, +, ++$ and possess strange partners $\Sigma(1385)$ of width ≈ 37 MeV with charges $-, 0, +$, and $\Xi(1530)$ of width ≈ 10 MeV with charges $-, 0$. When he looked at the masses of these excited states, he observed an about equal spacing on the Y -axis. When plotted in an $I_3 - Y$ plane, the particles fill an equilateral triangle except for a missing lower corner. See Fig. 24.8. Starting from these observations he put forward the hypothesis that just as nuclear forces are independent under isospin rotations, which form the group of unitary matrices in two dimensions, they should also be approximately invariant under the most direct extension of this group, which includes the additional quantum number of strangeness. So he postulated an approximate invariance of the strong interactions under the group of unitary matrices in three dimensions, $SU(3)$. Since the mass splittings are much larger than in the former $SU(2)$ -multiplets, this symmetry is much more broken in nature than the isotopic symmetry.

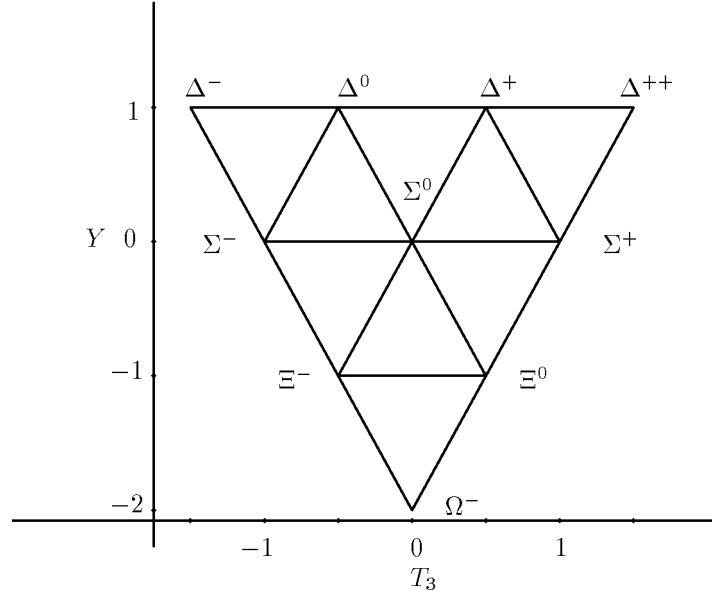


FIGURE 24.8 Baryon decuplet states associated with the first resonance of nucleons.

In field theory, the group theoretic implications of SU(3)-symmetry are studied by giving the relativistic fields an extra SU(3)-subscript. One introduces a fundamental Dirac field with subscripts $\alpha = 1, 2, 3$:

$$\psi(x) \rightarrow \psi_\alpha(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \end{pmatrix}, \quad (24.63)$$

which changes under SU(3)-transformations by group elements from the fundamental three-dimensional representation of SU(3), called 3. Such a Dirac field is called a *quark field*, and will be denoted by $q_\alpha(x)$. Omitting the spacetime arguments, the transformation law is:

$$3: q_\alpha \rightarrow U_\alpha^\beta q_\beta, \quad U \in \text{SU}(3). \quad (24.64)$$

The Hermitian adjoint of a quark field, $(q_\alpha)^\dagger \equiv (q^\dagger)^\alpha$. It transforms according to the complex conjugate representation, called 3^* . To emphasize the different transformation behavior we write $[U_\alpha^\beta]^\dagger$ as $(U^*)^\alpha_\beta$ so that

$$3^*: q^{\dagger\alpha} \rightarrow U^{*\alpha}_\beta q^{\dagger\beta}, \quad U \in \text{SU}(3). \quad (24.65)$$

The unitary scalar product $q^\dagger q \equiv (q^\dagger)^\alpha q_\alpha$ is an invariant, likewise the contraction of q_α with any other particle field, which transforms like $(q^\dagger)^\alpha$. For Dirac fields it is more convenient to work with the fields $\bar{q}(x) = q^\dagger(x)\gamma^0$ rather than $q^\dagger(x)$ because of their more favorable Lorentz transformation properties, in particular the Lorentz invariance of the scalar product $\bar{q}(x)q(x)$. Thus we shall work with conjugate quark fields

$$\bar{q}^\alpha = (\bar{q}^1, \bar{q}^2, \bar{q}^3). \quad (24.66)$$

This field is said to transform according to the representation $\bar{3}$ of SU(3). The contraction $\bar{q}^\alpha q_\alpha$ is obviously invariant under Lorentz- and SU(3)-transformations:

$$\bar{q}^\alpha q_\alpha = \text{invariant}. \quad (24.67)$$

We have seen in Eq. (7.308) that the charge-conjugate Dirac field is directly related to $\bar{q}$ by a similarity transformation of the Dirac indices, which for quark fields reads

$$q_C(x) = C\bar{q}^T(x). \quad (24.68)$$

The fields $\bar{q}$ annihilate antiparticles, and will therefore be referred to as *antiquark fields*, ignoring at this point the similarity transformation.

The traceless tensor field obtained from the direct product of q_α and $\bar{q}^\beta$,

$$M_\alpha{}^\beta \equiv q_\alpha \bar{q}^\beta - \frac{1}{3} \delta_\alpha{}^\beta q_\gamma \bar{q}^\gamma, \quad (24.69)$$

is in general a bilocal field containing $q_\alpha(\mathbf{x}, t)$ and $\bar{q}^\beta(\mathbf{x}', t')$ at different spacetime points which are irrelevant to the present discussion and therefore omitted. This field forms an invariant 8-dimensional representation space of SU(3), which Gell-Mann identified with the 8 meson states described above. This octet representation is irreducible. This means that every state of it can be reached by performing group operations on an arbitrary single fixed state. Gell-Mann called the fields up, down, and strange quark fields and denoted them by u, d, s :

$$q_\alpha = \begin{pmatrix} u \\ d \\ s \end{pmatrix}. \quad (24.70)$$

Similarly for the antiquarks:

$$\bar{q}^\alpha = (\bar{u}, \bar{d}, \bar{s}). \quad (24.71)$$

He associated the octet fields (24.69) with the pseudoscalar mesons as shown in Fig. 24.9. The field $M_\alpha{}^\beta$ annihilates the corresponding particle, for example $\pi^+ \equiv M_1{}^2 = \bar{d}u$ annihilates the particle π^+ . In contrast to isospin, the SU(3)-symmetry is strongly broken. The pion and the K mesons have quite different masses, namely 135 MeV and 490 MeV.

The operator which measures the third component of isospin, I_3 , is the number operator

$$\hat{I}_3 = \frac{1}{2}[(\hat{N}_u - \hat{N}_d) - (\hat{N}_{\bar{u}} - \hat{N}_{\bar{d}})]. \quad (24.72)$$

Here and in the sequel we denote by $\hat{N}_{u,d,s}$ the total number operator of the u, d, s -quarks and their antiparticles, respectively. Thus we have the commutation rules

$$-[\hat{N}_{u,d}, q_\alpha] = n_{u,d} q_\alpha, \quad \alpha(u, d, s) \quad (24.73)$$

with the eigenvalues

$$n_u = (1, 0, 0), \quad n_d = (0, 1, 0), \quad (24.74)$$

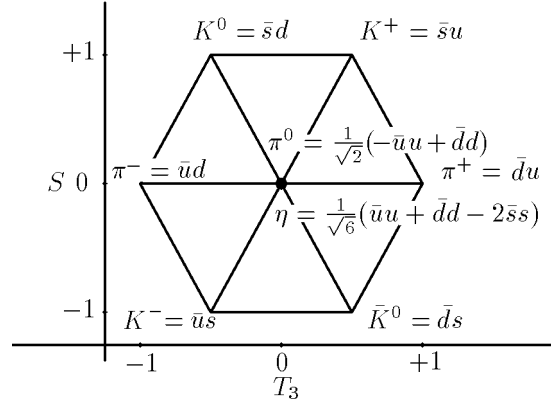


FIGURE 24.9 Quark content of the pseudoscalar meson octet. The particle- and quark-symbols denote the *annihilation* parts of the corresponding fields.

and similar relations between the number operators and the antiquarks $\bar{q}^\alpha = (\bar{u}, \bar{d}, \bar{s})$. The hypercharge of the mesons is given by

$$\hat{Y} = \frac{1}{3}[(\hat{N}_u + \hat{N}_d - 2\hat{N}_s) - (\hat{N}_{\bar{u}} + \hat{N}_{\bar{d}} - 2\hat{N}_{\bar{s}})], \quad (24.75)$$

where N_s counts the number of strange quarks, i.e., it is defined to have, for (u, d, s) and $(\bar{u}, \bar{d}, \bar{s})$, the eigenvalues $n_s = (0, 0, 1)$ and $(0, 0, -1)$, respectively, with corresponding eigenvalues of $N_{\bar{s}}$ for the antiquarks.

The group SU(3) is a $3 \cdot 3 - 1 = 8$ -parameter group. Its Lie algebra possesses 8 traceless Hermitian generators which are conventionally denoted by $\lambda^a/2$ ($a = 1, \dots, 8$) with the 3×3 traceless Hermitian matrices

$$\begin{aligned} \lambda^1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \lambda^4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \\ \lambda^6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \end{aligned} \quad (24.76)$$

Note that they have the same trace orthonormality relations as the Pauli matrices:

$$\text{tr}(\lambda^a \lambda^b) = 2\delta_{ab}. \quad (24.77)$$

It is easy to see that the 3×3 -matrices $U = e^{i\alpha_a \lambda^a/2}$ span the space to unitary 3×3 -matrices with unit determinants. The first three λ^a 's are the direct extension of the σ^i -matrices of isospin into three dimensions.

TABLE 24.2 Structure constants of SU(3). All elements not given in the table follow from the total antisymmetry.

abc	f_{abc}
123	1
147	1/2
156	-1/2
246	1/2
257	1/2
345	1/2
367	-1/2
458	$\sqrt{3}/2$
678	$\sqrt{3}/2$

The group structure is specified by the commutation rules of the generators

$$[\lambda^a, \lambda^b] = 2if_{abc}\lambda^c, \quad (24.78)$$

where the structure constants f_{abc} are totally antisymmetric in abc , due to the Jacobi identity satisfied by the commutators. Their values are given in Table 24.2. Let G_a be the operators in Hilbert space associated with these Lie algebra elements. These act on the three quark field operators of the fundamental representation as follows:

$$-[\hat{G}_a, q_\alpha] = (\lambda^a/2)_\alpha^\beta q_\beta. \quad (24.79)$$

An explicit operator expression for the generators can be given by assigning canonical commutation or anticommutation relations to the q -fields:

$$[q_\alpha, q^{\dagger\beta}] = \delta_\alpha^\beta \quad (24.80)$$

Then we can express the generators $\hat{G}_i$ simply as follows [recall Section 2.5]

$$G_a = q^{\dagger\alpha}(\lambda^a/2)_\alpha^\beta q_\beta. \quad (24.81)$$

It is easy to see that these operators $\hat{G}^a$ have indeed the same commutation relation as the matrices $\lambda^a/2$:

$$[\hat{G}_a, \hat{G}_b] = if_{abc}\hat{G}_c. \quad (24.82)$$

Besides these commutators, some calculations will involve the anticommutators of the λ^a -matrices. They are given by

$$\{\lambda^a, \lambda^b\} = 2d_{abc}\lambda^c + (4/3)\delta_{ab}, \quad (24.83)$$

where d_{abc} are completely symmetric in abc and have the nonzero matrix elements shown in Table 24.3.

TABLE 24.3 The symmetric couplings d_{abc} . All values not given explicitly are obtained from the total symmetry in abc .

abc	d_{abc}	abc	d_{abc}
118	$1/\sqrt{3}$	355	$1/2$
146	$1/2$	366	$-1/2$
157	$1/2$	377	$-1/2$
228	$1/\sqrt{3}$	448	$-1/2 \sqrt{3}$
247	$-1/2$	558	$-1/2 \sqrt{3}$
256	$1/2$	668	$-1/2 \sqrt{3}$
338	$1/\sqrt{3}$	778	$-1/2 \sqrt{3}$
344	$1/2$	888	$-1/\sqrt{3}$

Consider now the antiquark fields, which transform according to the representation 3^* of SU(3). Under commutation with $\hat{G}_a$, the antiquark fields behave as follows

$$-[\hat{G}_a, \bar{q}^\alpha] = -\bar{q}^\beta (\lambda^a/2)_\beta^\alpha = -(\lambda^{a*}/2)^\alpha_\beta \bar{q}^\beta. \quad (24.84)$$

The antiquark fields have the same commutation rules as the Hermitian conjugate of the quark fields, i.e., they commute like $(\bar{q}^\dagger)_\alpha \equiv (\bar{q}^\alpha)^\dagger$:

$$[\bar{q}^\beta, \bar{q}^\dagger_\alpha] = \delta^\beta_\alpha. \quad (24.85)$$

Thus, the generators of SU(3) have, for quark and antiquark fields, the operator representation:

$$\hat{G}_a = q^\dagger (\lambda^a/2) q - \bar{q}^\dagger (\lambda^{a*}/2) \bar{q}. \quad (24.86)$$

The generator of the third component of isospin is

$$\begin{aligned} \hat{I}_3 = \hat{G}_3 &= q^\dagger (\lambda^3/2) q - \bar{q}^\dagger (\lambda^3/2) \bar{q} \\ &= \frac{1}{2} (u^\dagger u - d^\dagger d) - \frac{1}{2} (\bar{u}^\dagger \bar{u} - \bar{d}^\dagger \bar{d}). \end{aligned} \quad (24.87)$$

Similarly, the hypercharge is given by

$$\begin{aligned} \hat{Y} &= \frac{2}{\sqrt{3}} \hat{G}_8 = \frac{2}{\sqrt{3}} [q^\dagger (\lambda^8/2) q - \bar{q}^\dagger (\lambda^8/2) \bar{q}] \\ &= \frac{1}{3} [(u^\dagger u + d^\dagger d - 2s^\dagger s) - (\bar{u}^\dagger \bar{u} + \bar{d}^\dagger \bar{d} - 2\bar{s}^\dagger \bar{s})], \end{aligned} \quad (24.88)$$

and the charge by

$$\begin{aligned} \hat{Q} &= Y/2 + I_3 \\ &= \frac{1}{3} [(2u^\dagger u - d^\dagger d - s^\dagger s) - (2\bar{u}^\dagger \bar{u} - \bar{d}^\dagger \bar{d} - \bar{s}^\dagger \bar{s})]. \end{aligned} \quad (24.89)$$

The raising and lowering of the third component is done with the operators

$$\begin{aligned}\hat{I}_{\pm} &= \frac{1}{2} \left[q^{\dagger} \lambda^{1 \pm i 2} q - \bar{q}^{\dagger} (\lambda^{1 \pm i 2})^* \bar{q} \right] \\ &= \begin{Bmatrix} u^{\dagger} d & - & \bar{d}^{\dagger} \bar{u} \\ d^{\dagger} u & - & \bar{u}^{\dagger} \bar{d} \end{Bmatrix},\end{aligned}\quad (24.90)$$

where $\lambda^{1 \pm i 2}$ is a short notation for $\lambda^1 \pm i \lambda^2$. A pair of operators which raise and lower the hypercharge by a unit (thereby also raising and lowering I_3 by half a unit) is¹

$$\begin{aligned}\hat{V}_{\pm} &= \frac{1}{2} \left[q^{\dagger} \lambda^{4 \pm i 5} q - \bar{q}^{\dagger} (\lambda^{4 \pm i 5})^* \bar{q} \right] \\ &= \begin{Bmatrix} u^{\dagger} s & - & \bar{u}^{\dagger} \bar{s} \\ s^{\dagger} u & - & \bar{s}^{\dagger} \bar{u} \end{Bmatrix}.\end{aligned}\quad (24.91)$$

The effect of these operators on the quark and antiquark states $|q_{\alpha}\rangle$ (created by the operators $(q^{\dagger})^{\alpha}$ when acting on the vacuum $|0\rangle$) is illustrated in Fig. 24.10 [this being the analog to the illustration in Fig. 4.3]. Note that there exists a related pair

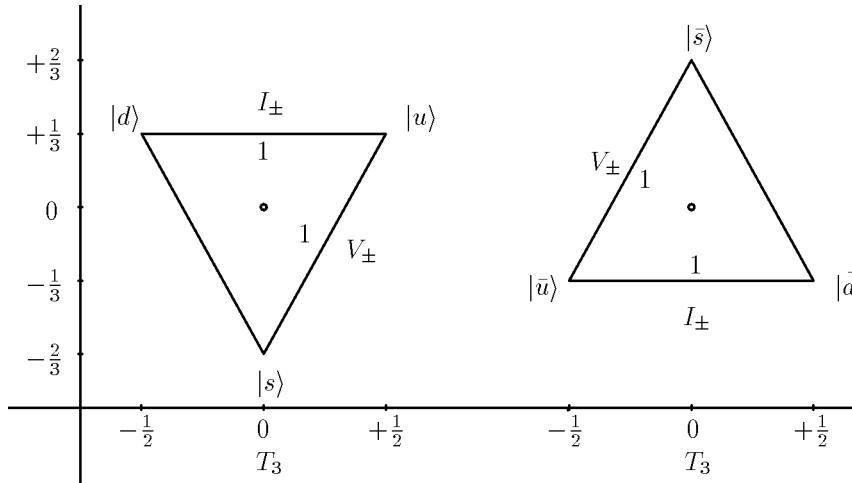


FIGURE 24.10 Effect of raising and lowering operators on quark and antiquark states. Here and in the subsequent weight diagrams the ket symbols of the states are omitted.

of operators which raise and lower hypercharge by a unit while acting oppositely to $V_{\pm}$ in the isospin:

$$\begin{aligned}\hat{U}_{\pm} &= \frac{1}{2} \left[q^{\dagger} \lambda^{6 \pm i 7} q - \bar{q}^{\dagger} (\lambda^{6 \pm i 7})^* \bar{q} \right] \\ &= \begin{Bmatrix} d^{\dagger} s & - & \bar{d}^{\dagger} \bar{s} \\ s^{\dagger} d & - & \bar{s}^{\dagger} \bar{d} \end{Bmatrix}.\end{aligned}\quad (24.92)$$

¹Note that there exists a third component to the two operators $V_{\pm}$, namely $V_3 = \frac{1}{2}(u^{\dagger}u - s^{\dagger}s) - \frac{1}{2}(\bar{u}^{\dagger}\bar{u} - \bar{s}^{\dagger}\bar{s})$, which commutes with $V_{\pm}$ in the same way as the isospin operators. The three operators form the so-called V -spin subgroup of $SU(3)$. A similar set of commutation rules holds for the $U_{\pm}$ operators of (24.92) and $U_3 = \frac{1}{2}(d^{\dagger}d - s^{\dagger}s) - \frac{1}{2}(\bar{d}^{\dagger}\bar{d} - \bar{s}^{\dagger}\bar{s})$.

These, however, will play no role in the future discussion.

Consider now the composite states associated with the product representation $3 \times \bar{3}$ of a quark and an antiquark assigned to the pseudoscalar mesons in (24.69). The quantum numbers I_3 and Y are additive so that the quantum numbers of the meson octet can be found by vector addition, i.e. by placing the $\bar{3}$ diagram with the (I_3, Y) origin once on each state of the 3 diagram and by adding up the vectors as shown in Fig. 24.11. In the theory of group representations the vectors $|I_3, Y\rangle$ of quarks and antiquarks are referred to as the *fundamental weights*. Using the

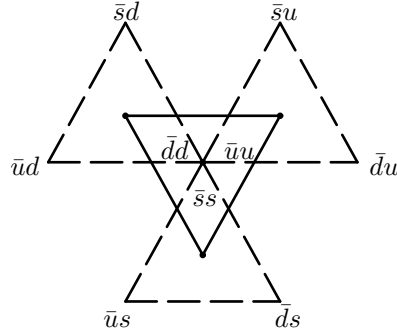


FIGURE 24.11 Addition of the fundamental weights in product representation space of 3 and $\bar{3}$ vectors.

raising and lowering operators $I_{\pm}, V_{\pm}$, it is easy to find all states of an irreducible representation starting out from any fixed state. For instance, the operator $\hat{I}_+$ acts upon the particle state $|\pi^-\rangle = |d\bar{u}\rangle$ as follows:

$$\hat{I}_+|\pi^-\rangle = |\bar{u}u - \bar{d}d\rangle \equiv \sqrt{2}|\pi^0\rangle, \quad (24.93)$$

whereas

$$\hat{I}_+|\pi^0\rangle = -\sqrt{2}|\bar{d}u\rangle \equiv -\sqrt{2}|\pi^+\rangle. \quad (24.94)$$

Similarly, the application of V_+ to $|\pi^-\rangle = |\bar{u}d\rangle$ yields

$$\hat{V}_+|\pi^-\rangle = -|\bar{s}d\rangle = -|K^0\rangle, \quad (24.95)$$

whereas applying $\hat{V}_+$ to $|\bar{K}^0\rangle$ we find

$$\hat{V}_+|\bar{K}^0\rangle = |\bar{u}u - \bar{s}s\rangle. \quad (24.96)$$

This state has the same (I_3, Y) -quantum numbers as $|\pi^0\rangle$, but it is not an eigenstate of total isospin I^2 . Such a state is given by

$$|\eta\rangle = \sqrt{\frac{1}{6}}|\bar{u}u + \bar{d}d - 2\bar{s}s\rangle, \quad (24.97)$$

so that $\hat{V}_+|\bar{K}^0\rangle$ can be decomposed into a π^0 - and an η -state as follows:

$$\begin{aligned}\hat{V}_+|\bar{K}^0\rangle &= \frac{1}{2}|\bar{u}u - \bar{d}d\rangle + \frac{1}{2}|\bar{u}u + \bar{d}d - 2\bar{s}s\rangle \\ &= \sqrt{\frac{1}{2}}|\pi^0\rangle + \sqrt{\frac{3}{2}}|\eta\rangle.\end{aligned}\quad (24.98)$$

It has become customary (de Swart-convention²) to change the phases to the $\bar{q}$ -states so that the matrix elements of $I_\pm$ and $V_\pm$ are all positive. This is achieved by changing the phases of the states of the representation 3^* as shown in Fig. 24.12. For

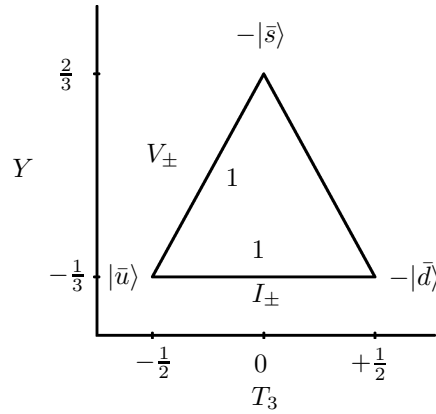


FIGURE 24.12 States of the $\bar{3}$ -representation with phases in the de Swart-convention.

the $SU(3)$ -representation matrices U^* , these phase-changes on the states correspond to a similarity transformation. The new matrices will be denoted by $\bar{U}$:

$$U^* \rightarrow \bar{U}. \quad (24.99)$$

Correspondingly, we shall say that the antiquark fields $\bar{q}$, after the appropriate phase changes, transform according to the $\bar{3}$ -representation.

The phases of all higher representations are adjusted accordingly. The meson octet states associated with the product of 3 and $\bar{3}$ -states are shown in Fig. 24.13. As a check we calculate a couple of phases:

$$\begin{aligned}\hat{V}_+|\pi^0\rangle &= \hat{V}_+\sqrt{\frac{1}{2}}|\bar{u}u - \bar{d}d\rangle \\ &= -\sqrt{\frac{1}{2}}|\bar{s}s\rangle = \sqrt{\frac{1}{2}}|K^+\rangle\end{aligned}\quad (24.100)$$

and

$$\hat{V}_+|\bar{K}^0\rangle = \hat{V}_+|-\bar{d}s\rangle = -|\bar{d}u\rangle = |\pi^+\rangle, \quad (24.101)$$

²J.J. de Swart, Rev. Mod. Phys. 35, 916 (1963).

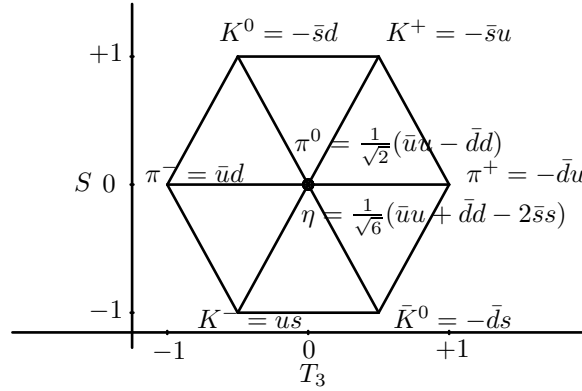


FIGURE 24.13 Quark-antiquark content of the meson octet states with phases in the de Swart-convention.

which are indeed positive.

Note that these quark-antiquark states can also be obtained by forming certain combinations of λ^a -matrices and sandwiching them between the creation operator parts of the quark and antiquark fields

$$q^{\dagger\alpha} = (u^{\dagger}, d^{\dagger}, s^{\dagger}), \quad (\bar{q}^{\dagger})_{\alpha} = (\bar{u}^{\dagger}, \bar{d}^{\dagger}, \bar{s}^{\dagger}), \quad (24.102)$$

and applying them to the vacuum. The creation operators of the meson octet states are

$$M_a^{\dagger} = q^{\dagger}(\lambda^a/\sqrt{2})\bar{q}^{\dagger}, \quad (24.103)$$

with the combinations indicated in Fig. 24.14. These combinations of λ^a indices are often used to specify octet states instead of the quark content. Any Hermitian octet operator $\hat{O}_a$ (for instance $\hat{G}_a$ itself and $M_a^{\dagger}$) with the indices $-(1+i2)/\sqrt{2}$ adds to a given state the quantum numbers of a π^+ . Let us verify the de Swart-phases of the assignments in Fig. 24.14 by applying $\hat{I}_{\pm}, \hat{V}_{\pm}$ to the meson states $|M_a\rangle = M_a^{\dagger}|0\rangle$ with the above index combinations. Using the commutation rules

$$[\hat{G}_a, M_b^{\dagger}] = if_{abc}M_c^{\dagger} \quad (24.104)$$

we have, for example,

$$\begin{aligned} [I_+, M_{\pi^-}^{\dagger}] &= \sqrt{2}f_{123}M_3^{\dagger} = \sqrt{2}M_{\pi^0}^{\dagger}, \\ [I_+, M_{\pi^0}^{\dagger}] &= if_{123}(-M_2^{\dagger} + iM_1^{\dagger}) = -\sqrt{2}M_{\pi^+}^{\dagger}, \\ [I_+, M_{K^0}^{\dagger}] &= (f_{174}M_4^{\dagger} - f_{165}M_5^{\dagger}) = M_{K^+}^{\dagger}. \end{aligned} \quad (24.105)$$

There is another simple way of constructing an octet representation of SU(3) from quark states without the use of antiquarks. By applying the product of three fields $q_{\alpha}^{\dagger}q_{\beta}^{\dagger}q_{\gamma}^{\dagger}$ at three different places³ to the vacuum one obtains 27-states. If these

³This assumption of different places is necessary to distinguish all 27-states, for otherwise some states will coincide due to particle identity.

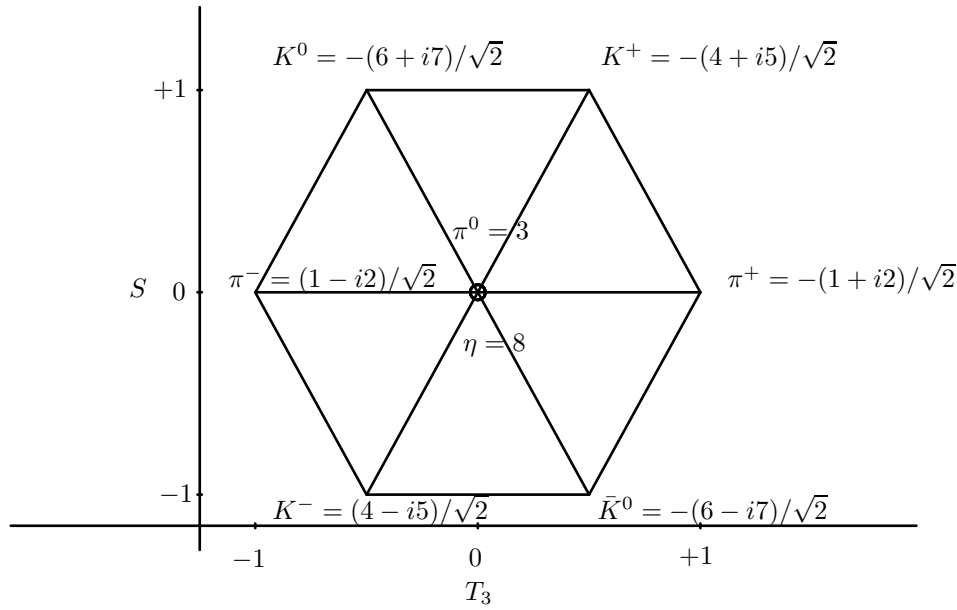


FIGURE 24.14 Combination of indices a in the pseudoscalar octet field $M_a^\dagger$ of (24.103). Here $-(1 \pm i2)/\sqrt{2}$ stands for $-(M_1^\dagger \pm iM_2^\dagger)/\sqrt{2}$.

are decomposed into the irreducible contents of $SU(3)$, they lead to the following multiplets

$$3 \times 3 \times 3 = 10 + 8 + 8 + 1. \quad (24.106)$$

The octet states can be identified with the nucleon octet states. In the decuplet there are doubly charged non-strange states which can be identified with the $I_3 = 3/2$ component of the first nucleon resonance $\Delta(1236)$. It is therefore suggestive to identify the other 10-states with the strange partners of this resonance. At the time when Gell-Mann proposed this identification, he could only match 9 of the decuplet states with known particles and resonances. There was one more state of strangeness 3 (at the bottom of the weight diagram to be constructed in Fig. 24.17) which closes it to a triangle. Since the masses within the two rows are almost degenerate and since they grow from row to row by about the same amount

$$\begin{aligned} m_\Delta - m_{\Sigma^*} &\approx -150, \\ m_{\Sigma^*} - m_{\Xi^*} &\approx -145, \end{aligned}$$

with the masses given in units MeV, Gell-Mann extrapolated the mass of the tenth particle to be

$$\begin{aligned} M &\approx M_\Delta + 3(M_{\Sigma^*} - M_\Delta) \\ &\approx 1232 + 3 \cdot 1567 \approx 1682. \end{aligned} \quad (24.107)$$

He therefore postulated the existence of a particle with this mass, a negative charge, and a hypercharge -2 as it resulted from the three quark content of the states. He

called this particle Ω^- . It was indeed found in 1964 at a mass of 1675 ± 8 Mev. This was celebrated as a triumph of the approximate SU(3)-symmetry hypothesis and the 10-assignment of the excited nucleons and their strange partners.

Let us explicitly construct the irreducible representations contained in the product $3 \times 3 \times 3$ and assign them to physical states. We perform the multiplication successively

$$3 \times 3 \times 3 = 3 \times (3 \times 3). \quad (24.108)$$

The product of two states 3×3 is easily reduced to

$$3 \times 3 = 6 + \bar{3}. \quad (24.109)$$

To see this we write down the symmetric and antisymmetric combinations as shown in Fig. 24.15. The first is a 6-representation, the second transforms in the same way

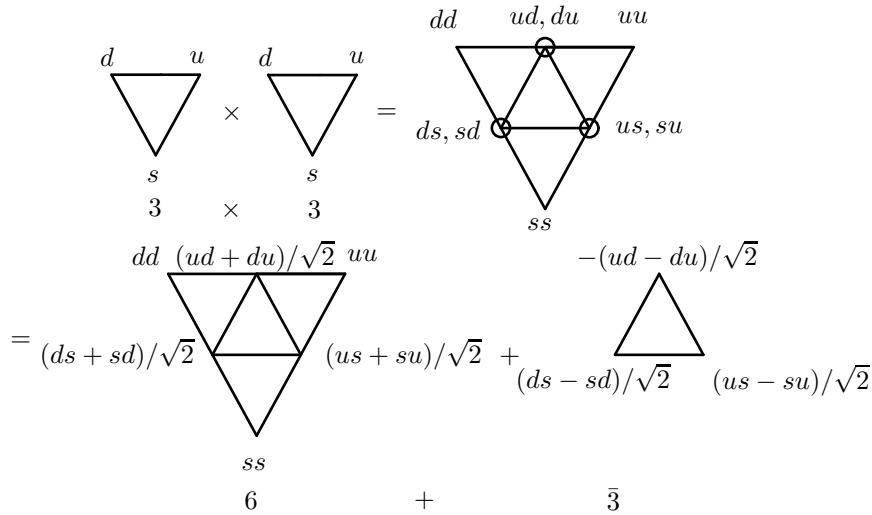


FIGURE 24.15 Quark content in the reduction of the product $3 \times 3 = 6 + \bar{3}$.

as an antiquark representation $\bar{3}$. As before we have assigned the phases to satisfy the de Swart-convention. After forming these products we continue the multiplication:

$$3 \times 3 \times 3 = 3 \times (6 + \bar{3}) = 3 \times 6 + 3 \times \bar{3}. \quad (24.110)$$

Let us now form 3×6 and $3 \times \bar{3}$. The product $3 \times \bar{3}$ has been calculated before in terms of quark-antiquark states:

$$3 \times \bar{3} = 8 + 1. \quad (24.111)$$

Now the octet states contain three quarks, as shown in Fig. 24.16. The octet states can be identified with the nucleons and their strange partners.

$$\begin{array}{ccc}
\begin{array}{c} d \quad u \\ \triangle \\ s \end{array} & \times & \begin{array}{c} -(ud - du)/\sqrt{2} \\ \triangle \\ (ds - sd)/\sqrt{2} \quad (us - su)/\sqrt{2} \end{array} \\
3 & \times & \bar{3} \\
\\
= \begin{array}{c} -d(ud - du)/\sqrt{2} \\ d(ds - sd)/\sqrt{2} \\ s(ds - sd)/\sqrt{2} \end{array} \begin{array}{c} \triangle \\ \triangle \\ \triangle \\ \triangle \\ \triangle \\ \triangle \end{array} \begin{array}{c} -u(ud - du)/\sqrt{2} \\ u(us - su)/\sqrt{2} \\ s(us - su)/\sqrt{2} \end{array} + \frac{1}{\sqrt{6}} \begin{pmatrix} +uds \\ -usd \\ +dsu \\ -dus \\ +sud \\ -sdu \end{pmatrix} \\
8 & + & 1
\end{array}$$

FIGURE 24.16 Octet and singlet states obtained from $3 \times \bar{3}$ in the product space of three-quarks.

The completely antisymmetric combination of uds -states is a singlet state under $SU(3)$ -transformations:

$$|\Lambda\rangle = \frac{1}{\sqrt{3!}}(|uds\rangle + |dsu\rangle + |sud\rangle + |dus\rangle + |sdu\rangle + |usd\rangle). \quad (24.112)$$

The proton state is

$$|p\rangle = \frac{1}{\sqrt{2}}|u(ud - du)\rangle. \quad (24.113)$$

The state $|\Sigma^0\rangle$ in the octet is found by applying $\hat{I}_-$ to the right most state $|\Sigma^+\rangle = -|u(us - su)\rangle$, thereby obtaining

$$|\Sigma^0\rangle = -\frac{1}{2}|d(us - su) + u(ds - sd)\rangle. \quad (24.114)$$

The isosinglet state $|\Lambda^0\rangle$ is obtained by applying $\hat{V}^-$ to $|p\rangle = |u(ud - du)\rangle/\sqrt{2}$ and by separating the result into a linear combination of $|\Sigma^0\rangle$ and an orthogonal state, which must be $|\Lambda^0\rangle$. First we have

$$\hat{V}^-|p\rangle = \sqrt{2}\frac{1}{2}|sud + usd - sdu - uds\rangle. \quad (24.115)$$

The scalar product with $|\Sigma^0\rangle$ gives

$$\langle\Sigma^0|\hat{V}^-|p\rangle = \frac{1}{\sqrt{2}}. \quad (24.116)$$

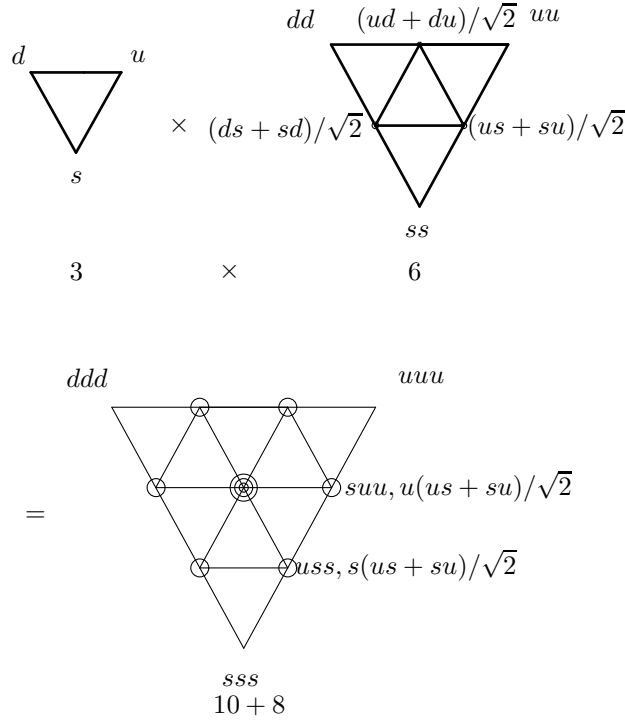


FIGURE 24.17 Irreducible three-quark states 10 and 8 in the product 3×6 (the symbol $(\dots)_s$ denotes complete symmetrization).

Hence we rewrite

$$V^-|p\rangle = \sqrt{2} \left(\frac{1}{2}|\Sigma^0\rangle + \frac{\sqrt{3}}{2}|\Lambda^0\rangle \right) \quad (24.117)$$

and identify

$$|\Lambda^0\rangle \equiv -\sqrt{1/12} |u(ds - sd) - d(us - su) - 2s(ud - du)\rangle. \quad (24.118)$$

Consider now the product 3×6 . It gives the states shown in Fig. 24.17. The state $|uuu\rangle$ is identified with the 1232 MeV resonance $\Delta^{++}(1232)$ of isospin and parity $3/2^+$. By applying the operators $I_\pm$ and $V_\pm$ to $|uuu\rangle$ we find the ten decuplet states

$$\begin{aligned}
|\Delta^{++}\rangle &= |uuu\rangle, \\
|\Delta^+\rangle &= \sqrt{\frac{1}{3}} |uud + udu + duu\rangle, \\
|\Delta^0\rangle &= \sqrt{\frac{1}{3}} |udd + dud + udd\rangle, \\
|\Delta^-\rangle &= |ddd\rangle, \\
|\Sigma^+\rangle &= \sqrt{\frac{1}{3}} |uus + usu + suu\rangle, \\
|\Sigma^0\rangle &= \sqrt{\frac{1}{6}} |uds + usd + dsu + dus + sud + sdu\rangle, \\
|\Sigma^-\rangle &= \sqrt{\frac{1}{3}} |dds + dsd + sdd\rangle, \\
|\Xi^0\rangle &= \sqrt{\frac{1}{3}} |uss + sus + ssu\rangle, \\
|\Xi^-\rangle &= \sqrt{\frac{1}{6}} |dss + sds + ssd\rangle, \\
|\Omega^-\rangle &= |sss\rangle
\end{aligned} \quad (24.119)$$

In addition to this decuplet, there is a further octet of particle states which can alternatively be assigned to the nucleon octet. Its quark states are found by constructing one state, say the proton, and applying the operators $I_{\pm}, V_{\pm}$ to it. The proton state is found by linearly composing $|uud\rangle$ and $|u(ud + du)\rangle/\sqrt{2}$ so that the result is orthogonal to $|\Delta^+\rangle$ in (24.119) and to $|p\rangle$ of (24.113):

$$|p'\rangle = \sqrt{\frac{1}{6}}|u(ud + du) - 2duu\rangle. \quad (24.120)$$

The prime in $|p'\rangle$ indicates that the quark wave function differs from (24.113). All other octet states associated with $|p'\rangle$ are then obtained by applying $I_{\pm}, V_{\pm}$ to $|p'\rangle$, for instance

$$|n'\rangle = \hat{I}_-|p'\rangle = -\sqrt{\frac{1}{6}}|d(ud + du) - 2udd\rangle. \quad (24.121)$$

As a first test of the octet assignment we calculate the mass differences within the nucleon octet assuming that the mass operator transforms like an SU(3) singlet, plus a term which behaves like a neutral isosinglet member of an octet, i.e., like η . Fortunately, the Clebsch-Gordan coefficients for the matrix elements

$$\langle 8_a | 8_b | 8_c \rangle \quad (24.122)$$

are already in our position. They are of two types, related to the traces $\text{tr}([\lambda^a, \lambda^b]\lambda^c) = f_{abc}$ and $\text{tr}(\{\lambda^a \lambda^b\}\lambda^c) = d_{abc}$. The first is antisymmetric, the second symmetric in abc . We therefore expand

$$\langle 8_a | 8_b | 8_c \rangle = F f_{abc} + D d_{abc}, \quad (24.123)$$

where F and D are two unknown irreducible matrix elements. To relate these to particles, we only have to multiply them with the SU(3)-polarization vectors $\epsilon_a(m)$ of the particles whose assignments are clear from Fig. (24.14). For instance

$$\epsilon_a(\pi^+) = -\frac{1}{\sqrt{2}}(1, i, 0, 0, 0, 0, 0, 0). \quad (24.124)$$

Then we have between octet states:

$$\langle 8m_2 | 8m | 8m_1 \rangle = \epsilon_a^*(m_2) \epsilon_b^*(m) (F f_{abc} + D d_{abc}) \epsilon_c(m_1). \quad (24.125)$$

We may also write

$$\langle 8m_2 | 8m | 8m_1 \rangle = F f_{m_2^* m^* m_1} + D d_{m_2^* m^* m_1}, \quad (24.126)$$

with obvious notation. The matrix associated with the $b = 8 \hat{=} \eta$ component is assumed to explain three mass differences. Two of them may be used to determine the two irreducible matrix elements F and D . The symmetry breaking will then allows us to derive one relation between the masses. Using the values of f_{abc} and

d_{abc} with $b = 8$ from Table 24.3, we have for the differences of the masses from some common SU(3) singlet mass m_{sg} :

$$\begin{aligned}\Delta m_N &= \langle p | 8_\eta | p \rangle = F f_{485} + D d_{484} = F\sqrt{3}/2 - D/2\sqrt{3}, \\ \Delta m_\Sigma &= \langle \Sigma^+ | 8_\eta | \Sigma^+ \rangle = D d_{181} = D/\sqrt{3}, \\ \Delta m_\Lambda &= \langle \Lambda^0 | 8_\eta | \Lambda^0 \rangle = D d_{888} = -D/\sqrt{3}, \\ \Delta m_\Xi &= \langle \Xi^0 | 8_\eta | \Xi^0 \rangle = F f_{687} + D d_{686} = -F\sqrt{3}/2 - D/2\sqrt{3}.\end{aligned}\quad (24.127)$$

Using these equations we readily find that the common singlet mass is

$$m_{\text{sg}} = \frac{1}{2}(m_\Sigma + m_\Lambda) = \frac{1}{2}(m_N + m_\Xi) + \frac{1}{4}(m_\Sigma - m_\Lambda), \quad (24.128)$$

so that the masses have to satisfy the famous Gell-Mann–Okubo relation

$$\frac{1}{2}(m_N + m_\Xi) = \frac{1}{4}(3m_\Lambda + m_\Sigma). \quad (24.129)$$

It holds reasonably well, the left-hand side being approximately equal to 1.128 GeV, the right-hand side equal to 1.134 GeV.

For the decuplet, the same ansatz reproduces the equal mass splittings between the rows that had led Gell-Mann to his prediction of the Ω -meson.

For the pseudoscalar meson octet the relative mass splitting is very large and the mass relation cannot be expected to be as good as for the baryon octet. If we use, however, the square masses, it is nevertheless in surprisingly good agreement with experiment:

$$m_K^2 = \frac{1}{4}(3m_\eta^2 + m_\pi^2). \quad (24.130)$$

The left-hand side is equal to 0.25 GeV², the right-hand side to 0.23 GeV². An argument for using square-masses is that, in contrast to the fermion Lagrangian, the boson Lagrangian has a mass term proportional to m^2 .

The vector meson octet has a smaller relative mass splitting and the mass relation should be good. If we insert, however, the experimental masses

$$m_{K^*}^2 = \frac{1}{4}(3m_\omega^2 + m_\rho^2), \quad (24.131)$$

there is a bad surprise: The left-hand side is equal to 0.80 GeV², considerably larger than the value 0.61 GeV² on the right hand. This disagreement can be resolved by postulating that the symmetry breaking part of the Lagrangian mixes the iso-singlet octet state with the SU(3) singlet state [5]. This is always possible with the symmetry breaking transforming like an η -meson. Specifically, if ω_0 , ϕ_0 denote the SU(3)-states, the physical particles can be

$$\begin{aligned}\omega &= \cos \theta \omega_0 - \sin \theta \phi_0, \\ \phi &= \sin \theta \omega_0 + \cos \theta \phi_0,\end{aligned}\quad (24.132)$$

with some unknown mixing angle θ . The symmetry breaking Lagrangian can contain the mass terms

$$\mathcal{L}_{\text{symm br}} = -m_8^2 \omega_0^2 - m_1^2 \phi_0^2 - m_{18}^2 \phi_0 \omega_0 + \dots, \quad (24.133)$$

with some SU(3) octet, singlet, and mixing mass parameters and the associated SU(3) fields. The octet mass parameter is determined from the Gell-Mann–Okubo relation (24.131) as

$$m_8 = 930 \text{ MeV}. \quad (24.134)$$

Between the physical states (24.132) this becomes diagonal, if the mixing angle θ is given by

$$\theta = \frac{1}{2} \arctan \frac{m_{18}^2}{m_9^2 - m_1^2}. \quad (24.135)$$

The diagonal masses are

$$m_\omega^2 = \frac{1}{2}(m_8^2 + m_1^2) - \frac{1}{2}[(m_8^2 - m_1^2)^2 - m_{18}^4], \quad (24.136)$$

$$m_\phi^2 = \frac{1}{2}(m_8^2 + m_1^2) + \frac{1}{2}[(m_8^2 - m_1^2)^2 - m_{18}^4]. \quad (24.137)$$

From the experimental numbers we determine the parameters

$$m_{18} \approx 0.65 \text{ MeV}, \quad \cos \theta \approx 0.77. \quad (24.138)$$

The mixing angle can be tested by experiment, since it determines the decay rate of the processes

$$\phi \rightarrow K^+ K^-, \quad (24.139)$$

which occurs with a width 2.2 MeV. Since the vector meson has spin 1, the pseudoscalar kaons must come out in a p -wave. Their orbital wave function is therefore antisymmetric. But for bosons the total wave function must be symmetric, which implies that the SU(3)-quantum numbers have to be coupled antisymmetrically. This, however, excludes the SU(3)-singlet part of ϕ from the decay (since its coupling would be proportional to δ_{ab} in the SU(3)-indices of the pseudoscalar mesons). The amplitude for the decay is therefore proportional to the SU(3)-Clebsch-Gordan coefficient $\cos \theta (8_{\omega_0} | 8_{K^+} | 8_{K^-}) \propto \cos \theta \langle 0, 0 | \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \rangle f_{845} = \cos \theta \times (1/\sqrt{2}) \times (\sqrt{3}/2)$. This should be compared with the decay $\rho^0 \rightarrow \pi^+ \pi^-$, whose amplitude is proportional to $(8_{\rho^0} | 8_{\pi^-} | 8_{\pi^+}) \propto \langle 1, 0 | 1, 1; 1, -1 \rangle f_{123} = (1/\sqrt{2}) \times 1$. Taking the squares, we find the ratio

$$\left| \frac{S(\phi \rightarrow K^+ K^-)}{S(\rho^0 \rightarrow \pi^+ \pi^-)} \right|^2 = \frac{3}{4} \cos^2 \theta \approx 0.44. \quad (24.140)$$

The decay rates contain a phase space factor

$$\Gamma \propto \frac{q^3}{M^2}, \quad (24.141)$$

where q is the momentum of the emerging pseudoscalar mesons, and M the mass of the decaying vector meson. In the processes at hand we have $q_K \approx 127$, $M_\phi \approx 1020$, $q_\pi \approx 359$, $M_\rho \approx 770$ MeV, so that the phase space factors are 0.0020 MeV and 0.078 MeV, respectively. Together with (24.140) this gives the ratio of decay rates

$$\left| \frac{\gamma(\phi \rightarrow K^+ K^-)}{\gamma(\rho^0 \rightarrow \pi^+ \pi^-)} \right|^2 \approx 0.011. \quad (24.142)$$

The experimental ratio is

$$\left| \frac{\gamma(\phi \rightarrow K^+ K^-)}{\gamma(\rho^0 \rightarrow \pi^+ \pi^-)} \right|_{exp}^2 \approx 0.014, \quad (24.143)$$

in reasonable agreement with SU(3)-symmetry.

For the pseudoscalar mesons the same type of mixing can occur between η - and η' - mesons. However, since their mass difference is relatively large compared to that between ω and ϕ , their mixing angle is much smaller, which explains why no mixing was needed to satisfy the Gell-Mann–Okubo relation (24.130).

As a further test of the octet assignment we may calculate branching ratios for the decay of the decuplet resonances in the nucleon and the meson octets. Also here the agreement with experimental data is reasonably good.

24.5 Newer Quarks

Particles discovered in the 1970s and the theoretical attempts to explain their interactions and decay properties suggested the existence of more quarks. They were named *charmed quark*, with the symbol c , *top quark*, with the symbol t , and *bottom quark*, with the symbol b . In Table 24.4 we have listed the masses and quantum numbers of the quarks discovered so far.

TABLE 24.4 List of Quarks and their properties taken from the Particle Data Group [11].

Quark	(I, I_3)	Charge	Strangeness	Mass (MeV)
u	$\frac{1}{2}, \frac{1}{2}$	$\frac{2}{3}$	0	$2.3_{-0.5}^{+0.7}$
d	$\frac{1}{2}, -\frac{1}{2}$	$-\frac{1}{3}$	0	$4.8_{-0.3}^{+0.5}$
s	0,0	$-\frac{1}{3}$	-1	95 ± 5
c	0,0	$\frac{2}{3}$	0	1275 ± 25
t	0,0	$\frac{2}{3}$	0	173070 ± 0.890
b	0,0	$-\frac{1}{3}$	0	4180 ± 30

It was tempting to incorporate these quarks into the above broken symmetry considerations and extend the basic quark antiquark SU(3)-multiplet by these additional quarks and antiquarks to higher multiplets, with an even larger broken symmetry group. This has led indeed to a reasonable particle classification if we add the lightest of the additional quarks, the charmed quark c , to the other three and forming a quartet u, d, s, c . This quartet can then be treated very approximately as a fundamental representation 4 of an internal symmetry group SU(4). Clearly, the corresponding antiquarks must be transformed according to the representation $\bar{4}$. The weight diagram of these representations is three-dimensional and contains an additional “charm” axis labeled by C in Fig. 24.18.

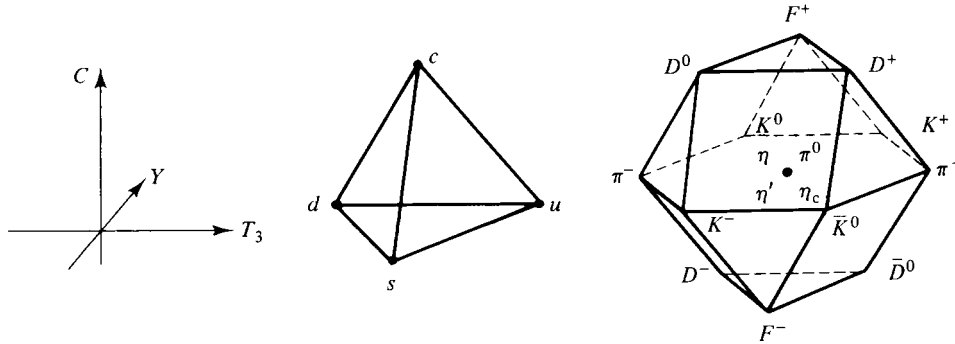


FIGURE 24.18 The four lowest quarks u, d, s, c and their position in the three-dimensional weight space with the quantum number “charm”. By combining a quark and an antiquark one finds the 16 states on the right-hand side, of which 15 form an irreducible representation of $SU(4)$. The new states D^0, D^+, F^+ and their antiparticles have been found in the laboratory.

24.6 Tensor Representations and Young Tableaux

A systematic construction of the tensor representation in direct product spaces such as $3 \times 3 \times 3$ is possible with the help of Young tableaux. The irreducible representations are obtained by forming tensors which transform irreducibly under permutations of the indices. They are of a definite symmetry type specified by the Young tableau introduced in Appendix 2A. The tableau $\begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline\end{array}$ indicates a tensor of com-

plete symmetry transforming like a 10-representation, while $\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline\end{array}$ corresponds to a

complete antisymmetric tensor transforming like an $SU(3)$ singlet. For the mixed tableau $\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline\end{array}$ we adopt the convention to first symmetrize the state $|q_\alpha q_\beta q_\gamma\rangle$ in

the first two indices, then antisymmetrize in the first and the third index. Equivalently we can use another tableau, say $\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline\end{array}$, or $\begin{array}{|c|c|} \hline 2 & 1 \\ \hline 3 & \\ \hline\end{array}$. Each gives an octet representation.

For instance, the proton wave function (24.113) arises from the symmetry operations of the Young tableau $\begin{array}{|c|c|} \hline 2 & 1 \\ \hline 3 & \\ \hline\end{array}$ applied to the state $|uud\rangle$. The symmetrization in the first two indices gives

$$|uud\rangle \rightarrow 2|uud\rangle \quad (\text{symmetry in } 21), \quad (24.144)$$

the antisymmetrization in the second and third index (of the original tensor $|q_\alpha q_\beta q_\gamma\rangle$)

$$|uud\rangle \rightarrow 2|u(ud - du)\rangle \quad (\text{antisymmetry in } 23). \quad (24.145)$$

Hence:

$$\begin{array}{|c|c|} \hline 2 & 1 \\ \hline 3 & \\ \hline\end{array} |uud\rangle = 2|u(ud - du)\rangle = 2\sqrt{2}|p\rangle. \quad (24.146)$$

Equivalent proton states could have been obtained from the tableau

$$\begin{array}{|c|} \hline 1 \\ \hline 3 \\ \hline \end{array} \begin{array}{|c|} \hline 2 \\ \hline \end{array} |uud\rangle = 2|uud - duu\rangle, \quad \begin{array}{|c|} \hline 1 \\ \hline 3 \\ \hline \end{array} \begin{array}{|c|} \hline 2 \\ \hline \end{array} |udu\rangle = 2|udu - duu\rangle, \quad (24.147)$$

or the sum of the two which gives

$$|u(ud + du) - 2duu\rangle. \quad (24.148)$$

This is once more the proton state $|p'\rangle$ of Eq. (24.120) found in the product 6×3 .

It cannot be decided by $SU(3)$ -symmetry alone, which mixture of the two independent three-quark wave functions corresponds to the proton in nature. This has to emerge from a dynamical model [6, 7]. We shall see later that the larger symmetry group $SU(6)$ makes definite predictions on this.

In general, the dimensionality of the $SU(n)$ -representation of a tableau is obtained from the following formula

$$d_{SU(n)} = \frac{D(l_1, l_2, \dots, l_n)}{D(n-1, n-2, \dots, 0)}, \quad (24.149)$$

where

$$D(x_1, \dots, x_n) \equiv \prod_{i < j} (x_i - x_j), \quad (24.150)$$

and

$$l_i \equiv n + m_i - i, \quad i = 1, 2, 3, \dots, n, \quad (24.151)$$

with m_i being the number of boxes in the i th row of the tableau. Note that also rows with no boxes have to be counted, up to $i = n$.

A useful alternative formula for the dimension is

$$d_{SU(n)} = \frac{l_1! l_2! \cdots l_n!}{0! 1! \cdots (n-1)!} \frac{1}{\prod_{i,j} h_{ij}}, \quad (24.152)$$

where h_{ij} is the sum of the number of boxes to the right of the element ij in the tableau plus the number of boxes below ij plus 1.

Take some examples. The trivial Young tableau $\square$ has $m_1 = 1, m_2 = 0, m_3 = 0, \dots, m_n = 0$ and thus $l_1 = n, l_2 = n-2, \dots, l_n = 0$. Hence

$$d \square = n. \quad (24.153)$$

The first non-trivial one $\square \square$ has $m_1 = 2, m_2 = 0, \dots, m_n = 0$ and thus $l_1 = n+1, l_2 = n-2, l_3 = n-3, \dots, l_n = 0$. Hence

$$d \square \square = n(n+1)/2, \quad (24.154)$$

which gives 6 for $SU(3)$. Further

$$d \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \end{array} = n(n-1)/2, \quad (24.155)$$

which gives 3 for $SU(3)$, the dimension of the representation $\bar{3}$. For 3-quark states, the dimensions are

$$d \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} = n(n+1)(n+2)/6, \quad (24.156)$$

$$d \begin{array}{|c|c|} \hline \square & \square \\ \hline \square \\ \hline \end{array} = (n-1)n(n+1)/3, \quad (24.157)$$

$$d \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = n(n-1)(n-2)/6, \quad (24.158)$$

which take the values 10, 8, 1, respectively, for $SU(3)$. Somewhat more generally, the dimensions of some simple tableaux are

$$d \begin{array}{|c|c|c| \dots |c|} \hline 1 & 2 & 3 & \dots & k \\ \hline \end{array} = \binom{n+k-1}{k}, \quad (24.159)$$

$$d \begin{array}{|c|c|c| \dots |c|} \hline 1 & 2 & 3 & \dots & k \\ \hline \square \\ \hline \end{array} = \binom{n+k-1}{k+1} k, \quad (24.160)$$

$$d \begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline \vdots \\ \hline k \\ \hline \end{array} = \binom{n}{k}. \quad (24.161)$$

A column with n boxes is completely antisymmetric in the corresponding indices and thus proportional to the invariant antisymmetric tensor $\epsilon_{i_1 i_2, \dots, i_n}$. This is why its dimensionality is 1. In constructing all Young tableaux any such column can be omitted. For instance, in $SU(3)$,

$$\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & & \end{array} = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array}. \quad (24.162)$$

One often indicates this cancellation by crossing out any complete column with a vertical line:

$$\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & & \end{array} \rightarrow \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \end{array}. \quad (24.163)$$

The representation associated with each Young tableaux occurs as often as dimensionality of the associated representation of the permutation group. This follows

from the fact that the representation matrices of the permutation group commute with those of $SU(3)$. They can therefore be brought simultaneously to a block form

$$\begin{pmatrix} \boxed{D_1} & & & \\ & \boxed{D_1} & & \\ & & \boxed{D_2} & \\ & & & \ddots \end{pmatrix}. \quad (24.164)$$

Along the diagonal there are n_i identical irreducible representation blocks D_i of dimensionality d_i , etc. Now, according to Schur's lemma, any matrix commuting with such a block matrix must be itself a block matrix with the dual form, that consists of d_i identical blocks of dimensionality n_i . The formulas for the dimensionality of the irreducible representations of the permutation group were given in App. 2A. If the Young tableau has r boxes, the dimensionality is given by

$$d_{S_r} = \frac{r!}{\prod_{ij} h_{ij}}, \quad (24.165)$$

where the numbers h_{ij} are the same as in (24.149).

Using this formula we find, for instance, that the product of three-quark states

$\square \times \square \times \square$ decompose into *one* $SU(3)$ decuplet $\square\square\square$, *two* octets $\begin{smallmatrix} \square & \square \\ & \square \end{smallmatrix}$,

and *one* singlet $\begin{smallmatrix} \square \\ \square \\ \square \end{smallmatrix}$:

$$3 \times 3 \times 3 = 10 + 8 + 8 + 1. \quad (24.166)$$

The Young tableau can also be used to find the irreducible contents in a product of two or more irreducible representations. For instance, suppose we want to know

the irreducible contents of 8×8 . We take the two Young tableaux $\begin{smallmatrix} \square & \square \\ & \square \end{smallmatrix} \times \begin{smallmatrix} \square & \square \\ & \square \end{smallmatrix}$

and distinguish the rows of boxes in the second factor by $a, b, c, \dots$, in the example

$$\begin{smallmatrix} \boxed{a} & \boxed{a} \\ \boxed{b} \end{smallmatrix}.$$

Then we add the lettered boxes to the first tableau in the following way:

- add all a 's in such a way that one obtains all proper tableaux (i.e., with $m_{i+1} \geq m_i$) which have no more than one a in each column;
- add the b 's, following the same rule;
- add the c 's, following the same rule.

In our example we thus obtain the expansion

$$\begin{array}{c}
 \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} \times \begin{array}{|c|c|} \hline a & a \\ \hline b & \\ \hline \end{array} = \begin{array}{|c|c|c|c|} \hline \square & \square & a & a \\ \hline \square & b & & \\ \hline \end{array} + \begin{array}{|c|c|c|c|} \hline \square & \square & a & a \\ \hline \square & \phi & & \\ \hline \end{array} \\
 8 \times 8 \qquad \qquad \qquad 27 \qquad \qquad \qquad 10 \\
 \\
 + \begin{array}{|c|c|c|} \hline \square & \square & a \\ \hline \square & a & b \\ \hline \end{array} + \begin{array}{|c|c|c|} \hline \square & \square & a \\ \hline \square & a & \\ \hline \phi & & \\ \hline \end{array} \\
 \qquad \qquad \qquad \overline{10} \qquad \qquad \qquad 8 \\
 \\
 + \begin{array}{|c|c|c|} \hline \square & \square & a \\ \hline \square & b & \\ \hline a & & \\ \hline \end{array} + \begin{array}{|c|c|c|} \hline \square & \square & \\ \hline \square & a & \\ \hline a & b & \\ \hline \end{array} \\
 \qquad \qquad \qquad 8 \qquad \qquad \qquad 1
 \end{array} \tag{24.167}$$

In accordance with the rule given earlier we have dropped all complete columns. Note that due to the antisymmetry of any complete column, an *incomplete* column is equivalent to the complex conjugate representation, i.e., a tableau that would be obtained from the missing boxes necessary to complete it (indicated by a box with a circle), for instance

$$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \circ \\ \hline \end{array} = \begin{array}{|c|} \hline \circ \\ \hline \circ \\ \hline \square \\ \hline \end{array} . \tag{24.168}$$

This is how we can see immediately that the representation associated with the tableau $\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \end{array}$ is a $\overline{10}$

$$\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \circ & \circ & \circ \\ \hline \end{array} = \begin{array}{|c|c|c|} \hline \circ & \circ & \circ \\ \hline \circ & \circ & \circ \\ \hline \square & \square & \square \\ \hline \end{array} . \tag{24.169}$$

The octet representation, being the adjoint representation of SU(3) is real [its generators are $(G_a)_{bc} = -if_{abc}$ with real antisymmetric matrices $(f_a)_{bc}$; recall (4.83)].

From the Young tableau of the octet $\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array}$ this is obvious since the missing boxes

in $\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \circ \\ \hline \circ & \circ \\ \hline \end{array}$ form once more the same tableau $\begin{array}{|c|c|} \hline \circ & \circ \\ \hline \circ & \square \\ \hline \end{array}$, so the representation is equal to the complex conjugate of itself and thus real.

24.7 Effective Interactions among Hadrons

There exists a great variety of strongly interacting particles with many possible interactions between them. Let us study a few of them.

24.7.1 The Pion-Nucleon Interaction

The most important strong interaction is the one between pions and nucleons since it gives rise to the dominant part of the forces which keep the nuclei together. If we neglect electromagnetic interactions, this interaction exhibits isospin symmetry of pions and nucleons, so that a system of fields π_a and N has the following effective action

$$\mathcal{A} = \mathcal{A}_\pi + \mathcal{A}_N + \mathcal{A}_{\pi NN}, \quad (24.170)$$

with

$$\mathcal{A}_\pi = \int d^4x \frac{1}{2} \{ [\partial \pi_a(x)]^2 - m_\pi^2 \pi_a^2(x) \}, \quad (24.171)$$

$$\mathcal{A}_N = \int d^4x \bar{N}(x) (i \not{\partial} - M_N) N(x), \quad (24.172)$$

$$\mathcal{A}_{\pi NN} = g_{\pi NN} \int d^4x \bar{N}(x) i \gamma_5 \tau^a N(x) \pi_a(x). \quad (24.173)$$

Here $\pi_a(x)$ is an isovector field and $N(x)$ a Dirac spinor field with an additional isospinor index, which is not explicitly written down. The matrices τ^a are 2×2 Pauli matrices acting on the isospinor indices of $N(x)$. Studies of pion nucleon scattering amplitudes determine the size of the pseudoscalar coupling constant $g_{\pi NN}$ to be

$$\frac{g_{\pi NN}^2}{4\pi} \approx 14.4 \pm .4. \quad (24.174)$$

In some analyses, the pion nucleon interaction (24.173) is parametrized in the axial vector form

$$\mathcal{A}_{\pi NN} = \frac{f_{\pi NN}}{M_\pi} \int d^4x \bar{N}(x) \gamma^\mu \gamma_5 \tau^a N(x) \partial_\mu \pi_a. \quad (24.175)$$

For physical nucleons on the mass shell, the two interactions are the same with a relation between the two coupling constants

$$f_{\pi NN} = -\frac{M_\pi}{2M_N} g. \quad (24.176)$$

Thus

$$f_{\pi NN}^2 = 0.081 \pm 0.002. \quad (24.177)$$

In either form, the coupling strength is too large to perform perturbative calculations with the interaction $\mathcal{A}_{\pi NN}$.

It is useful to find the SU(3)-symmetric extension of the pion nucleon interaction. In SU(3), there are two ways of coupling three octets with each other, an antisymmetric one f_{ijk} and a symmetric one, d_{ijk} . The easiest way to do the calculation is by writing the nucleon octet as a 3×3 -matrix.

$$B = \begin{pmatrix} \frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda^0 & \Sigma^+ & p \\ \Sigma^- & -\frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda^0 & n \\ -\Xi^- & \Xi^0 & -\frac{2}{\sqrt{6}}\Lambda^0 \end{pmatrix}, \quad (24.178)$$

and the pseudoscalar octet as

$$P = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta^0 & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta^0 & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta^0 \end{pmatrix}. \quad (24.179)$$

In this context the phases of $\pi^\pm$ are chosen as $\pi^\pm \equiv (\pi_1 \pm i\pi_2)/\sqrt{2}$ so that P is a Hermitian matrix. Then the interaction Lagrangian has a simple explicit form

$$\mathcal{L}_{\text{PBB}} = g \frac{F}{F+D} \text{tr}([\bar{B}, B]P) + g \frac{D}{F+D} \text{tr}(\{\bar{B}, B\}P), \quad (24.180)$$

where $g \equiv g_{\pi NN}$ is the pion nucleon coupling constant and F/D the so-called “ F -over- D -ratio”, which gives the relative strength of antisymmetric and symmetric coupling. Working out the different components, this yields the expansion in terms of isospinors

$$\begin{aligned} \mathcal{L}_{\text{int}} = & g \left\{ (\bar{N}\boldsymbol{\tau}N) \cdot \boldsymbol{\pi} + (1-2\alpha)(\bar{\Xi}\boldsymbol{\tau}\Xi) \cdot \boldsymbol{\pi} + \frac{3-4\alpha}{\sqrt{3}}\bar{N}N\eta^0 \right. \\ & - \frac{3-2\alpha}{\sqrt{3}}\bar{\Xi}\Xi\eta^0 - (1-2\alpha)(\bar{N}\boldsymbol{\tau}K) \cdot \boldsymbol{\Sigma} - (\bar{\Xi}\boldsymbol{\tau}K^c) \cdot \boldsymbol{\Sigma} \\ & - (1-2\alpha)\bar{\Sigma} \cdot (K^\dagger\boldsymbol{\tau}N) - \bar{\Sigma} \cdot (K^{c\dagger}\boldsymbol{\tau}\Xi) - \frac{3-2\alpha}{\sqrt{3}}\bar{N}\Lambda K \\ & - \frac{3-2\alpha}{\sqrt{3}}K^\dagger\bar{\Lambda}N + \frac{3-4\alpha}{\sqrt{3}}\bar{\Xi}\Lambda K^c + \frac{3-4\alpha}{\sqrt{3}}K^{c\dagger}\bar{\Lambda}\Xi \\ & + i(1-\alpha)(\bar{\Sigma} \times \boldsymbol{\Sigma}) \cdot \boldsymbol{\pi} + \frac{2\alpha}{\sqrt{3}}(\bar{\Sigma}\Lambda) \cdot \boldsymbol{\pi} + \frac{2\alpha}{\sqrt{3}}(\bar{\Lambda}\Sigma) \cdot \boldsymbol{\pi} \\ & \left. + \frac{2\alpha}{\sqrt{3}}(\bar{\Sigma} \cdot \boldsymbol{\Sigma})\eta^0 - \frac{2\alpha}{\sqrt{3}}\bar{\Lambda}\Lambda\eta^0 \right\}. \end{aligned} \quad (24.181)$$

Here we have used the isospinors

$$N \equiv \begin{pmatrix} p \\ n \end{pmatrix}, \quad \Xi \equiv \begin{pmatrix} \Xi^0 \\ \Xi^- \end{pmatrix}, \quad (24.182)$$

and

$$K \equiv \begin{pmatrix} K^+ \\ K^0 \end{pmatrix}, \quad K^c \equiv \begin{pmatrix} \bar{K}^0 \\ -K^- \end{pmatrix}. \quad (24.183)$$

Note that K^c is the charge conjugate spinor $C\bar{K}^*$. The parameter α is defined by

$$\alpha \equiv \frac{D}{F+D} \quad (24.184)$$

so that

$$F/D = (1 - \alpha)/\alpha. \quad (24.185)$$

The two numbers $g = g_{\pi NN}$ and F/D parametrize all couplings.

The pion nucleon coupling was written down in Eq. (24.174). The F/D -ratio is determined experimentally from an analysis of the production process

$$\pi^- p \rightarrow \Sigma^0 K^+ \quad (24.186)$$

which contains the coupling

$$\begin{aligned} g_{n\Sigma^- K^+} &\equiv -\sqrt{2}g(1 - 2\alpha) \\ &= -\sqrt{2}g \frac{F - D}{F + D}. \end{aligned} \quad (24.187)$$

From the experimental data one finds

$$\frac{F}{D} \approx \frac{2}{3}. \quad (24.188)$$

For the coupling between pions and Σ -particles, the interaction Lagrangian (24.181) yields

$$g_{\Sigma\Sigma\pi} = g(1 - \alpha) = g \frac{F}{F + D}. \quad (24.189)$$

The SU(3)-relations between coupling constants in the Lagrangian (24.181) are, of course, in agreement with standard SU(3)-Clebsch-Gordan coefficients. The coefficients of the SU(2)-subgroup can be taken from Table 4.2 in Chapter 4.1, The isoscalar factors from Table 24.5 in Appendix 24A on p. 1378.

Take, for instance, the matrix element $\langle p|\pi^0|p\rangle$. The SU(2) Clebsch-Gordan coefficient is $1/\sqrt{3}$. The antisymmetric and symmetric isoscalar factors are $\sqrt{3}/\sqrt{12} = 1/2$ and $\sqrt{9}/\sqrt{20} = 3/2\sqrt{5}$, respectively. Hence, with the normalization factors of (24A.13), we have

$$\langle p|\pi^0|p\rangle = \frac{F + D}{2}. \quad (24.190)$$

The matrix element $\langle \Sigma^+|\pi^0|\Sigma^+\rangle$ has an SU(2)-Clebsch-Gordan $1/\sqrt{2}$ and the isoscalar factors $\sqrt{2/3}$ and 0, respectively, so that

$$\langle \Sigma^+|\pi^0|\Sigma^+\rangle = F, \quad (24.191)$$

just as before in (24.189).

Let us also calculate the coupling $g_{n\Sigma^-K^+}$ for which the Clebsch-Gordan coefficient is $-\sqrt{2/3}$ and the isoscalar factors are $1/2$ and $-3/2\sqrt{5}$, respectively. Thus

$$\langle n|K^+|\Sigma^-\rangle = \frac{1}{\sqrt{2}}(F - D), \quad (24.192)$$

and

$$g_{n\Sigma^-K^+} = -g\sqrt{2}\frac{F - D}{F + D}, \quad (24.193)$$

as in (24.187).

In Appendix 24A we have collected a few useful formulas for $SU(3)$ -calculations.

24.7.2 The Decay $\Delta(1232) \rightarrow N\pi$

The interactions between the various members of the nucleon octet with pseudoscalar mesons and the decuplet resonances of spin-parity $J^P = 3/2^+$ are all determined by only one $SU(3)$ -invariant matrix element. This, in turn, may be chosen to coincide with the coupling between the proton, the π^+ , and the $\Delta^{++}(1232)$ -resonance. The Lagrangian for this specific interaction is conventionally written as

$$\mathcal{L}_{\Delta^{++}pn^+} = \frac{g^*}{M_N} \left(\bar{\psi}_\mu^{++} \psi^+ \partial_\mu \pi^+ + \text{c.c.} \right), \quad (24.194)$$

where ψ_μ is a Rarita-Schwinger spinor for the spin $3/2$ particle $\Delta^{++}(1232)$. Some people write $4h/M_\pi$ instead of g^*/M_N .

The isospin structure can be incorporated by multiplying the Lagrangian by the Clebsch-Gordan factor

$$\frac{\langle \frac{3}{2}c | \frac{1}{2}a1b \rangle}{\langle \frac{3}{2}\frac{3}{2} | \frac{1}{2}\frac{1}{2}11 \rangle}, \quad (24.195)$$

where c, a, b are the isospin orientations of Δ, N and π . Alternatively, we can use Rarita-Schwinger isospinors Δ_a for the Δ -particle (each of the three components $\Delta_1, \Delta_2, \Delta_3$ is a two-component isospinor), and we can write in isospace (suppressing the Lorentz indices):

$$\mathcal{L} = \frac{g^*}{M_N} \left(\bar{\Delta} N - \bar{N} \Delta \right) \cdot \boldsymbol{\pi}. \quad (24.196)$$

Indeed, the isospinor for the Δ^{++} -resonance has only a $+$ -component with isospin up, so that $\bar{\Delta} N \boldsymbol{\pi}$ contains the particles Δ^{++}, p , and π^+ in the form $\bar{\Delta}^{++} p \pi^+$, as in (24.194).

For calculations it is useful to record the completeness relation of Rarita-Schwinger isospinors

$$\sum_{s_3} \Delta_a \bar{\Delta}_b = \delta_{ab} 1 - \frac{1}{3} \tau_a \tau_b = \frac{2}{3} \delta_{ab} 1 - \frac{1}{6} [\tau_a, \tau_b], \quad (24.197)$$

where 1 stands for the 2×2 unit matrix in isospace.

The coupling g^* can be determined by an analysis of the strength of the Δ^{++} resonance in the π^+p scattering amplitude. This gives

$$g^* \approx 12.43 g \approx 0.92 g \quad (24.198)$$

corresponding to

$$h \approx 0.457 g. \quad (24.199)$$

If we assume the Δ resonance to be very narrow, we can immediately calculate the decay rate from the interaction (24.194). The decay amplitude is found as follows: We consider a Δ^{++} -resonance in its rest frame and use helicity amplitudes along the direction of the momentum of the emerging proton, which we assume to run in the 3-direction. The Δ helicity can be $\pm 3/2$ or $\pm 1/2$. Only the latter two orientations allow to conserve angular momentum with the helicities of the proton being $\pm 1/2$. The two orientations decay with the same rate, so we only need to study one case, say the helicity $+1/2$. The Rarita-Schwinger spinor is a Clebsch-Gordan combination of spin $J, M = 1, 0$ with $1/2, 1/2$ and of $J, M = 1, 1$ with $1/2 - 1/2$:

$$u_\mu(\mathbf{0}; \frac{3}{2}, \frac{1}{2}) = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} u(\mathbf{0}, \frac{1}{2}) - \frac{1}{\sqrt{6}} \begin{pmatrix} 0 \\ 1 \\ i \\ 0 \end{pmatrix} u(\mathbf{0}, -\frac{1}{2}). \quad (24.200)$$

Between the state

$$a_{\pi^+}^\dagger a_p^\dagger |0\rangle \quad (24.201)$$

and a Δ -state at rest $\langle 0|a_\Delta$ with unit normalization in a finite volume V , the wave functions for the pion and the nucleon are

$$\frac{1}{\sqrt{2E_\pi V}} e^{-iq_\pi x} \frac{1}{\sqrt{V}} u(\mathbf{p}_N, s'_3), \quad (24.202)$$

and for the Δ -resonance

$$\frac{1}{\sqrt{V}} u_\mu(\mathbf{p}_\Delta, s_3). \quad (24.203)$$

We therefore find the decay amplitude [matrix element of the t -matrix (9.290)]:

$$t = \frac{g^*}{M_N} \bar{u}_\mu u q^\mu \frac{1}{\sqrt{V}^3} \frac{1}{\sqrt{2E_\pi}} \frac{1}{\sqrt{E_N/M_N}} \quad (24.204)$$

$$= \frac{g^*}{M_N} \sqrt{\frac{2}{3}} \cosh \frac{\zeta}{2} p_N \frac{1}{\sqrt{2E_\pi}} \frac{1}{\sqrt{V}^3} \frac{1}{\sqrt{E_N/M_N}}, \quad (24.205)$$

where

$$u(p_N, \tfrac{1}{2})u(0, \tfrac{1}{2}) = \cosh \frac{\zeta}{2} = \frac{1}{2M_N}(E_N + M_N), \quad (24.206)$$

with E_N, E_π being the energies of proton and pion in the rest frame of the decaying Δ -resonance, and p_N the momentum of the nucleon emerging in the z -direction. The decay rate is found from formula (9.338), yielding for the helicity $h = 1/2$ -state:

$$\begin{aligned} \Gamma_{\Delta^{h=1/2} \rightarrow N\pi} &= \frac{1}{(2\pi)^3} 2\pi \frac{E_N E_\pi}{M_\Delta} \int d\Omega |t|^2 \\ &= \frac{4\pi}{(2\pi)^3} 2\pi \frac{p_N}{M_\Delta} \frac{g^{*2}}{M_N^2} \frac{2}{3} p_N^2 \frac{1}{4} (E_N + M_N) \\ &= \frac{g^{*2}}{4\pi} \frac{2}{3} \frac{p_N^3}{M_N^2 M_\Delta} (E_N + M_N). \end{aligned} \quad (24.207)$$

Since the resonance Δ is, with probability $1/2$, in the helicity- $3/2$ state, where it cannot decay, the final decay rate is only one half of the value (24.207), i.e.,

$$\Gamma = \frac{g^{*2}}{4\pi} \frac{1}{3} \frac{p_N^3}{M_N^2 M_\Delta} (E_N + M_N). \quad (24.208)$$

In terms of the three particle masses involved, the energy E_N is given by

$$E_N = \frac{M_\Delta^2 + M_N^2 - M_\pi^2}{2M_\Delta}, \quad (24.209)$$

and the momentum p_N of the outcoming proton (equal to that of the pion) is

$$p_N = \sqrt{[M_\Delta^2 - (M_N + M_\pi)^2][M_\Delta^2 - (M_N - M_\pi)^2]}/2M_\Delta. \quad (24.210)$$

Using the experimental width

$$\Gamma_\Delta \approx 115 \text{ MeV}, \quad (24.211)$$

we obtain

$$g^* \approx 14.43 \approx 1.07g, \quad (24.212)$$

corresponding to

$$h \approx 0.53, \quad (24.213)$$

in reasonable agreement with the independent determination (24.199) from the pion-nucleon scattering.

24.7.3 Vector Meson Decay $\rho(770) \rightarrow \pi\pi$

Among mesons, the most directly observable coupling is the $\rho\pi\pi$ -coupling. It governs the strength of the most prominent resonance in the p -wave pion-pion scattering amplitude. Since ρ is a vector meson of isospin 1, it is coupled to the two pions in a p -wave. The Lagrangian interaction is given by

$$\mathcal{L} = \frac{g_{\rho\pi\pi}}{2} \mathbf{\rho}^\mu \cdot \left(\boldsymbol{\pi} \times \overleftrightarrow{\partial}_\mu \boldsymbol{\pi} \right). \quad (24.214)$$

For the decay $\rho^+ \rightarrow \pi^0 \pi^+$, the invariant t -matrix element [defined in (9.290)] is given by

$$\langle \pi^0 \pi^+ | t | \rho^+ \rangle = -g_{\rho\pi\pi} \frac{1}{\sqrt{2V E_{pi}^2}} \frac{1}{\sqrt{2V M_\rho}} 2p_\pi^\mu \epsilon_\mu(\mathbf{p}_\rho, s_3), \quad (24.215)$$

where $\epsilon_\mu(p_\rho, s_3)$ is the polarization vector of the ρ meson and the decay rate is, according to formula (9.339),

$$\Gamma_{\rho^+ \rightarrow \pi^0 \pi^+} = g_{\rho\pi\pi}^2 \frac{4\pi}{(2\pi)^2} \frac{p_{\text{CM}}}{M_\rho^2} \frac{1}{2^3} 4 |p_\pi^\mu \epsilon_\mu|^2. \quad (24.216)$$

The average over the initial polarization gives

$$\frac{1}{3} p_\pi^\mu p_\pi^\nu \sum_{s_3} \epsilon^\mu(p_\rho, s_3) \epsilon^\nu(p_\rho, s_3) = -\frac{1}{3} p_\pi^\mu p_\pi^\nu \left(g_{\mu\nu} - \frac{p_\rho^\mu p_\rho^\nu}{p_\rho^2} \right) = \frac{1}{3} p_{\text{CM}\pi}^2, \quad (24.217)$$

where $p_{\text{CM}\pi}$ is the momentum of the pions in the rest frame of the decaying ρ -meson:

$$p_{\text{CM}\pi} = \frac{1}{2} \left(M_\rho^2 - 4m_\pi^2 \right)^{1/2}. \quad (24.218)$$

This brings (24.216) to the form

$$\Gamma_{\rho^+ \rightarrow \pi^0 \pi^+} = \frac{g_{\rho\pi\pi}^2}{4\pi} \frac{2}{3} \frac{p_{\text{CM}\pi}^3}{M_\rho^2} = \frac{g_{\rho\pi\pi}^2}{4\pi} \frac{2}{3} \frac{\left(M_\rho^2 - 4m_\pi^2 \right)^{3/2}}{8M_\rho^2}. \quad (24.219)$$

The experimental decay width is

$$\Gamma_{\rho\pi\pi} \approx 153 \text{ MeV}. \quad (24.220)$$

From this one finds the coupling constant

$$\frac{g_{\rho\pi\pi}^2}{4\pi} \approx 2.85. \quad (24.221)$$

24.7.4 Vector Meson Decays $\omega(783) \rightarrow \rho\pi$ and $\omega(783) \rightarrow \pi\pi\pi$

Another important coupling is that between ω , ρ , and π :

$$\mathcal{L}_{\omega\rho\pi} = g_{\omega\rho\pi} \epsilon_{\mu\nu\lambda\kappa} \partial^\mu \omega^\nu \partial^\lambda \rho^\kappa \cdot \boldsymbol{\pi}. \quad (24.222)$$

It is responsible for the decay

$$\omega \rightarrow \pi\pi\pi, \quad (24.223)$$

which proceeds at a rate

$$\Gamma_{\omega \rightarrow \pi\pi\pi} = 9.8 \pm 0.3 \text{ MeV}. \quad (24.224)$$

The $\pi\pi$ -channels are dominated by the ρ -resonance. One can therefore assume a sequential decay, finding

$$\begin{aligned} \Gamma_{\omega \rightarrow 3\pi} &= (M_\omega - 3M_\pi)^4 (M_\rho^2 - 4M_\pi^2)^{-2} M_\omega M_\pi^2 \frac{1}{\sqrt{27}} \frac{1}{4} \frac{g_{\rho\pi\pi}^2}{4\pi} \frac{g_{\omega\rho\pi}^2}{4\pi} \times 3.56 \\ &\approx 10.3 \text{ MeV} \frac{g_{\rho\pi\pi}^2}{4\pi} \frac{g_{\omega\rho\pi}^2}{4\pi}, \end{aligned} \quad (24.225)$$

where the number 3.56 is due to the numeric integration of a phase space integral [8]. The experimental rate gives

$$\frac{g_{\rho\pi\pi}^2}{4\pi} \approx \frac{0.95}{M_\pi^2}, \quad (24.226)$$

and hence

$$\frac{g_{\omega\rho\pi}^2}{g_{\rho\pi\pi}^2} \approx \frac{0.117}{M_\pi^2} \approx 6.14 \frac{1}{\text{GeV}^2}. \quad (24.227)$$

24.7.5 Vector Meson Decays $K^*(892) \rightarrow K\pi$

In πK -scattering one observes the SU(3)-partner of the ρ -meson, the strange vector meson K^* (892). Its coupling is written as

$$\mathcal{L}_{K^*K\pi} = \frac{1}{2} g_{K^*K\pi} (K^{\dagger\mu} \boldsymbol{\tau} K)_i \overset{\leftrightarrow}{\partial}_\mu \boldsymbol{\pi}. \quad (24.228)$$

Its decay width is

$$\Gamma_{K^*K\pi} = 3 \frac{\left(\frac{1}{2} g_{K^*K\pi}\right)^2}{4\pi} \frac{2}{3} \frac{p_{\text{CM}K^*}^3}{M_K^2}, \quad (24.229)$$

where

$$p_{\text{CM}K^*} = \frac{1}{2M_{K^*}} \sqrt{[M_{K^*}^2 - (M_{K^*} + M_\pi)^2] [M_{K^*}^2 - (M_{K^*} - M_\pi)^2]} \quad (24.230)$$

is the momentum of the decay products in the rest frame of K^* . This implies a ratio with respect to the $\rho\pi\pi$ -width:

$$\frac{\Gamma_{K^*K\pi}}{\Gamma_{\rho\pi\pi}} = \frac{3}{4} \frac{g_{K^*K\pi}^2}{g_{\rho\pi\pi}^2} \frac{M_\rho^2}{M_{K^*}^2} \frac{p_{\text{CM}K^*}^3}{p_{\text{CM}\rho}^3} \approx \frac{3}{4} \frac{g_{K^*K\pi}^2}{g_{\rho\pi\pi}^2} \times 0.385. \quad (24.231)$$

The experimental width of K^* is

$$\Gamma_{K^*K\pi} = (51.8 \pm 0.8) \text{ MeV}, \quad (24.232)$$

so that its ratio with respect to the ρ -width (24.220) is 0.3406. Inserting this into (24.231), we extract a ratio of coupling constants

$$\frac{g_{K^*K\pi}}{g_{\rho\pi\pi}} \approx 1.086. \quad (24.233)$$

By SU(3)-symmetry, this ratio is predicted to be unity, in good agreement with experiments.

24.7.6 Axial Vector Meson Decay $a_1(1270) \rightarrow \rho\pi$

A more involved coupling governs the decay of the axial vector meson $a_1(1270)$. It is seen as a resonance of mass 1270 MeV and width

$$\Gamma_{a_1\rho\pi} \approx 316 \pm 45 \text{ MeV} \quad (24.234)$$

in the $\rho\pi$ -scattering amplitude. Angular momentum and parity allow s - and d -wave interactions, so that there exist two independent coupling constants with a Lagrangian density

$$\mathcal{L} = g_{a_1\rho\pi} (\mathbf{a}_\mu \times \boldsymbol{\rho}^\mu) \cdot \boldsymbol{\pi} + h_{a_1\rho\pi} (\partial_\mu \mathbf{a}^\nu \times \partial_\nu \boldsymbol{\rho}^\mu) \cdot \boldsymbol{\pi}. \quad (24.235)$$

Let $\epsilon(p), \epsilon(q)$ denote the polarization vectors of the a_1 and ρ meson, respectively, and k the momentum of the outgoing pion. Then the invariant t -matrix element for $A^+ \rightarrow \rho^- \pi^+$ reads

$$t_{ba} = \frac{1}{\sqrt{2V^3}} \frac{1}{\sqrt{p_0 q_0 k_0}} \left[g_{a_1\rho\pi} \epsilon_\mu^*(p) \epsilon^\mu(q) - h_{a_1\rho\pi} q_\nu \epsilon^{*\nu}(p) p^\mu \epsilon_\mu(q) \right]. \quad (24.236)$$

For the calculation of decay rates it is better to use a more complicated-looking decomposition into a longitudinal and a transverse helicity amplitude

$$\begin{aligned} t^L &= \frac{1}{\sqrt{2V^3}} \frac{1}{\sqrt{p_0 q_0 k_0}} g_L P_\mu q^\nu \left(g_{\mu\lambda} - \frac{q_\mu q_\lambda}{q^2} \right) \left(g_{\nu\kappa} - \frac{p_\nu p_\kappa}{p^2} \right) \epsilon^* * \kappa(p) \epsilon^\lambda(q), \\ t^T &= -\frac{g_T}{m_a^2} \epsilon^{\mu\alpha'\beta'}{}_\gamma \epsilon^{\lambda\alpha\beta\gamma} q_\beta p_\alpha q_{\beta'} p_{\alpha'} \epsilon_\lambda^*(p) \epsilon_\mu(q). \end{aligned} \quad (24.237)$$

The relation between them is

$$\begin{aligned} -h_{a_1\rho\pi} &= g_L + g_T \frac{m_{a_1}^2 + m_\rho^2 - m_\pi^2}{2m_{a_1}^2}, \\ -g_{a_1\rho\pi} &= \frac{g_T}{m_{a_1}^2} \left[\left(\frac{m_{a_1}^2 + m_\rho^2 - m_\pi^2}{2} \right)^2 - m_{a_1}^2 m_\rho^2 \right]. \end{aligned} \quad (24.238)$$

The advantage of these amplitudes is, that they are decoupled in the decay process. A somewhat tedious calculation (see Appendix 24B) gives

$$\Gamma_{a_1\rho\pi} = \Gamma_{a_1\rho\pi}^L + \Gamma_{a_1\rho\pi}^T, \quad (24.239)$$

where

$$\Gamma_{a_1\rho\pi}^L = \frac{g_L^2}{n\pi} \frac{1}{3} \frac{p_\rho^5}{m_\rho^2}, \quad \Gamma_{a_1\rho\pi}^T = \frac{g_T^2}{n\pi} \frac{2}{3} \frac{p_\rho^5}{m_{a_1}^2}. \quad (24.240)$$

Since the experimental masses have the ratio

$$\frac{m_{a_1}^2}{m_\rho^2} \approx 2.72, \quad (24.241)$$

we get

$$\Gamma_{a_1\rho\pi} \approx 5.5 \times 10^{-5} (g_L^2 + 2.735 g_T^2) \text{ GeV}, \quad (24.242)$$

and find for the coupling constants the relation

$$g_L^2 + \frac{2m_\rho^2}{m_{a_1}^2} g_T^2 \approx g_L^2 + 0.68 g_T^2 \approx 75.1. \quad (24.243)$$

The ratio between the coupling constants g_L and g_T has to be determined by some other method.

24.7.7 Coupling of $\rho(770)$ to Nucleons

The coupling is defined by the non-minimal Lagrangian density

$$\mathcal{L} = g_{\rho NN} \left[\mathbf{p}_\mu \bar{\psi} \gamma^\mu \boldsymbol{\tau} \psi + \frac{\kappa_{\rho NN}}{2M} (\partial_\mu \mathbf{p}_\nu - \partial_\nu \mathbf{p}_\mu) \bar{\psi} \sigma^{\mu\nu} \boldsymbol{\tau} \psi \right]. \quad (24.244)$$

An analysis of the phase shifts in $\pi\pi \rightarrow N\bar{N}$ yields the coupling strengths [9]

$$\frac{g_{\rho NN}^2}{4\pi} = 0.6 \pm 0.1, \quad \kappa_{\rho NN} = 6.6 \pm 1.0. \quad (24.245)$$

Appendix 24A Useful SU(3)-Formulas

The matrix elements of an octet operator between two octets labeled by the real indices $i = 1, 2, 3, \dots, 8$ of the adjoint representation 8 can be written as follows:

$$\langle 8_i | 8_k 8_j \rangle = F(-if_{kij}) + Dd_{kij} = F(\hat{F}_k)_{ij} + D(\hat{D}_k)_{ij}, \quad (24A.1)$$

where f_{ijk} are the structure constants of SU(3), and d_{ijk} those of the anticommutators

$$\{\lambda_i, \lambda_j\} = d_{ijk}\lambda_k + \frac{4}{3}\delta_{ij}.$$

The SU(3)-vector e^i associated with a specific particle is found from the assignment of the nucleon octet to the 3×3 -matrix elements

$$N = \begin{pmatrix} \frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda & \Sigma^+ & p \\ \Sigma^- & -\frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda & n \\ \Xi^- & \Xi^0 & -\frac{1}{\sqrt{6}}2\Lambda \end{pmatrix}, \quad (24A.2)$$

by contraction with the λ -matrices:

$$e^i = \frac{1}{\sqrt{2}}\text{tr}(\lambda^i N). \quad (24A.3)$$

The proton, for example, corresponds to the octet vector

$$e^i(p) = \frac{1}{\sqrt{2}}\text{tr}\left[\lambda^i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]. \quad (24A.4)$$

It has the non-zero components

$$e^4(p) = \frac{1}{\sqrt{2}}, \quad e^5(p) = \frac{i}{\sqrt{2}}. \quad (24A.5)$$

For the π^0 -couplings we calculate the matrix elements $\hat{F}_{0ij}$ and $\hat{D}_{0ij}$ between two proton states as follows:

$$\langle p | \hat{F}_0 | p \rangle = \frac{1}{2}, \quad \langle p | \hat{D}_0 | p \rangle = \frac{1}{2}. \quad (24A.6)$$

Hence

$$\langle p | \pi_0 | p \rangle = \frac{F + D}{2}. \quad (24A.7)$$

Similarly, the SU(3)-vector of the Σ^+ -particle is

$$e^i(\Sigma^+) = \frac{1}{\sqrt{2}}\text{tr}\left[\lambda^i \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]. \quad (24A.8)$$

It has the non-zero components

$$e^1(\Sigma^+) = \frac{1}{\sqrt{2}}, \quad e^2(\Sigma^+) = \frac{i}{\sqrt{2}}. \quad (24A.9)$$

For the coupling of π^0 to Σ -particles we need the matrix elements $(\hat{F}_0)_{ij}$ and $(\hat{D}_0)_{ij}$ between Σ^+ -states:

$$\langle \Sigma^+ | \hat{F}_0 | \Sigma^+ \rangle = 1, \quad \langle \Sigma^+ | \hat{D}_0 | \Sigma^+ \rangle = 0. \quad (24A.10)$$

Hence

$$\langle \Sigma^+ | \pi^0 | \Sigma^+ \rangle = F. \quad (24A.11)$$

The matrix elements of π^+ between $\Sigma^+ \Sigma^+$ and pp have therefore the ratio

$$\frac{\Sigma^+ \pi^+ \Sigma^+}{p \pi p} = \frac{2F}{F + D}, \quad (24A.12)$$

just as in (24.189), (24.191), and (25.100).

The SU(3)-matrix elements may also be calculated by using tables of the SU(3)-Clebsch-Gordan coefficients. The matrices $\hat{F}_i$ $\hat{D}_i$ correspond to the coefficients

$$\hat{F}_i = \sqrt{3} \langle 8_a | 88 \rangle, \quad \hat{D}_i = \sqrt{\frac{5}{3}} \langle 8_s | 88 \rangle. \quad (24A.13)$$

The Clebsch-Gordan coefficients can be decomposed into a product of an isospin SU(2)-Clebsch-Gordan coefficient and a so-called isoscalar factor

$$\langle 8_a i | 8j; 8k \rangle = \langle \langle 8_a Y_i | 8Y_j; 8Y_k \rangle \rangle \langle T^i, T_3^i | T^j, T_3^j; T^k, T_3^k \rangle, \quad (24A.14)$$

where T^i, T_3^i is the isospin content of the SU(3)-index i . The isoscalar factors are listed in Table 24.5.

TABLE 24.5 Isoscalar factors of SU(3). We have omitted the square roots of the number in the arrays on the right-hand sides, i.e., -3 stands for $-\sqrt{3}$. This is indicated by the superscript $1/2$ on each array. The table is from the Particle Data Properties Booklet [10].

$$\begin{aligned} & \mathbf{1} \rightarrow \mathbf{8} \otimes \mathbf{8} \\ & (\Lambda) \rightarrow (N\bar{K} \ \Sigma\pi \ \Lambda\eta \ \Xi K) = \frac{1}{\sqrt{8}} \begin{pmatrix} 2 & 3 & -1 & -2 \end{pmatrix}^{1/2} \\ & \mathbf{8}_1 \rightarrow \mathbf{8} \otimes \mathbf{8} \\ & \begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix} \rightarrow \begin{pmatrix} N\pi \ N\eta \ \Sigma K \ \Lambda K \\ N\bar{K} \ \Sigma\pi \ \Lambda\pi \ \Sigma\eta \ \Xi K \\ N\bar{K} \ \Sigma\pi \ \Lambda\eta \ \Xi K \\ \Sigma\bar{K} \ \Lambda\bar{K} \ \Xi\pi \ \Xi\eta \end{pmatrix} = \frac{1}{\sqrt{20}} \begin{pmatrix} 9 & -1 & -9 & -1 \\ -6 & 0 & 4 & 4 & -6 \\ 2 & -12 & -4 & -2 \\ 9 & -1 & -9 & -1 \end{pmatrix}^{1/2} \\ & \mathbf{8}_3 \rightarrow \mathbf{8} \otimes \mathbf{8} \\ & \begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix} \rightarrow \begin{pmatrix} N\pi \ N\eta \ \Sigma K \ \Lambda K \\ N\bar{K} \ \Sigma\pi \ \Lambda\pi \ \Sigma\eta \ \Xi K \\ N\bar{K} \ \Sigma\pi \ \Lambda\eta \ \Xi K \\ \Sigma\bar{K} \ \Lambda\bar{K} \ \Xi\pi \ \Xi\eta \end{pmatrix} = \frac{1}{\sqrt{12}} \begin{pmatrix} 3 & 3 & 3 & -3 \\ 2 & 8 & 0 & 0 & -2 \\ 6 & 0 & 0 & 6 \\ 3 & 3 & 3 & -3 \end{pmatrix}^{1/2} \\ & \mathbf{10} \rightarrow \mathbf{8} \otimes \mathbf{8} \\ & \begin{pmatrix} \Delta \\ \Sigma \\ \Xi \\ \Omega \end{pmatrix} \rightarrow \begin{pmatrix} N\pi \ N\eta \\ N\bar{K} \ \Sigma\pi \ \Lambda\pi \ \Sigma\eta \ \Xi K \\ \Sigma\bar{K} \ \Lambda\bar{K} \ \Xi\pi \ \Xi\eta \\ \Xi\bar{K} \end{pmatrix} = \frac{1}{\sqrt{12}} \begin{pmatrix} -6 & 6 \\ -2 & 2 & -3 & 3 & 3 \\ 3 & -3 & 3 & 3 \\ 12 \end{pmatrix}^{1/2} \\ & \mathbf{8} \rightarrow \mathbf{10} \otimes \mathbf{8} \\ & \begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix} \rightarrow \begin{pmatrix} \Delta\pi \ \Sigma K \\ \Delta\bar{K} \ \Sigma\pi \ \Sigma\eta \ \Xi K \\ \Sigma\pi \ \Xi K \\ \Sigma\bar{K} \ \Xi\pi \ \Xi\eta \ \Omega K \end{pmatrix} = \frac{1}{\sqrt{15}} \begin{pmatrix} -12 & 3 \\ 8 & -2 & -3 & 2 \\ -9 & 6 \\ 3 & -3 & -3 & 6 \end{pmatrix}^{1/2} \\ & \mathbf{10} \rightarrow \mathbf{10} \otimes \mathbf{8} \\ & \begin{pmatrix} \Delta \\ \Sigma \\ \Xi \\ \Omega \end{pmatrix} \rightarrow \begin{pmatrix} \Delta\pi \ \Delta\pi \ \Sigma K \\ \Delta\bar{K} \ \Sigma\pi \ \Sigma\eta \ \Xi K \\ \Sigma\bar{K} \ \Xi\pi \ \Xi\eta \ \Omega K \\ \Xi\bar{K} \ \Omega\eta \end{pmatrix} = \frac{1}{\sqrt{24}} \begin{pmatrix} 15 & 3 & -6 \\ 8 & 8 & 0 & -8 \\ 12 & 3 & -3 & -6 \\ 12 & -12 \end{pmatrix}^{1/2} \end{aligned}$$

Appendix 24B Decay Rate for $a_1 \rightarrow \rho\pi$

Denoting the polarization vectors $\epsilon(p)$ and $\epsilon(q)$ of a_1 and ρ mesons by ϵ and ϵ' , and using the transversality properties $p_\mu \epsilon^\mu = 0$, $q_\mu \epsilon'^\mu = 0$, respectively, the amplitudes are (dropping the normalization factors $1/\sqrt{2Nq_0}$ associated with the three particles)

$$\begin{aligned} t &= g_L(p\epsilon'^*)(q\epsilon) + \frac{g_T}{M_{a_1}^2} \begin{vmatrix} \epsilon'^*\epsilon & \epsilon'^*q & \epsilon'^*p \\ \epsilon q & q^2 & qp \\ \epsilon p & qp & p^2 \end{vmatrix} \\ &= g_L(p\epsilon')(q\epsilon) + \frac{g_T}{M_{a_1}^2} [M_{a_1}^2 M_\rho^2 (\epsilon'^*\epsilon) + (p\epsilon'^*)qp - (\epsilon'^*\epsilon)(qp)^2]. \end{aligned} \quad (24B.1)$$

This expression shows directly the relation of the couplings g_L and g_T with the couplings $g_{a_1, \rho\pi}$ and $h_{a_1 \rho\pi}$. We now put a_1 in its rest frame, so that $p^\mu = (M_{a_1}, 0, 0, 0)$, and we find the scalar products

$$\epsilon'^*(q, 1)\epsilon^*(p, 1) = -1, \quad \epsilon'^*(q, 2)\epsilon^*(p, 2) = -1, \quad \epsilon'^*(q, 3)\epsilon(p, 3) = -\frac{q_0}{M_\rho},$$

and further

$$\begin{aligned} (q\epsilon(p, 1)) &= 0, & (p\epsilon'^*(q, 1)) &= 0, \\ (q\epsilon(p, 2)) &= 0, & (p\epsilon'^*(q, 2)) &= 0, \\ (q\epsilon(p, 3)) &= -p_{\text{CM}}, & (p\epsilon'^*(q, 3)) &= \frac{p_{\text{CM}}}{M_\rho} M_{a_1}, \end{aligned} \quad (24B.2)$$

where

$$p_{\text{CM}} = \frac{1}{2M_{a_1}} \sqrt{[M_{a_1}^2 - (M_\rho - M_\pi)^2][M_{a_1}^2 - (M_\rho + M_\pi)^2]} \quad (24B.3)$$

is the center-of-mass momentum of the ρ -meson. We therefore find the helicity amplitudes (writing the helicities as superscripts in parentheses)

$$\begin{aligned} \langle \rho^{(0)} \pi_1 | t | a_1(0) \rangle &= -g_L p_{\text{CM}}^2 \frac{M_{a_1}}{M_\rho}, \\ \langle \rho^{\frac{1}{2}} \pi | t | a_1^{\frac{1}{2}} \rangle &= \frac{g_T}{M_{a_1}^2} (-M_{a_1}^2 M_\rho^2 + E_{\text{CM}}^2 M_{a_1}^2) = g_T p_{\text{CM}}^2, \end{aligned} \quad (24B.4)$$

where

$$E_{\text{CM}} = \frac{M_{a_1}^2 + M_\rho^2 - M_\pi^2}{2M_{a_1}} \quad (24B.5)$$

is the energy of the ρ meson in the center-of-mass frame. From this we obtain directly the longitudinal width

$$\Gamma_{a_1 \rightarrow \rho\pi}^L = \frac{g_L^2}{4\pi} \frac{2}{6} \frac{p_{\text{CM}}^5}{M_\rho^2}, \quad (24B.6)$$

having inserted a factor 2 due to isospin, and a transversal width

$$\Gamma_{a_1 \rightarrow \rho\pi}^T = \frac{g_T^2}{4\pi} \frac{2}{6} \cdot 2 \frac{p_{\text{CM}}^5}{M_{a_1}^2}. \quad (24B.7)$$

Notes and References

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*Paradise is exactly like where you are right now.
... only much, much better.*
LAURIE ANDERSON (1947)

25

Symmetries Linking Internal and Spacetime Properties. Supersymmetry

Besides space-time symmetries under Lorentz- and Poincaré-group, and under approximate internal symmetries groups SU(2), SU(3), etc., there exists a further class of approximate symmetries which combine external and internal indices. Historically, the first example for this class of symmetries arose in nuclear physics where isospin was combined with spin to form the larger group SU(4).

25.1 Approximate SU(4)-Symmetry of Nuclear Forces

Soon after the discovery of the approximate isospin symmetry in nuclear physics, the search went on for higher approximate symmetries. It turned out that the nuclear forces exhibited also an approximate independence of spin. Moreover, this could be combined with isospin to form an approximate invariance under the larger group SU(4). The different terms in the potential between nucleons are conventionally classified by their behavior under certain interchange operators acting upon two-nucleon wave functions. These are defined as follows:

$$\begin{aligned} P^M \psi(x_1 a_1, x_2 a_2) &\equiv \psi(x_2 a_1, x_1 a_2) \text{ Majorana operator,} \\ P^B \psi(x_1 a_1, x_2 a_2) &\equiv \psi(x_1 a_2, x_2 a_1) \text{ Bartlett operator,} \\ P^H \psi(x_1 a_1, x_2 a_2) &\equiv \psi(x_2 a_2, x_1 a_1) \text{ Heisenberg operator,} \end{aligned} \quad (25.1)$$

where x denotes the positions and a the third components of the spins of the particles. The effect of the interchange operators on two-nucleon wave functions of definite orbital angular momentum l and spin (singlet or triplet) is shown in Table 25.1. Using these operators, the most general two-particle potential can be written as follows:

$$\begin{aligned} V = V_W(r) + V_M(r)P^M + V_B(r)P^B + V_H(r)P^H \\ + V_{TW}(r)S_{12} + V_{TM}(r)S_{12}P^M, \end{aligned} \quad (25.2)$$

where S_{12} is the spin-orbit coupling operator

$$S_{12} \equiv 3(\boldsymbol{\sigma}_1 \hat{\mathbf{r}})(\boldsymbol{\sigma}_2 \hat{\mathbf{r}}) - (\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2). \quad (25.3)$$

TABLE 25.1 Action of the different interchange operators.

	even l		odd l	
	triplet	singlet	triplet	singlet
P^M	1	1	-1	-1
P^B	1	-1	1	-1
P^H	1	-1	-1	1

Here $\hat{\mathbf{r}} \equiv \mathbf{r}/|\mathbf{r}|$ is the direction of the distance vector $\mathbf{r}$ between the two particles. The $\boldsymbol{\sigma}$ -matrices $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$ act on the spin indices of the particles 1, 2, respectively. This is, in fact, the most general way of describing noncentral forces which can be derived from a potential. The potential $V_W(r)$ is called *Wigner potential*, which is purely central. The potential V_{TW} that is proportional to the operator S_{12} parametrizes the so-called *tensor force* that is responsible for mixing the ${}^3_1D$ wave into the ${}^3_1S$ ground state wave function¹ of the deuteron ($\approx 2 - 6\%$). Note that for a spin singlet state, the eigenvalue of S_{12} is zero. The potential V_M is called Majorana potential. The Bartlett operator P_B can be expressed in terms of the Pauli spin matrices as follows:

$$P^B = \frac{1}{2}(1 + \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2). \quad (25.4)$$

In this parametrization, each of the six V -terms in (25.8) is proportional to the unit matrix in the space of charge indices.

Let us now define, in this space, the operator

$$P^\tau \equiv \frac{1}{2}(1 + \boldsymbol{\tau}_1 \boldsymbol{\tau}_2), \quad (25.5)$$

where $\boldsymbol{\tau}$ denotes a three-component vector of Pauli matrices $\boldsymbol{\tau} = (\tau^1, \tau^2, \tau^3)$, which, instead of acting on spin indices, acts on the isospin indices of the nucleons. It is easy to verify that the operators P^H and P^τ have opposite signs

$$P^H = -P^\tau, \quad (25.6)$$

when acting on wave functions satisfying the Pauli principle. We can also verify that

$$P^M = P^B P^H. \quad (25.7)$$

The action of the spin-isospin operators is shown in Table 25.2.

From this we see that it is possible to rewrite the potential (25.1) in terms of the $\boldsymbol{\tau}$ -matrices as follows:

$$\begin{aligned} V = & V_a(r) + V_\sigma(r)(\boldsymbol{\sigma}^1 \boldsymbol{\sigma}^2) + V_\tau(r)(\boldsymbol{\tau}^1 \boldsymbol{\tau}^2) + V_{\sigma\tau}(\boldsymbol{\sigma}^1 \boldsymbol{\sigma}^2)(\boldsymbol{\tau}^1 \boldsymbol{\tau}^2) \\ & + V_{Td}(r)S_{12} + V_{T\tau}(\boldsymbol{\tau}^1 \boldsymbol{\tau}^2)S_{12}. \end{aligned} \quad (25.8)$$

¹Notation: ${}^J_S L$ where L is the orbital angular momentum, S the combined spin, and J the total angular momentum.

TABLE 25.2 Action of spin and isospin operators in the expansion (25.8).

	even l		odd l	
	triplet	singlet	triplet	singlet
$\boldsymbol{\sigma}^1 \boldsymbol{\sigma}^2$	-3	1	-3	1
$\boldsymbol{\tau}^1 \boldsymbol{\tau}^2$	1	-3	-3	1
$(\boldsymbol{\sigma}^1 \boldsymbol{\sigma}^2)(\boldsymbol{\tau}^1 \boldsymbol{\tau}^2)$	-3	-3	9	1

The coefficient functions are related to the earlier ones by

$$\begin{aligned}
 V_a &= V_W + \frac{1}{2}V_B - \frac{1}{2}V_H - \frac{1}{4}V_M, & V_\sigma &= \frac{1}{2}V_B - \frac{1}{4}V_M, \\
 V_\tau &= -\frac{1}{2}V_H - \frac{1}{4}V_M, & V_{\sigma\tau} &= -\frac{1}{4}V_M, \\
 V_{Td} &= V_{TW} - \frac{1}{2}V_{TM}, & V_{T\tau} &= -\frac{1}{2}V_{TM}.
 \end{aligned} \tag{25.9}$$

In 1937, Wigner observed [1] that if the spin-orbit forces are small and Wigner and Majorana forces are dominant, the potential can be written as

$$V = V_1(r) + V_2(r)(1 + \boldsymbol{\sigma}^1 \boldsymbol{\sigma}^2)(1 + \boldsymbol{\tau}^1 \boldsymbol{\tau}^2). \tag{25.10}$$

This would be invariant under spin rotations, isospin rotations, and the extension of these two $SU(2)$ -groups to $SU(4)$. Experimentally, however,

$$\frac{V_H}{V_M} \approx 0.4 - 0.5, \tag{25.11}$$

so that there exists really quite a large symmetry breaking. Nevertheless, the group has turned out to be useful in understanding nuclear spectra.

The group $SU(4)$ is generated by the fifteen 4×4 matrices acting on a nucleon field $N_{\alpha\alpha'}$ with isospin index α ($\alpha = 1, 2$) and spin index α' ($\alpha' = 1, 2$):

$$\frac{\boldsymbol{\tau}}{2} \times 1, \quad 1 \times \frac{\boldsymbol{\sigma}}{2}, \quad \frac{\boldsymbol{\tau}}{2} \times \frac{\boldsymbol{\sigma}}{2}. \tag{25.12}$$

The commutation rules are given by the known ones for $\boldsymbol{\sigma}, \boldsymbol{\tau}$, an additional set of obvious commutation rules between the $\boldsymbol{\sigma}$'s and $\boldsymbol{\tau}$'s, and the combined generators $(\boldsymbol{\tau}/2) \times (\boldsymbol{\sigma}/2)$. They express their vector nature with respect to each subgroup, plus the new ones

$$\left[\frac{\tau^a \times \sigma^i}{2}, \frac{\tau^b \times \sigma^j}{2} \right] = i\delta_{ab}\epsilon_{ijk}1 \times \frac{\sigma^k}{2} + i\epsilon_{abc}\delta_{ij}\frac{\tau^c}{2} \times 1. \tag{25.13}$$

If $SU(4)$ is a good approximate symmetry of nuclear forces, then nuclei should occur in irreducible multiplets of $SU(4)$. Moreover, since both isospin and spin are invariant under space reflections, each multiplet should have the same parity.

The fundamental representation of $SU(4)$ is four-dimensional and denoted by 4. Its four components are identified with the four states of the nucleon as follows:

$$N = \begin{pmatrix} p^\uparrow \\ p^\downarrow \\ n^\uparrow \\ n^\downarrow \end{pmatrix}. \tag{25.14}$$

The higher representations are obtained as usual. One forms an appropriate multi-nucleon state of highest spin and isospin and applies the lowering operators

$$\frac{\tau^-}{2} \times 1, \quad 1 \times \frac{\sigma^-}{2}, \quad \frac{\tau^- \times \sigma^3}{4}, \quad \frac{\tau^3 \times \sigma^-}{4}, \quad \frac{\tau^- \times \sigma^-}{4} \quad (25.15)$$

to generate irreducible multiplets.

Consider the symmetric Young tableau $\square\square$ and take the state of highest weight in isospin and spin

$$|1, 1; 1, 1\rangle \equiv |p^\uparrow p^\uparrow\rangle, \quad (25.16)$$

where the notation on the left-hand side specifies the isospins and spins T, S , and their third components as $|T, T_3; S, S_3\rangle$.² From the state (25.16) we run through the entire isovector triplet of spin 1 by repeated application of the lowering operator τ^- . For these the other spin components are obtained by applying σ^- .

The application of $\tau^-/2$ to (25.16) gives the state

$$|1, 0; 1, 1\rangle = \frac{1}{\sqrt{2}} |n^\uparrow p^\uparrow + p^\uparrow n^\uparrow\rangle, \quad (25.17)$$

whereas $\sigma^-/2$ leads to

$$|1, 0; 1, 0\rangle = \frac{1}{2} |n^\downarrow p^\uparrow + n^\uparrow p^\downarrow + p^\downarrow n^\uparrow + p^\uparrow n^\downarrow\rangle. \quad (25.18)$$

Since the two operators τ^- , σ^- are taken from the $SU(2)_T \times SU(2)_S$ subgroup, they do not change T, S . This is only possible by applying a proper $SU(4)$ generator such as $\tau^- \times \sigma^-/4$. It creates the mixed state

$$\frac{1}{\sqrt{2}} |n^\downarrow p^\uparrow + p^\uparrow n^\downarrow\rangle. \quad (25.19)$$

Combining this with (25.18), we now form the state

$$|0, 0; 0, 0\rangle = \frac{1}{\sqrt{4}} |n^\downarrow p^\uparrow - p^\downarrow n^\uparrow - n^\uparrow p^\downarrow + p^\uparrow n^\downarrow\rangle, \quad (25.20)$$

which is orthogonal to (25.18) and has the properties:

$$\frac{\tau^-}{2} |0, 0; 0, 0\rangle = \frac{1}{2} |n^\downarrow n^\uparrow - n^\uparrow n^\downarrow - n^\uparrow n^\downarrow + n^\uparrow n^\downarrow\rangle = 0, \quad (25.21)$$

$$\frac{\sigma^-}{2} |0, 0; 0, 0\rangle = \frac{1}{2} |n^\downarrow n^\downarrow - p^\downarrow n^\downarrow - n^\downarrow p^\downarrow + p^\downarrow n^\downarrow\rangle = 0, \quad (25.22)$$

showing that it is a singlet under isospin and spin operations, as indicated by the zeros in the ket on the left-hand side of (25.20). Thus we have found an irreducible decuplet of $SU(4)$ with 10 states, and the $[T, S]$ decomposition

$$10 = [1, 1] + [0, 0]. \quad (25.23)$$

²In accordance with the standard names for isospin and spin matrices $\boldsymbol{\tau}, \boldsymbol{\sigma}$ we shall denote half the isospin generators $\boldsymbol{\tau}/2$ by $\mathbf{T}$ rather than $\mathbf{I}$, as is customary in nuclear physics, and $\boldsymbol{\sigma}/2$ by $\mathbf{S}$.

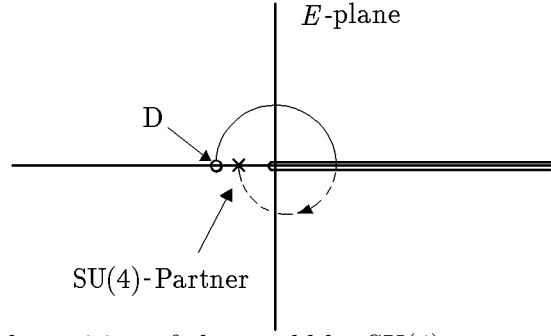


FIGURE 25.1 Pole position of the would-be $SU(4)$ -partner of the deuteron with spin-1 and isospin-0. It is close to the D-pole but not a particle since it hides in the complex energy plane just below the two-particle cut.

In addition, there is a six-dimensional representation consisting of the states

$$\begin{aligned}
 |0, 0; 1, 1\rangle &= \frac{1}{\sqrt{2}} |p^\uparrow n^\uparrow - n^\uparrow p^\uparrow\rangle, \\
 \frac{\sigma^-}{2} |0, 0; 1, 1\rangle &= \frac{1}{\sqrt{2}} |p^\downarrow n^\uparrow + p^\uparrow n^\downarrow - n^\downarrow p^\uparrow - n^\uparrow p^\downarrow\rangle = \sqrt{2} |0, 0; 1, 0\rangle, \\
 \frac{\sigma^-}{2} |0, 0; 1, 0\rangle &= |p^\downarrow n^\downarrow - n^\downarrow p^\downarrow\rangle = \sqrt{2} |0, 0; 1, -1\rangle \\
 \frac{\sigma^- \times \tau^-}{4} |0, 0; 1, 1\rangle &= \frac{1}{\sqrt{2}} |-n^\downarrow n^\uparrow + n^\uparrow n^\downarrow\rangle = |1, -1; 0, 0\rangle \\
 \frac{\tau^+}{2} |1, -1; 0, 0\rangle &= \frac{1}{\sqrt{2}} |-p^\downarrow n^\uparrow - n^\downarrow p^\uparrow + p^\uparrow n^\downarrow + n^\uparrow p^\downarrow\rangle = \sqrt{2} |1, 0; 0, 0\rangle \\
 \frac{\tau^+}{2} |1, 0; 0, 0\rangle &= |-p^\downarrow p^\uparrow + p^\uparrow p^\downarrow\rangle = \sqrt{2} |1, 1; 0, 0\rangle.
 \end{aligned} \tag{25.24}$$

These have the $[T, S]$ -content denoted by

$$6 = [1, 0] + [0, 1]. \tag{25.25}$$

The representation 6 is an irreducible content of the tensor product, i.e.,

$$4 \times 4 = 10 + 6. \tag{25.26}$$

The deuteron is a state in the irreducible representation 6. It has $[T, S] = [0, 1]$, i.e., it is an isosinglet vector particle transforming like the $SU(4)$ generator $\boldsymbol{\tau}/2 \times 1$. If $SU(4)$ is supposed to be a good approximate symmetry, there should also be a partner $[1, 0]$, i.e., a spin-zero isotriplet transforming like the $SU(4)$ generator $1 \times \boldsymbol{\sigma}/2$. This does not really exist. However, the singlet NN scattering length is very large in the $T = 1$ state, indicating a bound state just around the cut of the two-particle continuum in the energy plane. The symmetry breaking prevents these $SU(4)$ partners from appearing as physical particles [2].

In elementary-particle physics, the group $SU(4)$ combining isospin and spin has played quite an important historical role. There, up and down quarks with spin up and down are identified with the representation 4 of $SU(4)$:

$$4 = \begin{pmatrix} u^\uparrow \\ u^\downarrow \\ d^\uparrow \\ d^\downarrow \end{pmatrix}. \quad (25.27)$$

For mesons, the representation 15 in $4 \times \bar{4} = 15 + 1$ extends the isospin triplet pseudoscalars π^+, π^0, π^- , which transform in the same way as the generators of the isospin subgroup τ^a . The vector mesons ρ^+, ρ^0, ρ^- are assigned to the generators $\tau^a \times \sigma^i$, plus an isosinglet σ^i which is identified with the ω meson. The symmetry breaking, however, is extremely large since

$$\begin{aligned} m_\pi &\approx 135 \text{ MeV}, \\ m_\rho &\approx 770 \text{ MeV}, \\ m_\omega &\approx 783 \text{ MeV}. \end{aligned} \quad (25.28)$$

For the nucleons p, n , the $SU(4)$ symmetry is much better. Taking three up and down quarks with spin up and down, the three Young tableaux

$$\begin{array}{|c|c|c|}, & \begin{array}{|c|c|} \hline & \\ \hline & \\ \hline \end{array}, & \begin{array}{|c|} \hline \\ \hline \\ \hline \\ \hline \end{array} \end{array} \quad (25.29)$$

possess, according to the general dimension formulas (24.156)–(24.158), the dimensions

$$\frac{n(n+1)(n+2)}{6}, \quad \frac{(n-1)n(n+1)}{3}, \quad \frac{n(n-1)(n-2)}{6}, \quad (25.30)$$

the second appearing twice. These tableaux represent a symmetric representation 20, two mixed representations 20, and one antisymmetric representation 4. Actually, the latter 4 is equivalent to the complex conjugate $\bar{4}$ of the fundamental representation. To see this we note that the completely antisymmetric representation

$$\begin{array}{|c|} \hline \\ \hline \\ \hline \\ \hline \end{array} \quad (25.31)$$

of rank 4 is one-dimensional which means that the antisymmetric 4 must have met with a $\bar{4}$ to form an invariant.

In order to find the isospin and spin contents of the representations (25.29), we write the $SU(4)$ index as α, α' , where α are the two isospin indices and α' the spin indices. The representation 4 is a doublet with respect to each subgroup

$$\boxed{a\alpha} = 2 \times 2. \quad (25.32)$$

The Young tableau $\square\square = 10$ is symmetric under the simultaneous exchange of both indices. Hence, with respect to the two subgroups it can become a product of symmetric tensors or antisymmetric tensors

$$\begin{array}{c} \boxed{a\alpha}\boxed{b\beta} \\ 10 \end{array} = \begin{array}{c} \boxed{a}\boxed{b} \\ 3 \end{array} \times \begin{array}{c} \boxed{\alpha}\boxed{\beta} \\ 3 \end{array} + \begin{array}{c} \boxed{a} \\ 1 \end{array} \times \begin{array}{c} \boxed{\alpha} \\ 1 \end{array} \times \begin{array}{c} \boxed{b} \\ 1 \end{array} \times \begin{array}{c} \boxed{\beta} \\ 1 \end{array}. \quad (25.33)$$

Similarly

$$\begin{array}{c} \boxed{a\alpha} \\ \boxed{b\beta} \\ 6 \end{array} = \begin{array}{c} \boxed{a} \\ \boxed{b} \\ 1 \end{array} \times \begin{array}{c} \boxed{\alpha}\boxed{\beta} \\ 3 \end{array} + \begin{array}{c} \boxed{a}\boxed{b} \\ 3 \end{array} \times \begin{array}{c} \boxed{\alpha} \\ \boxed{\beta} \\ 1 \end{array}. \quad (25.34)$$

To obtain all irreducible tensors of rank 3 we multiply $\square\square$ and $\begin{array}{c} \square \\ \square \end{array}$ by another box, and find within $SU(4)$ the decomposition

$$\begin{array}{c} \square\square \\ 10 \end{array} \times \begin{array}{c} \square \\ 4 \end{array} = \begin{array}{c} \square\square\square \\ 20 \end{array} + \begin{array}{c} \square\square \\ \square \\ 20 \end{array}, \quad (25.35)$$

and

$$\begin{array}{c} \square \\ \square \\ 6 \end{array} \times \begin{array}{c} \square \\ 4 \end{array} = \begin{array}{c} \square\square \\ \square \\ 20 \end{array} + \begin{array}{c} \square \\ \square \\ \square \\ 4 \end{array}. \quad (25.36)$$

As far as the isospin and spin contents are concerned, we multiply the decomposition (25.33) of the 10 by

$$\begin{array}{c} \square \\ 4 \end{array} = \begin{array}{c} \square \\ 2 \end{array} \times \begin{array}{c} \square \\ 2 \end{array}. \quad (25.37)$$

Thus the product 10×4 contains the isospin and spin products

$$\begin{array}{c} \square\square \\ 3 \end{array} \times \begin{array}{c} \square \\ 2 \end{array} = \begin{array}{c} \square\square\square \\ 4 \end{array} + \begin{array}{c} \square\square \\ \square \\ 2 \end{array} \quad (25.38)$$

$$\begin{array}{c} \square \\ \square \\ 1 \end{array} \times \begin{array}{c} \square \\ 2 \end{array} = \begin{array}{c} \square\square \\ \square \\ 2 \end{array}. \quad (25.39)$$

In the second case there is only one product since $\begin{array}{c} \square \\ \square \end{array}$ is one-dimensional. Hence we can decompose 10×4 as follows

$$\begin{array}{c} \square\square \\ 10 \end{array} \times \begin{array}{c} \square \\ 4 \end{array} = \left(\begin{array}{c} \square\square\square \\ 4 \end{array} + \begin{array}{c} \square\square \\ \square \\ 2 \end{array} \right) \times \left(\begin{array}{c} \square\square\square \\ 4 \end{array} + \begin{array}{c} \square\square \\ \square \\ 2 \end{array} \right) \quad (25.40)$$

$$+ \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} . \quad (25.41)$$

On the left-hand side, the product reduces to

$$\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} + \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} . \quad (25.42)$$

20 20

It is easy to read off which products on the right-hand side belong to these two representations:

$$\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} = \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} \times \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} + \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \quad (25.43)$$

20 4 4 2 2

$$\begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} = \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} + \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \times \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array} \\ + \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} . \quad (25.44)$$

20 4 2 2 4 2 2

Thus the symmetric representation 20 consists of a spin- $\frac{1}{2}$ isospin- $\frac{1}{2}$, and a spin- $\frac{3}{2}$ isospin- $\frac{3}{2}$ multiplet. They are associated with the following particles: The spin- $\frac{1}{2}$ isospin- $\frac{1}{2}$ states are the two isospin states of the nucleon p and n . The spin- $\frac{3}{2}$ isospin- $\frac{3}{2}$ states contain the first pion-nucleon resonance $\Delta(1230)$, plus its isospin partners with the charge states $-, 0, +, ++$. All particles have intrinsic parity $+$. The mixed 20 consists of a spin- $\frac{3}{2}$ isospin- $\frac{1}{2}$, a spin- $\frac{1}{2}$ isospin- $\frac{3}{2}$, and spin- $\frac{1}{2}$ isospin- $\frac{1}{2}$ multiplet. These states are also found experimentally in pion-nucleon scattering as resonances of negative parity.

The content of the antisymmetric SU(4) representation

$$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = \bar{4}$$

is obviously 2×2 , i.e., an isospin- $\frac{1}{2}$ spin- $\frac{1}{2}$ multiplet. It is associated with the spin-parity pion-nucleon resonance $N(1440)$ of spin-parity $S^P = \frac{1}{2}^+$.

25.2 Approximate SU(6)-Symmetry in Strong Interactions

With the success of the approximate symmetry SU(4) in nuclear and particle physics, the question arose whether there exists an extension of the symmetry group which

includes also the internal symmetry SU(3). The three quarks with spin-up and -down form a sextet of particles

$$q = \begin{pmatrix} u^\uparrow \\ u^\downarrow \\ d^\uparrow \\ d^\downarrow \\ s^\uparrow \\ s^\downarrow \end{pmatrix}. \quad (25.45)$$

Hence the most straightforward extension would be SU(6). This group is generated by the 35 matrices

$$\frac{\lambda^a}{2} \times 1, \quad 1 \times \frac{\sigma^i}{2}, \quad \frac{\lambda^a}{2} \times \frac{\sigma^i}{2}. \quad (25.46)$$

The only non-trivial commutation rules are

$$\left[\frac{\lambda^a \times \sigma^i}{2}, \frac{\lambda^b \times \sigma^j}{2} \right] = i d_{abc} \epsilon_{ijk} \frac{1}{2} \lambda^c \times \sigma^k + i f_{abc} \delta_{ij} \frac{1}{2} \lambda^c \times 1 + i \frac{2}{3} \delta_{ab} \epsilon_{ijk} 1 \times \frac{1}{2} \sigma^k. \quad (25.47)$$

Since in SU(4) the representation 4×4 contains the pseudoscalar π and vector mesons ρ, ω , we expect the representation $6 \times \bar{6}$ to extend these multiplets by their SU(3)-partners. The representation $6 \times \bar{6}$ decomposes into $35 + 1$, with the particles in the 35-representation having the transformation properties of the 35 group generators (25.46). Thus there is now an SU(3)-octet of pseudoscalar mesons which transform like the generators $\lambda^a \times 1/2$. In addition, there is an SU(3)-octet of vector mesons ρ, ω, K^* . These are 24 states which transform like the generators $\lambda^a \times \sigma^i/2$, and there is an SU(3)-singlet vector meson $\varphi(1020)$ which transforms like the three generators $1 \times \sigma^i/2$. More accurately the states ω and ϕ will be mixed with each other.

These meson multiplets are quite widely separated in mass, implying that the symmetry SU(6) is strongly broken. Still, this would-be symmetry group organizes nicely the most important low-lying meson states, as illustrated in Fig. 25.2.

As in the case of SU(4)-symmetry, the situation is much better for baryons. The nucleons and their strange partners as well as the first nucleon resonances and their strange partners all lie in a single irreducible multiplet of three-quark states. They decompose as follows:

$$\begin{array}{c} \square \\ 6 \end{array} \times \begin{array}{c} \square \\ 6 \end{array} \times \begin{array}{c} \square \\ 6 \end{array} = \begin{array}{c} \square \square \square \\ 56 \end{array} + 2 \times \begin{array}{c} \square \square \\ \square \\ 70 \end{array} + \begin{array}{c} \square \\ \square \\ \square \\ 20 \end{array}. \quad (25.48)$$

In order to find the SU(3)- and spin-contents of these multiplets we decompose, as in the case of SU(4),

$$\begin{array}{c} \square \\ \alpha\alpha \\ 6 \end{array} = \begin{array}{c} \square \\ a \\ 3 \end{array} \times \begin{array}{c} \square \\ \alpha \\ 2 \end{array}, \quad (25.49)$$

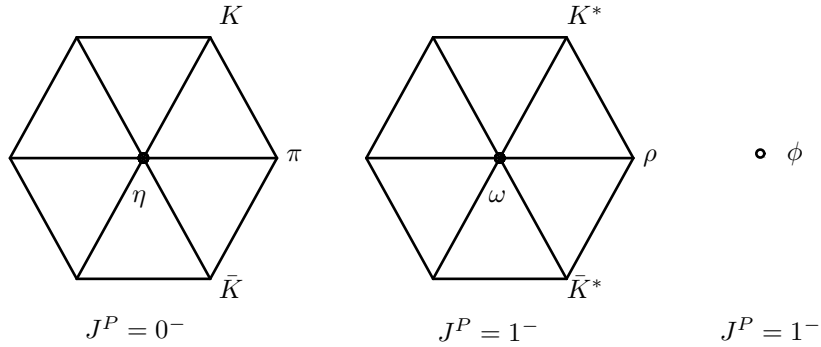


FIGURE 25.2 Pseudoscalar and vector mesons of the 35-representation of SU(6).

and form the symmetric and antisymmetric products of two representations 6. They are 21- and 15-dimensional and their SU(3) and spin contents are given by

$$\begin{array}{c} \boxed{a\alpha} \boxed{b\beta} \\ 21 \end{array} = \begin{array}{c} \boxed{a} \boxed{b} \\ 6 \end{array} \times \begin{array}{c} \boxed{\alpha} \boxed{\beta} \\ 3 \end{array} + \begin{array}{c} \boxed{a} \\ \boxed{b} \\ \bar{3} \end{array} \times \begin{array}{c} \boxed{\alpha} \\ \boxed{\beta} \\ 1 \end{array},$$

$$\begin{array}{c} \boxed{a\alpha} \\ \boxed{b\beta} \\ 15 \end{array} = \begin{array}{c} \boxed{a} \boxed{b} \\ 6 \end{array} \times \begin{array}{c} \boxed{\alpha} \\ \boxed{\beta} \\ 1 \end{array} + \begin{array}{c} \boxed{a} \\ \boxed{b} \\ \bar{3} \end{array} \times \begin{array}{c} \boxed{\alpha} \boxed{\beta} \\ 3 \end{array}.$$

Multiplying the 21 by a further 6, we find

$$\begin{aligned} \begin{array}{c} \boxed{} \boxed{} \\ 21 \end{array} \times \begin{array}{c} \boxed{} \\ 6 \end{array} &= \begin{array}{c} \boxed{} \boxed{} \boxed{} \\ 56 \end{array} + \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 70 \end{array} \\ &= \left(\begin{array}{c} \boxed{} \boxed{} \\ 10 \end{array} + \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 8 \end{array} \right) \times \left(\begin{array}{c} \boxed{} \boxed{} \boxed{} \\ 4 \end{array} + \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 2 \end{array} \right) \\ &\quad + \left(\begin{array}{c} \boxed{} \\ \boxed{} \\ \boxed{} \\ 1 \end{array} \times \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 8 \end{array} \right) \times \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 2 \end{array}. \end{aligned} \quad (25.50)$$

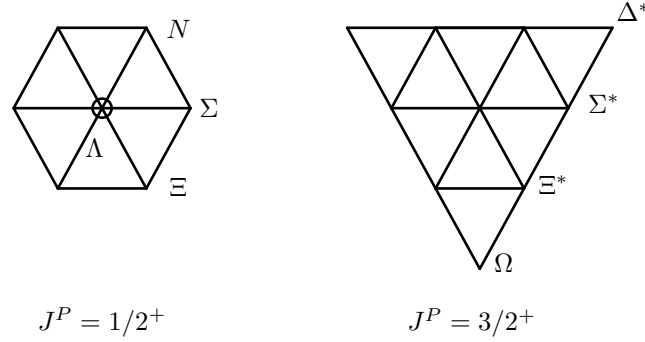
It is then easy to read off the SU(3) and spin contents on the right-hand side

$$\begin{array}{c} \boxed{} \boxed{} \boxed{} \\ 56 \end{array} = \begin{array}{c} \boxed{} \boxed{} \boxed{} \\ 10 \end{array} \times \begin{array}{c} \boxed{} \boxed{} \boxed{} \\ 4 \end{array} + \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 8 \end{array} \times \begin{array}{c} \boxed{} \boxed{} \\ \boxed{} \\ 2 \end{array},$$

$$\begin{array}{c} \square \square \\ \square \end{array} = \begin{array}{c} \square \square \square \\ 10 \end{array} \times \begin{array}{c} \square \square \\ \square \\ 2 \end{array} + \begin{array}{c} \square \square \\ \square \\ 8 \end{array} \times \begin{array}{c} \square \square \square \\ 4 \end{array} \\
+ \begin{array}{c} \square \square \\ \square \\ 8 \end{array} \times \begin{array}{c} \square \square \\ \square \\ 2 \end{array} + \begin{array}{c} \square \\ \square \\ \square \\ 1 \end{array} \times \begin{array}{c} \square \square \\ \square \\ 2 \end{array}. \quad (25.51)$$

Thus the 56 consists of a decuplet of spin $\frac{3}{2}$ and an octet of spin $\frac{1}{2}$. These can be associated with the decuplet of nucleon resonances and the nucleon octet, all of positive parity as shown in Fig. 25.3.

FIGURE 25.3 The $SU(3)$ -content of particles in the 56-representation of $SU(6)$ containing the $J^P = 1/2^+$ nucleons and the $J^P = 3/2^+$ resonances.



The 70 consists of a decuplet of spin $\frac{1}{2}$, an octet of spin $\frac{3}{2}$, an octet of spin $\frac{1}{2}$, and a singlet of spin- $\frac{1}{2}$ states, thus extending the isospin $SU(4)$ -multiplets of negative parity in Eq. (25.44) by their $SU(3)$ -partners as shown in Fig. 25.4.

The $SU(3) \times SU(2)$ -contents of the antisymmetric $SU(6)$ representation

$$\begin{array}{c} \square \\ \square \\ \square \\ 20 \end{array}$$

are easily written down as

$$\begin{array}{c} \square \\ \square \\ \square \\ 20 \end{array} = \begin{array}{c} \square \square \square \\ 8 \end{array} \times \begin{array}{c} \square \\ \square \\ \square \\ 2 \end{array} + \begin{array}{c} \square \\ \square \\ \square \\ 1 \end{array} \times \begin{array}{c} \square \square \square \\ 4 \end{array}. \quad (25.52)$$

The octet states could possibly be the spin $\frac{1}{2}$ -particles of positive parity shown in Fig. 25.5. The $SU(3)$ -singlet $\frac{3}{2}^+$ partner of them has not yet been found.

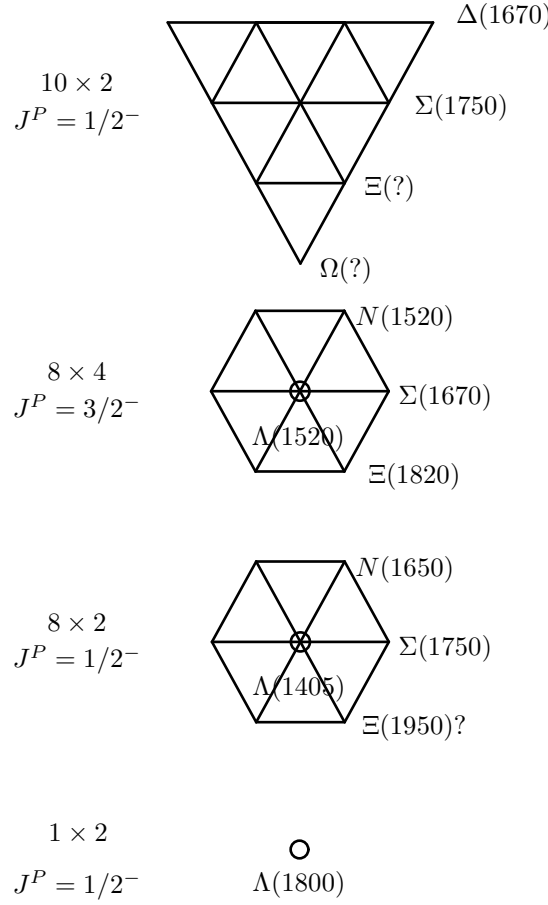


FIGURE 25.4 Nucleon resonances of negative parity in the 70-representation of SU(6).

Let us now study the states of the 56-representation in more detail. The state of highest weight is the $\Delta^{++}(1235)$ resonance of spin $\frac{3}{2}$

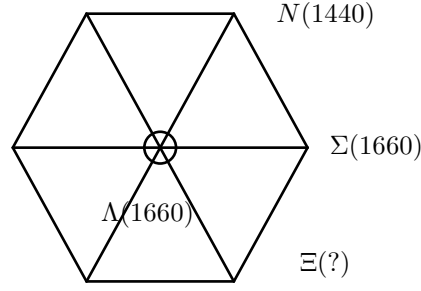
$$\Delta^{++}(1235)^{\uparrow\uparrow} = |u^{\uparrow}u^{\uparrow}u^{\uparrow}\rangle. \quad (25.53)$$

By lowering the third components of spin and isospin once, we obtain the normalized state

$$\begin{aligned} \Delta^{+}(1235)^{\uparrow} = \frac{1}{3} & \left| d^{\downarrow}u^{\uparrow}u^{\uparrow} + u^{\downarrow}d^{\uparrow}u^{\uparrow} + u^{\downarrow}u^{\uparrow}d^{\uparrow} \right. \\ & + d^{\uparrow}u^{\downarrow}u^{\uparrow} + u^{\uparrow}d^{\downarrow}u^{\uparrow} + u^{\uparrow}u^{\downarrow}d^{\uparrow} \\ & \left. + d^{\uparrow}u^{\uparrow}u^{\downarrow} + u^{\uparrow}d^{\uparrow}u^{\downarrow} + u^{\uparrow}u^{\uparrow}d^{\downarrow} \right\rangle. \end{aligned} \quad (25.54)$$

Applying to this the operator $\lambda^3\sigma^3$, we find

$$\lambda^3\sigma^3\Delta^{+}(1235)^{\uparrow} = \frac{1}{3} \left| 3(d^{\downarrow}u^{\uparrow}u^{\uparrow} + u^{\uparrow}d^{\downarrow}u^{\uparrow} + u^{\uparrow}u^{\uparrow}d^{\downarrow}) \right|$$

FIGURE 25.5 Octet of spin-parity $\frac{1}{2}^+$ -baryons.

$$-(u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\downarrow u^\uparrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow) \rangle. \quad (25.55)$$

This should be a mixture of $\Delta^+(1235)^\uparrow$ and a proton $p^\uparrow$.

Since the proton is orthogonal to $\Delta^+(1235)^\uparrow$, we can immediately guess a normalized proton state:

$$p^\uparrow = \frac{\sqrt{2}}{3} \left| d^\downarrow u^\uparrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\uparrow d^\downarrow \right. \\ \left. - \frac{1}{2} (u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow) \right\rangle. \quad (25.56)$$

To ensure that it is a pure proton state we simply apply the isospin raising operator and find that the state is annihilated, thus guaranteeing the total isospin to be $1/2$. Applying the isospin lowering operator, we obtain the neutron state

$$n^\uparrow = -\frac{\sqrt{2}}{3} \left| d^\uparrow d^\uparrow u^\downarrow + d^\uparrow u^\downarrow d^\uparrow + u^\downarrow d^\uparrow d^\uparrow \right. \\ \left. - \frac{1}{2} (d^\downarrow u^\uparrow d^\uparrow + d^\downarrow d^\uparrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow d^\downarrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow u^\uparrow d^\downarrow) \right\rangle. \quad (25.57)$$

As an interesting consequence of $SU(6)$, we calculate the ratio between the magnetic moment of neutron and proton. For this we assume that the magnetic moment operator transforms under $SU(3)$ like the charge operator which is given by the generators

$$Q = \lambda^Q = \frac{1}{2} \left(\lambda^3 + \frac{1}{\sqrt{3}} \lambda^8 \right). \quad (25.58)$$

Under rotations, it must transform like a spin operator $\boldsymbol{\sigma}$. Thus the magnetic moment operator should be proportional to the following generator in $SU(6)$:

$$\boldsymbol{\mu} = \frac{1}{2} \left(\lambda^3 + \frac{1}{\sqrt{3}} \lambda^8 \right) \times \boldsymbol{\sigma}. \quad (25.59)$$

We now apply the third component of this

$$\mu_3 = \frac{1}{2} \left(\lambda^3 + \frac{1}{\sqrt{3}} \lambda^8 \right) \times \sigma^3, \quad (25.60)$$

to the quark states and use the eigenvalues listed in Table 25.3. In front of the states $|p^\uparrow\rangle$ and $|n^\uparrow\rangle$, this yields

$$\mu_3|p^\uparrow\rangle = \frac{\sqrt{2}}{3} \left| \frac{5}{3} (d^\downarrow u^\uparrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\uparrow d^\downarrow) \right. \\ \left. - \frac{1}{2} \left(-\frac{1}{3} \right) (u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow) \right\rangle, \quad (25.61)$$

$$\mu_3|n^\uparrow\rangle = \frac{\sqrt{2}}{3} \left| -\frac{4}{3} (d^\uparrow d^\uparrow u^\downarrow + d^\uparrow u^\downarrow d^\uparrow + u^\downarrow d^\uparrow d^\uparrow) \right. \\ \left. - \frac{1}{2} \left(\frac{2}{3} \right) (d^\downarrow u^\uparrow d^\uparrow + d^\downarrow d^\uparrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow d^\downarrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow u^\uparrow d^\downarrow) \right\rangle. \quad (25.62)$$

Hence we find the matrix elements of the magnetic moments as being proportional to

$$\langle p^\uparrow | \mu_3 | p^\uparrow \rangle = \frac{2}{9} \left(\frac{5}{3} \cdot 3 - \frac{1}{3} \cdot \frac{6}{4} \right) = 1, \quad (25.63)$$

$$\langle n^\uparrow | \mu_3 | n^\uparrow \rangle = \frac{2}{9} \left(-\frac{4}{3} \cdot 3 + \frac{2}{3} \cdot \frac{6}{4} \right) = -\frac{2}{3}. \quad (25.64)$$

These imply a ratio of magnetic moments

$$\frac{\mu_n}{\mu_p} = -\frac{2}{3}. \quad (25.65)$$

Experimentally, the magnetic moments are

$$\begin{aligned} \mu_p &= 2.7928444 \pm 0.0000011, \\ \mu_n &= -1.91304308 \pm 0.00000054, \end{aligned} \quad (25.66)$$

in units of $c\hbar/2m_p c = 505 \times 10^{-24}$ erg/Gauss. Thus the ratio is $\approx -2.055/3$, in excellent agreement with the SU(6)-prediction (25.65).

By the same method we can calculate all rates of the radiative decays of the decuplet resonances $10 \rightarrow 8 + \gamma$ in terms of only one unknown overall size parameter.

The prediction of the ratios of the magnetic moments is possible due to the fact that in the irreducible multiplet 56 of the symmetry group SU(6), the SU(3)-octet operator $\lambda^a \times \sigma^3/2$ has, between the octet states of nucleons, a specific ratio of

TABLE 25.3 Eigenvalues of charge and other operators on quark states.

q	$u^\uparrow$	$u^\downarrow$	$d^\uparrow$	$d^\downarrow$	$s^\uparrow$	$s^\downarrow$
$\lambda^3 \times \sigma^3$	1	-1	1	-1	0	0
$(\lambda^8/\sqrt{3}) \times \sigma^3$	$\frac{1}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{2}{3}$	$\frac{2}{3}$
$Q \times \sigma_3$	$\frac{2}{3}$	$-\frac{2}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$

symmetric and antisymmetric couplings (which within $SU(3)$ would be arbitrary). Let us express the two couplings in terms of the irreducible matrix elements F and D as follows

$$\begin{aligned} \left\langle b \left| \frac{\lambda^a}{2} \times \sigma^3 \right| c \right\rangle &= F \cdot (-if_{ab^*c}) + D \cdot (d_{ab^*c}) \\ &\equiv F \cdot (F_a)_{b^*c} + D \cdot (D_a)_{b^*c}. \end{aligned} \quad (25.67)$$

Then we find between protons with the octet components $(4 + i\sqrt{5})/\sqrt{2}$

$$(F_3)_{pp} = f_{345} = \frac{1}{2}, \quad (D_3)_{pp} = d_{344} = \frac{1}{2}, \quad (25.68)$$

and between neutrons with the components $(6 + i7)/\sqrt{2}$

$$(F_3)_{nn} = -f_{367} = -\frac{1}{2}, \quad (D_3)_{nn} = d_{366} = -\frac{1}{2}. \quad (25.69)$$

The $a = 8$ components of F_a, D_a have the matrix elements

$$\begin{aligned} (F_8)_{pp} = f_{845} &= \sqrt{\frac{3}{2}}, & (D_8)_{pp} = d_{866} &= -\frac{1}{2\sqrt{3}} \\ (F_8)_{nn} = f_{867} &= \sqrt{\frac{3}{2}}, & (D_8)_{nn} = d_{866} &= -\frac{1}{2\sqrt{3}}. \end{aligned} \quad (25.70)$$

The matrix elements of the magnetic moment operator

$$\mu_3 = \lambda^Q \times \sigma^3 \equiv \frac{1}{2}(\lambda^3 + \frac{1}{\sqrt{3}}\lambda^8)\sigma^3 \quad (25.71)$$

are therefore given in terms of the irreducible matrix elements F and D by

$$\begin{aligned} \langle p | \mu_3 | p \rangle &= F \cdot \left(\frac{1}{2} + \frac{1}{2} \right) + D \cdot \left(\frac{1}{2} - \frac{1}{6} \right) = \left(F + \frac{1}{3}D \right), \\ \langle n | \mu_3 | n \rangle &= F \cdot \left(-\frac{1}{2} + \frac{1}{2} \right) + D \cdot \left(-\frac{1}{2} - \frac{1}{6} \right) = -\frac{2}{3}D. \end{aligned} \quad (25.72)$$

The ratio is

$$\frac{\langle p | \mu_3 | p \rangle}{\langle n | \mu_3 | n \rangle} = \frac{F/D + \frac{1}{3}}{-\frac{2}{3}}. \quad (25.73)$$

This holds on the basis of only $SU(3)$ symmetry. Inserting the $SU(6)$ result (25.65), we see that $SU(6)$ fixes the F/D ratio

$$\frac{F}{D} = \frac{2}{3}. \quad (25.74)$$

The absolute values of the irreducible matrix elements of the operators

$$\frac{\lambda^3}{2} \times \sigma^3, \quad \frac{\lambda^8}{2} \times \sigma^3 \quad (25.75)$$

are also known from the above results(25.63) and (25.64):

$$F + D \frac{1}{3} = 1, \quad -\frac{2}{3}D = -\frac{2}{3}, \quad (25.76)$$

so that

$$F = \frac{2}{3}, \quad D = 1. \quad (25.77)$$

It is straight-forward to calculate the magnetic moment of any other members of the octet, for instance of $\Sigma^+ \triangleq (1 + i2)/\sqrt{2}$:

$$\begin{aligned} \langle \Sigma^+ | \mu_3 | \Sigma^+ \rangle &= F \cdot (-if_{Q12}) + D \cdot d_{Q11} \\ &= F \cdot \left[\frac{1}{2} \left(f_{312} + \frac{1}{\sqrt{3}} f_{812} \right) \right] + D \cdot \left[\frac{1}{2} \left(d_{311} + \frac{1}{\sqrt{3}} d_{811} \right) \right] \\ &= \frac{1}{2}F + \frac{1}{6}D = \frac{1}{2}. \end{aligned} \quad (25.78)$$

This implies the ratio

$$\frac{\langle p | \mu_3 | p \rangle}{\langle \Sigma^+ | \mu_3 | \Sigma^+ \rangle} = 2. \quad (25.79)$$

In fact, the fastest way to find the F/D -ratio is by calculating the matrix elements of $\lambda^3 \times \sigma^3/2$ from the SU(6) wave functions. Between protons we find immediately

$$\left\langle p \left| \frac{\lambda^3}{2} \times \sigma^3 \right| p \right\rangle = \frac{5}{6}. \quad (25.80)$$

Using the wave function

$$\begin{aligned} |\Sigma^{+\uparrow}\rangle &= \frac{\sqrt{2}}{3} \left(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow \right) \\ &\quad - \frac{1}{2} (u^\uparrow u^\downarrow s^\uparrow + u^\downarrow s^\uparrow u^\uparrow + s^\uparrow u^\uparrow u^\downarrow + u^\downarrow u^\uparrow s^\uparrow + u^\uparrow s^\uparrow u^\downarrow + s^\uparrow u^\downarrow u^\uparrow), \end{aligned} \quad (25.81)$$

we obtain

$$\left\langle \Sigma^+ \left| \frac{\lambda^3}{2} \times \sigma^3 \right| \Sigma^+ \right\rangle = \frac{2}{3}. \quad (25.82)$$

In terms of the irreducible matrix elements F, D , the corresponding matrix elements would be in general

$$\left\langle p \left| \frac{\lambda^3}{2} \times \sigma^3 \right| p \right\rangle = \frac{F}{2} + \frac{D}{2}, \quad \left\langle \Sigma^+ \left| \frac{\lambda^3}{2} \times \sigma^3 \right| p \right\rangle = F. \quad (25.83)$$

Hence we identify, once more,

$$F = \frac{2}{3}, \quad D = 1. \quad (25.84)$$

The magnetic moment μ^* for the transition $p \rightarrow \Delta$ is found by multiplying $\mu_3 |p^\uparrow\rangle$ from the left by $\langle\Delta^{+\uparrow}|$. This gives

$$\mu^* \equiv \langle\Delta^{+\uparrow}|\mu_3|p^\uparrow\rangle = \frac{\sqrt{2}}{9} \left[\frac{5}{3} \cdot 3 + \frac{1}{6} \cdot 6 \right] = \frac{2}{3}\sqrt{2}. \quad (25.85)$$

A comparison with the proton matrix element (25.63) yields the $SU(6)$ prediction

$$\mu^* = \frac{2}{3}\sqrt{2}\mu_p. \quad (25.86)$$

Experimentally one finds, from the $\Delta(1236)$ resonance in the cross section of the photoproduction process

$$\gamma + p \rightarrow \pi^0 + p, \quad (25.87)$$

the value

$$\mu_{\text{exp}}^* \approx (1.28 - 0.01) \cdot \mu^*. \quad (25.88)$$

This is not in quite such a good agreement as the proton-to-neutron ratio (25.65). We must, however, keep in mind that the symmetry $SU(6)$ is significantly broken, and that the comparison with the data requires matrix elements of μ between states whose normalization factors can depend on the masses of the particles. Thus one is bound to commit errors of the order of the relative mass differences within the experimental multiplets, herethere between the $\Delta(1232)$ and the proton $p(938)$. These can easily account for the 28 % discrepancy in the magnetic moment prediction (25.88).

It should be noted that the ratio $g^*/g \approx 1.07$, found in Eq. (24.212) from the experimental decay rates of the Δ -resonance, is a manifestation of $SU(4)$ -symmetry. Since the Δ -resonance and the nucleon are in the same $SU(4)$ -multiplet 20 (corresponding to the $SU(6)$ -multiplet 56), all pion couplings are controlled by only one irreducible matrix element. In calculating them we have to remember that, in order to preserve parity, the pseudoscalar pion must emerge in a p -wave. The matrix element between a Δ^+ -resonance and a proton

$$\frac{1}{M_N} \bar{u}_\mu(\mathbf{0}, \tfrac{1}{2}) u(\mathbf{p}_N, s'_3) i q_\pi^\mu \quad (25.89)$$

has, for small momentum p_N in the z -direction, the limiting form

$$-i \left[\sqrt{\frac{2}{3}} \frac{p_N}{M_N} \bar{u}(\mathbf{0}, \tfrac{1}{2}) u(\mathbf{0}, \tfrac{1}{2}) + \frac{1}{\sqrt{6} M_N} (p_N^1 - i p_N^2) u(0, \tfrac{1}{2}) \right]. \quad (25.90)$$

Thus it can be written in terms of two component spinors as

$$-2\sqrt{\frac{2}{3}} \frac{\mathbf{p}_N}{M_N} \chi(\tfrac{1}{2}) \boldsymbol{\sigma} \chi(\tfrac{1}{2}). \quad (25.91)$$

The p -wave emission leads to the appearance of a spin matrix σ^i acting upon the helicity index of the nucleon. The same thing is observed for the matrix elements in the pseudoscalar pion nucleon coupling

$$\bar{u}(\mathbf{0}, \tfrac{1}{2}) i\gamma_5 u(\mathbf{p}_N, \tfrac{1}{2}). \quad (25.92)$$

For small momentum, this becomes

$$-i(\chi(\tfrac{1}{2}), \chi(\tfrac{1}{2})) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \gamma_0 \begin{pmatrix} e^{-\zeta\sigma/2} \chi(\tfrac{1}{2}) \\ e^{\zeta\sigma/2} \chi(\tfrac{1}{2}) \end{pmatrix} \approx -i \frac{\mathbf{p}_N}{M_N} \chi(\tfrac{1}{2}) \boldsymbol{\sigma} \chi(\tfrac{1}{2}). \quad (25.93)$$

We now add the internal SU(2)-structure and the SU(4)-matrix associated with the emission of the pion in the z -direction of Δ^+ . The pion transforms like the tensor operator

$$\pi^a \hat{=} \tau^a \sigma^3, \quad (25.94)$$

so that the ratio of the couplings $p\pi^0 p$ and $\Delta^+ \pi^0 p$ can be found quite simply by applying $\tau^3 \sigma^3$ to the proton state

$$p = \frac{\sqrt{2}}{3} \left[u^\uparrow u^\uparrow d^\downarrow + u^\uparrow d^\downarrow u^\uparrow + d^\downarrow u^\uparrow u^\uparrow - \frac{1}{2} (u^\uparrow u^\downarrow d^\uparrow + u^\uparrow d^\uparrow u^\downarrow + u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + d^\uparrow u^\downarrow u^\uparrow) \right], \quad (25.95)$$

which gives

$$\begin{aligned} \tau^3 \sigma^3 p &= \frac{\sqrt{2}}{3} \left[3(u^\uparrow u^\uparrow d^\downarrow + u^\uparrow u^\downarrow u^\uparrow + d^\downarrow u^\uparrow u^\uparrow) \right. \\ &\quad \left. + \frac{1}{2} (u^\uparrow u^\downarrow d^\uparrow + u^\uparrow d^\uparrow u^\downarrow + u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + d^\uparrow u^\downarrow u^\uparrow) \right]. \end{aligned} \quad (25.96)$$

From these equations and (25.54) we extract the matrix elements

$$\begin{aligned} p \tau^3 \sigma^3 p &= \frac{2}{9} \left(3 \cdot 3 - \frac{1}{4} \cdot 6 \right) = \frac{5}{3}, \\ \Delta^+ \tau^3 \sigma^3 p &= \frac{\sqrt{2}}{9} \left(3 \cdot 3 + \frac{1}{2} \cdot 6 \right) = \frac{4}{3} \sqrt{2}. \end{aligned} \quad (25.97)$$

For the ratio between g and g^* , we have to go from $\Delta^+ \tau^3 \sigma^3 p$ to the matrix element $\Delta^{++} \tau^+ \sigma^3 p$ which involves a Clebsch-Gordan factor

$$\Delta^{++} \tau^+ \sigma^3 p = \frac{1}{\sqrt{2}} \frac{4}{3} \sqrt{2} = \frac{4}{3}. \quad (25.98)$$

Thus we obtain

$$\frac{g^*}{g} = \frac{4}{3} \frac{5}{3} = \frac{4}{5} = 0.8, \quad (25.99)$$

in reasonable agreement with the experimental ratio 0.92 from the analysis of pion-nucleon scattering amplitudes.

By a similar quark calculation, we can predict from SU(6)-symmetry the F/D -ratio of the coupling between nucleon octets and pseudoscalar mesons fitted to experimental data in Eq. (24.188). According to the interaction Lagrangian (24.181), the coupling $\Sigma^+\Sigma^+\pi^0$ is given by

$$g_{\Sigma^+\Sigma^+\pi^0} = g(1 - \alpha) = g \frac{2F}{F + D}. \quad (25.100)$$

But this matrix element is easily calculated. The SU(6) state is obtained from $\Sigma^{+\uparrow}$ by applying V_- to it which changes the d -quark into an s -quark. Hence

$$\begin{aligned} \Sigma^{+\uparrow} = & -\frac{\sqrt{2}}{3}(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow) \\ & -\frac{1}{2}(u^\uparrow u^\downarrow s^\uparrow + u^\uparrow s^\uparrow u^\downarrow + s^\uparrow u^\uparrow u^\downarrow + u^\downarrow u^\uparrow s^\uparrow + u^\downarrow s^\uparrow u^\uparrow + s^\uparrow u^\downarrow u^\uparrow). \end{aligned} \quad (25.101)$$

Applying $\tau_3\sigma_3$ gives

$$\tau_3\sigma_3\Sigma^{+\uparrow} = -\frac{\sqrt{2}}{3}2(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow), \quad (25.102)$$

leading to a scalar product with $\Sigma^{+\uparrow}$:

$$\Sigma^{+\uparrow}\tau_3\sigma_3\Sigma^{+\uparrow} = \frac{4}{3}. \quad (25.103)$$

In comparison with the pion-nucleon matrix element $g_{\pi NN} = g$, this amounts to the relation

$$g_{\pi^0\Sigma^+\Sigma^+} = \frac{4}{5}g. \quad (25.104)$$

We therefore find, for the F/D -ratio, the SU(6)-value

$$F/D = 2/3, \quad (25.105)$$

in good agreement with the experimental determination.

25.3 From SU(6) to Current Algebra

Historically, the SU(6) symmetry had an important impact upon the development of the quark model. Since the symmetry is only approximate there was need to find a way of controlling the symmetry-breaking corrections. For the group SU(6) this has remained impossible. For an important subgroup of SU(6), however, this can be done. It is the subgroup generated by $\lambda^a/2, \lambda^a\sigma^3/2$. It is called $SU(3)_R \times SU(3)_L$, and its generators are taken to be the combinations of

$$Q_\pm^a = \frac{\lambda^a}{2} \times \frac{(1 \pm \sigma^3)}{2}. \quad (25.106)$$

These generators are intimately related to the $SU(3) \times SU(3)$ -current algebra which was discussed before in the context of chiral symmetries. The charges and axial charges observed in electromagnetic and weak interactions are related to $Q_{\pm}^a$ as follows:

$$Q^a = Q_+^a + Q_-^a, \quad Q_5^a = Q_+^a - Q_-^a. \quad (25.107)$$

This relation makes it possible to calculate the symmetry-breaking corrections in terms of experimentally observable quantities.

The good $SU(6)$ -results for the magnetic moments were based on the prediction of the F/D ratio $2/3$ and the ratio $\langle p|\mu_3|p\rangle / \langle \Delta^+|\mu_3|p\rangle = 2\sqrt{2}/3$. It is gratifying to observe that these predictions are also contained in the $SU(3)_R \times SU(3)_L$ subgroup of $SU(6)$. Within the framework of current algebra it will, moreover, be possible to calculate symmetry-breaking corrections to these ratios.

The representations 56 and 70 of $SU(6)$ have the following irreducible contents with respect to this subgroup

$$56 = \begin{pmatrix} \frac{3}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ (10, 1) & (6, 3)_{10} & -(\bar{3}, 6)_{10} & (1, 10) \\ & (6, 3)_8 & (3, 6)_8 & \end{pmatrix}, \quad (25.108)$$

$$70 = \begin{pmatrix} \frac{3}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ (8, 1) & \frac{1}{\sqrt{2}}[(6, 3) - (\bar{3}, 3)]_8 & \frac{1}{\sqrt{2}}[(3, 6) + (3, \bar{3})]_8 & -(1, 8) \\ & \frac{1}{\sqrt{2}}[(6, 3) + (\bar{3}, 3)]_8 & \frac{1}{\sqrt{2}}[(3, 6) - (3, \bar{3})]_8 & \\ & (6, 3)_{10} & (3, 6)_{10} & \\ & (\bar{3}, 3)_1 & - (3, \bar{3})_1 & \end{pmatrix}. \quad (25.109)$$

The columns in these matrices are ordered according to the third component of the spin, s_3 , pointing along the direction of the momentum of the particle, which is indicated in the upper row, and the subscripts denote the coupling of the two parts of $SU(3)_R \times SU(3)_L$ with respect to the ordinary $SU(3)$ symmetry group generated by $Q_+^a + Q_-^a$. Within this subgroup, the F/D ratio $2/3$ is the F/D ratio found for the operator $Q_+^a - Q_-^a$ between two $(6, 3)_8$ representations. The transition $\Delta \rightarrow p$ comes from the matrix element of $Q_+^a - Q_-^a = \lambda^a \sigma^3/2$. The representation $(6, 3)$ contains an $SU(3)$ -octet and a decuplet which can be identified with the nucleon octet and the first resonance decuplet at helicity $s_3 = 1/2$.

At this point it is useful to realize that the commutation rules of $SU(3)_L \times SU(3)_R$ can be rephrased as sum rules for the irreducible matrix elements of Q^a, Q_5^a . Take, for example, the commutation rules between the axial charges

$$[Q_5^a, Q_5^b] = if_{abc}Q^c, \quad (25.110)$$

and choose the commutator with the indices $a = 1 + i2$, $b = 1 - i2$, $c = 3$:

$$[Q_5^+, Q_5^-] = 2Q^3. \quad (25.111)$$

Sandwiching this between proton states gives

$$\langle p|Q_5^+Q_5^-|p\rangle - \langle p|Q_5^-Q_5^+|p\rangle = 2\langle p|Q^3|p\rangle. \quad (25.112)$$

Inserting a complete set of intermediate states between the axial charges, we obtain

$$\left| \langle n | Q_5^- | p \rangle \right|^2 + \left| \langle \Delta^0 | Q_5^- | p \rangle \right|^2 - \left| \langle \Delta^{++} | Q_5^+ | p \rangle \right|^2 = 2 \langle p | Q^3 | p \rangle. \quad (25.113)$$

We now introduce irreducible matrix elements of the axial charge Q_5^a with respect to the $SU(2)$ subgroup by defining between protons:

$$\langle p | Q_5^3 | p \rangle \equiv \frac{1}{2} G_A. \quad (25.114)$$

Then

$$\langle n | Q_5^- | p \rangle \equiv G_A. \quad (25.115)$$

This can either be derived directly by using the generator $\lambda^- \sigma^3 / 2$, or via the Wigner-Eckart-theorem for $SU(2)$ -vector operators. We only have to keep in mind that Q_5^3 creates the quantum numbers of π^0 , while $Q_5^\pm$ creates those of $\sqrt{2}\pi^+$, $-\sqrt{2}\pi^-$ if we assume that π^+ , π^0 , π^- satisfy the Condon-Shortley phase convention³. We define further between a proton and a Δ -resonance

$$\langle \Delta^+ | Q_5^3 | p \rangle \equiv \frac{1}{\sqrt{2}} G^* \quad (25.116)$$

and find, from the Wigner-Eckart theorem,

$$\begin{aligned} \langle \Delta^{++} | Q_5^+ | p \rangle &\equiv -\sqrt{\frac{3}{2}} G^*, \\ \langle \Delta^0 | Q_5^- | p \rangle &= \frac{1}{\sqrt{2}} G^*. \end{aligned} \quad (25.117)$$

With the right-hand side of (25.113) being the isospin value of the proton $1/2$ we obtain the sum rule

$$G_A^2 - G^{*2} = 1. \quad (25.118)$$

Similarly, we can take the commutator (25.111) between two Δ^{++} states and have the sum rule

$$\left| \langle p | Q_5^- | \Delta^{++} \rangle \right|^2 + \left| \langle \Delta^+ | Q_5^- | \Delta^{++} \rangle \right|^2 = 3. \quad (25.119)$$

Let us now introduce the irreducible matrix element G_A^* of the axial charge between two Δ -states via

$$\langle \Delta^+ | Q_5^0 | \Delta^+ \rangle = \frac{1}{2} G_A^*. \quad (25.120)$$

Then, by the Wigner-Eckart theorem we have

$$\langle \Delta^+ | Q_5^- | \Delta^{++} \rangle = -\sqrt{3} G_A^*, \quad (25.121)$$

and Eq. (25.119) becomes

$$\frac{1}{2} G^{*2} + G_A^{*2} = 1. \quad (25.122)$$

³One may verify this by applying $Q^\pm$ to Q^3 giving $\pm Q^\mp$.

Between p and Δ^+ , finally, the commutator (25.111) yields

$$\begin{aligned} \langle \Delta^+ | Q_5^+ | n \rangle \langle n | Q_5^- | p \rangle + \langle \Delta^+ | Q_5^+ | \Delta^0 \rangle \langle \Delta^0 | Q_5^- | p \rangle \\ - \langle \Delta^+ | Q_5^- | \Delta^{++} \rangle \langle \Delta^{++} | Q_5^+ | p \rangle = 0, \end{aligned} \quad (25.123)$$

and this amounts to the sum rule

$$G^* G_A - 5 G_A^* G^* = 0. \quad (25.124)$$

The unique solution to these $SU(2) \times SU(2)$ sum rules is

$$G_A = \frac{5}{3}, \quad G^* = \frac{4}{3}, \quad G_A^* = \frac{1}{3}. \quad (25.125)$$

A more covariant looking derivation of these sum rules is possible by rewriting the matrix elements of Q_5^a for $a = 1, 2, 3$ between isospin- $\frac{1}{2}$ and $-\frac{3}{2}$ spinors as follows:

$$\begin{aligned} NN : \quad (Q_5^a)_{mm'}^{11} &= G_A \chi^\dagger(m) \frac{\tau^a}{2} \chi(m') = G \frac{\sqrt{3}}{2} \langle \tfrac{1}{2}, m | 1, a; \tfrac{1}{2}, m' \rangle \\ \Delta N : \quad (Q_5^a)_{mm'}^{31} &= G^* \frac{\sqrt{3}}{2} \chi_a^\dagger(m) \chi(m') = G^* \frac{\sqrt{3}}{2} \langle \tfrac{3}{2}, m | 1, a; \tfrac{1}{2}, m' \rangle, \\ \Delta\Delta : \quad (Q_5^a)_{mm'}^{33} &= G_A^* \frac{3}{2} i \epsilon_{abc} \chi_b^+(m) \chi_c(m') = G_A^* \frac{\sqrt{15}}{2} \langle \tfrac{3}{2}, m | 1, a; \tfrac{3}{2}, m' \rangle. \end{aligned} \quad (25.126)$$

Here $\langle SM | s_1 m_1 s_2 m_2 \rangle$ are the usual $SU(2)$ Clebsch-Gordan coefficients and χ_a are Rarita-Schwinger isospinors. They are obtained by coupling an ordinary isospinor χ with an isovector v_a by a Clebsch-Gordan coefficient

$$\chi_a(m) = \langle \tfrac{3}{2}, m | 1, m_1; \tfrac{1}{2}, m_2 \rangle v_a(m_1) \chi(m_2). \quad (25.127)$$

They satisfy the constraint

$$\tau^a \chi_a(m) = 0 \quad (25.128)$$

and the identities

$$i \epsilon_{abc} \tau^b \chi_c = \chi_a, \quad \tau^a \chi_b = -i \epsilon_{abc} \chi_c. \quad (25.129)$$

Using these we can calculate the matrix elements by sandwiching the commutation relations (25.110) between nucleon and Δ -states, and summing over a complete set of intermediate states.

When employing the matrix elements (25.126), we can do the summation easily the help of the completeness relations

$$\begin{aligned} \sum_m \chi_\alpha(m) \chi_\beta^*(m) &= \delta_{\alpha\beta}, \\ \sum_m \chi_a(m) \chi_b^*(m) &= \frac{2}{3} \delta_{ab} - \frac{1}{6} [\tau^a, \tau^a]. \end{aligned} \quad (25.130)$$

In this way we obtain once more the sum rules (25.118), (25.122), and (25.124).

So far, these relations hold for the $SU(2)_L \times SU(2)_R$ subgroup of $SU(3)_L \times SU(3)_R$. Extending the procedure from $SU(2)$ to $SU(3)$, we decompose the irreducible matrix of Q_5^3 between protons and remember (25.68) to see that

$$G_A = F + D. \quad (25.131)$$

Considering once more the commutator (25.111) between Σ^+ states gives

$$\left| \langle \Sigma^0 | Q_5^- | \Sigma^+ \rangle \right|^2 + \left| \langle \Lambda | Q_5^- | \Sigma^+ \rangle \right|^2 + \left| \langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle \right|^2 = 2, \quad (25.132)$$

where Σ^{*0} is the strange partner of the Δ^0 resonance. Using the same $SU(3)$ -decomposition as in Eq. (25.67), the matrix element Q_5^3 between two Σ^+ states is

$$\langle \Sigma^+ | Q_5^0 | \Sigma^+ \rangle = F. \quad (25.133)$$

Hence, by the Wigner-Eckart theorem for the $SU(2)$ subgroup we have

$$\langle \Sigma^0 | Q_5^- | \Sigma^+ \rangle = \sqrt{2}F. \quad (25.134)$$

Using once more the $SU(3)$ -decomposition (25.67), we calculate the matrix element

$$\begin{aligned} \langle \Lambda^0 | Q_5^- | \Sigma^+ \rangle &= F \cdot \left(-if_{1-i2,8,(1+i2)/\sqrt{2}} \right) + D \cdot d_{1-i2,8,(1+i2)/\sqrt{2}} \\ &= D \frac{1}{\sqrt{2}} (d_{118} + d_{228}) = \sqrt{\frac{2}{3}} D. \end{aligned} \quad (25.135)$$

Similarly, the matrix element

$$\langle \Delta^0 | Q_5^- | p \rangle = \frac{1}{\sqrt{2}} G^* \quad (25.136)$$

is related to $\langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle$ by $SU(3)$ -symmetry. Using the Clebsch-Gordan coefficients of Table 4.2 on p. 381 and the isoscalar factors of Table 24.5 on page 1378 we have

$$\begin{aligned} \langle \Delta^0 | Q_5^- | p \rangle &= - \left\langle \frac{3}{2}, -\frac{1}{2} \middle| 1, -1; \frac{1}{2}, \frac{1}{2} \right\rangle \left(-\sqrt{\frac{1}{2}} \right) a, \\ &= \frac{1}{\sqrt{6}} a \\ \langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle &= - \langle 1, 0 | 1, -1; 1, 1 \rangle \frac{1}{\sqrt{6}} a \\ &= \frac{1}{\sqrt{12}} a, \end{aligned} \quad (25.137)$$

where a is some number. Using these equations we find from (25.136)

$$\langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle = \frac{1}{2} G^*. \quad (25.138)$$

The sum rule (25.132) becomes therefore

$$F^2 + \frac{1}{3}D^2 + \frac{1}{8}G^{*2} = 1. \quad (25.139)$$

Given the solution of the $SU(2) \times SU(2)$ -algebra (25.125), we find from this once more the F/D ratio $\frac{2}{3}$.

For completeness, let us also look at the commutation rule (25.111) between Ξ^+ particles, which gives the sum rule

$$\left| \langle \Xi^0 | Q_5^- | \Xi^+ \rangle \right|^2 + \left| \langle \Xi^{*0} | Q_5^- | \Xi^+ \rangle \right|^2 = 1. \quad (25.140)$$

Within $SU(3)$, the particles Ξ^+ and Ξ^0 have the vector indices $(6 - i7)/\sqrt{2}$ and $(4 - i5)/\sqrt{2}$, so that the decomposition (25.67) reads

$$\begin{aligned} \langle \Xi^- | Q_5^- | \Xi^+ \rangle &= F \cdot (-if_{1-i2, (4+i5)/\sqrt{2}, -(6-i7)/\sqrt{2}}) + D \cdot d_{1-i2, (4+i5)/\sqrt{2}, -(6-i7)/\sqrt{2}} \\ &= F \cdot (f_{146} + f_{157}) + D \cdot (-d_{146} - d_{157}) = 2F \cdot f_{146} + D \cdot (-2d_{146}) \\ &= F - D. \end{aligned} \quad (25.141)$$

The matrix element between $\Xi^{*0}(1530)$ and Ξ^+ , on the other hand, comes from the $SU(3)$ -matrix elements (which is found again by combining the Clebsch-Gordan coefficients of Table 4.2 on p. 381 and the isoscalar factors of Table 24.5 on page 1378):

$$\begin{aligned} \langle \Xi^{*0} | Q^- | \Xi^+ \rangle &= \langle \tfrac{1}{2}, -\tfrac{1}{2} | 1, -1; \tfrac{1}{2}, \tfrac{1}{2} \rangle \frac{1}{2}a \\ &= \left(-\sqrt{\frac{2}{3}} \right) \frac{1}{2}a. \end{aligned} \quad (25.142)$$

This has to be compared with

$$\begin{aligned} \langle \Delta^0 | Q_5^- | p \rangle &= \langle \tfrac{3}{2}, -\tfrac{1}{2} | 1, -1; \tfrac{1}{2}, \tfrac{1}{2} \rangle \left(-\frac{1}{\sqrt{2}} \right) a \\ &= \frac{1}{\sqrt{3}} \left(-\frac{1}{\sqrt{2}} \right) a. \end{aligned} \quad (25.143)$$

Hence

$$\langle \Xi^{*0} | Q_5^- | \Xi^+ \rangle = \frac{1}{\sqrt{2}} G^*, \quad (25.144)$$

and the sum rule reads

$$(F - D)^2 + \frac{1}{2}G^{*2} = 1. \quad (25.145)$$

This is satisfied by

$$F = \frac{2}{3}, \quad D = \frac{1}{3}, \quad G^* = \frac{4}{3}. \quad (25.146)$$

25.4 Supersymmetry

Until 1967, a search was going on to combine the approximate internal symmetries $SU(3)$ or $SU(6)$ with the external symmetry of spacetime. That search went on until 1967 when Coleman and Mandula proved a no-go theorem [4]. This stated that the only combination between the two groups is the trivial direct product.

In 1974, a new type of symmetry was discovered [5], which extended the Poincaré group in a completely novel way. Its representations possess irreducible multiplets which contain at the same time both types of particles, fermions and bosons. The basic example is given by the free action

$$\mathcal{A} = \int d^4x \left[\frac{1}{2}(\partial A)^2 + \frac{1}{2}(\partial B)^2 + \frac{1}{2}F^2 + \frac{1}{2}G^2 + M(FA + GB) + \frac{1}{2}\bar{\chi}(\not{\partial} - M)\chi \right], \quad (25.147)$$

where A, B, C, D are four real scalar fields, and χ is a four-component real Majorana spinor. The four scalar fields can be transformed into the four components of the Majorana field by the following transformations

$$\begin{aligned} \delta\chi &= [F + i\gamma_5 G - i\not{\partial}(A + i\gamma_5 B)]\epsilon, \\ \delta\bar{\chi} &= \bar{\epsilon}[F + i\gamma_5 G + i(A + i\gamma_5 B)\not{\partial}], \end{aligned} \quad (25.148)$$

$$\begin{aligned} \delta A &= \bar{\epsilon}\chi, & \delta F &= \bar{\epsilon}(-i\not{\partial}\chi), \\ \delta B &= \bar{\epsilon}i\gamma_5\chi, & \delta G &= \bar{\epsilon}[-i\not{\partial}(-i\gamma_5)]\chi. \end{aligned} \quad (25.149)$$

Here ϵ is a four-component real parameter with spinor indices. The spinor character makes it necessary to require ϵ and χ to be Grassmann variables which anticommute with each other

$$\epsilon_\alpha\chi_\beta = -\chi_\beta\epsilon_\alpha. \quad (25.150)$$

It is easy to verify that these transformations leave the action invariant. For the mass terms we calculate:

$$\delta(FA) = \bar{\epsilon}(-i\not{\partial}\chi)A + F\bar{\epsilon}\chi, \quad (25.151)$$

$$\delta(CB) = \bar{\epsilon}[-i\not{\partial}(-i\gamma_5)\chi]B + G\bar{\epsilon}i\gamma_5\chi, \quad (25.152)$$

$$\delta\bar{\chi}\chi = \bar{\chi}[F + i\gamma_5 G - i\not{\partial}(A + i\gamma_5 B)]\epsilon + \bar{\epsilon}[F + i\gamma_5 G + i(A + i\gamma_5 B)\not{\partial}]\chi. \quad (25.153)$$

The real Majorana spinor satisfies (recall Section 4.13)

$$\bar{\chi}^T = \gamma_0\chi = C\chi = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} \chi, \quad (25.154)$$

so that

$$\begin{aligned} \bar{\chi}\epsilon &= \chi^T\gamma_0^T\epsilon = -\epsilon^T\gamma_0\chi = \epsilon^T\gamma_0^T\chi = \bar{\epsilon}\chi, \\ \bar{\chi}\gamma_5\epsilon &= \chi^T\gamma_0^T\gamma_5\gamma_0\bar{\epsilon}^T = \chi^T\gamma_5\epsilon^T = -\bar{\epsilon}\gamma_5^T\chi = \bar{\epsilon}\gamma_5\chi. \end{aligned} \quad (25.155)$$

Recall that in the Majorana representation

$$\gamma_5 = \begin{pmatrix} \sigma^2 & 0 \\ 0 & -\sigma^2 \end{pmatrix}, \quad (25.156)$$

so that $\gamma_5^T = -\gamma_5$. Hence the F - and G -terms in the transformation (25.153) can be combined to

$$\delta(\bar{\chi}\chi) = 2\bar{\epsilon}(F + i\gamma_5 G)\chi, \quad (25.157)$$

thus canceling in the transformation of the total mass term

$$FA + GB - \frac{1}{2}\bar{\chi}\chi. \quad (25.158)$$

What about the A - and B -terms? We write these in (25.153) as

$$\begin{aligned} \delta(\bar{\chi}\chi) &= \partial^\mu \{ \bar{\chi} [-i\gamma_\mu(A + i\gamma_5 B)]\epsilon + \bar{\epsilon} i(A + i\gamma_5 B)\gamma_\mu\chi \} \\ &\quad - \left\{ -\bar{\chi} \overleftarrow{\not{D}} i(A + i\gamma_5 B)\epsilon - \bar{\epsilon} i(A + i\gamma_5 B) \overrightarrow{\not{D}} \chi \right\}. \end{aligned} \quad (25.159)$$

The first term is a pure surface term and does not contribute to the total action. In the third term we use

$$\bar{\chi}\gamma_\mu\epsilon = -\bar{\epsilon}\gamma_\mu\chi, \quad \bar{\chi}\gamma_\mu\gamma_5\epsilon = -\bar{\epsilon}\gamma_5\gamma_\mu\chi, \quad (25.160)$$

and see that it is equal to the fourth term. Both together cancel the AB -terms in $\delta(FA + GB)$. Thus the total action is invariant. The transformations are called *supersymmetry transformation* and the action *supersymmetric*.

Note that the fields F, G carry no gradients in the action and are therefore not dynamical. In principle they could be eliminated from the action using the equations of motion, but then the verification of the supersymmetry would be much more involved. Only if they are explicitly present, the four components of χ have four real scalar counterparts A, B, G, F . In a free field theory, the equations of motion make F, G vanish. When interactions are included, they are still non-dynamical, but no longer zero.

In particle physics, no indication of some broken supersymmetry has so far been discovered. There exists, however, a supersymmetry between the unphysical content in gauge fields and the Faddeev-Popov ghost fields in QED. This is essential for removing the vacuum energy of the two unphysical modes. Recall the Lagrangian (7.525):

$$\mathcal{L}_{\text{tot}} = \mathcal{L} + \mathcal{L}_{\text{GF}} + \mathcal{L}_{\text{ghost}} = -\frac{1}{4}F_{\mu\nu}^2 - D(x)\partial^\mu A_\mu(x) + \alpha D^2(x)/2 - i\partial_\mu \bar{C}\partial^\mu C. \quad (25.161)$$

It is invariant under the following two sets of supersymmetry transformations:

$$\begin{aligned} \delta A_\mu &= i\partial_\mu C, \\ \delta \bar{C} &= D, \\ \delta C &= \delta D = 0, \end{aligned} \quad (25.162)$$

and

$$\begin{aligned}\bar{\delta}A_\mu &= i\partial_\mu\bar{C}, \\ \bar{\delta}C &= -D, \\ \bar{\delta}\bar{C} &= \bar{\delta}D = 0.\end{aligned}\tag{25.163}$$

These are known as the BRS transformations (see Footnote 14 in Chapter 7).

The BRS supersymmetry is generated by charges

$$\begin{aligned}Q &= \sum_{\mathbf{k}} \omega_{\mathbf{k}}(a_{\mathbf{k},l}c_{\mathbf{k}} + \text{h.c.}), \\ \bar{Q} &= \sum_{\mathbf{k}} \omega_{\mathbf{k}}(a_{\mathbf{k},l}\bar{c}_{\mathbf{k}} + \text{h.c.}).\end{aligned}\tag{25.164}$$

Together with the subsidiary conditions (7.523), the conditions

$$Q|0\rangle = 0, \quad \bar{Q}|0\rangle = 0\tag{25.165}$$

are seen to enforce precisely the Gupta-Bleuler subsidiary condition (7.502) (see Ref. [3]). The full power of the BRS supersymmetry is needed in the renormalization of nonabelian gauge theories. This is necessary for extracting finite results from higher-order perturbative calculations of weak interaction processes within the standard model of electroweak interactions.

Note that by postulating the absence of ghosts from the Hilbert space at a specific time, they are excluded for *all* times since the Lagrangian conserves ghost charge. This is a consequence of its invariance under

$$C \rightarrow e^\alpha C, \quad \bar{C} \rightarrow e^{-\alpha}\bar{C}.\tag{25.166}$$

The ghost charge conservation follows from Noether's theorem (recall Chapter 8).

Notes and References

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*Science is facts; just as houses are made of stones,
so is science made of facts; but a pile of stones is not a house
and a collection of facts is not necessarily science.*

HENRI POINCARÉ (1854–1912)

26

Hadronization of Quark Theories

In this chapter we shall study a simple model of quantum field theory which shows how quark theories can be converted into bilocal field theories via functional techniques. The new basic field quanta of the converted theory approximate the quark-antiquark meson bound states. They are obtained by solving the Bethe-Salpeter bound-state equation in the ladder approximation. These will be called *bare mesons* and we shall introduce mesonic Feynman graphs describing their propagation. In the limit of infinitely heavy gluon masses, the bilocal fields become local and describe π -, ρ -, A_1 -, and σ -mesons. Their fluctuations are governed by a collective chirally invariant Lagrange density, which is an $SU(3)$ -symmetric extension of the Gell-Mann–Lévy linear σ -model [1].

Many interesting relations are found between meson- and quark-properties such as $m_\rho^2 \approx 6M^2$, where M is the non-strange quark mass *after* spontaneous breakdown of chiral symmetry, the so-called *constituent quark mass*. There is a simple formula linking these quark masses with the small bare masses appearing as parameters in the Lagrange density. The quark masses also determine the vacuum expectations of scalar densities.

26.1 Introduction

In attempting to understand the physics of strongly interacting particles, the *hadrons* (recall the classification in Section 24.1), two fundamentally different theoretical approaches have been developed. One of them, the dual approach, is based on complete democracy among all strongly interacting particles. Within this approach, an elaborate set of rules assures the construction of certain lowest order vertex functions for any number of mesons [1]. The other approach assumes the existence of a local field equation involving fundamental quarks bound together by vector gluons [3]. Here strong interaction effects on electromagnetic and weak currents of hadrons can be analyzed in a straight-forward fashion without detailed dynamical computations [4]. Either approach has its weakness, where the other is powerful. Dual models have, until now, given no access to currents, while quark theories have

left the problem of mesonic vertex function intractable. Not even an approximate bound state calculation is available (except in 1+1 dimensions [12] or by substituting the field couplings by simple ad-hoc forces [13]).

At present it appears that a Lagrangian field theory of the Yang-Mills type is the correct fundamental theory of elementary particles. The gluon fields form flux tubes between quarks and antiquarks which have a fixed diameter of the order of the Compton wavelength of the pion. Since the field energy is to lowest order proportional to the square of the field strength, the energy of the flux tube grows linearly with its length and leads to quark confinement. For large distances, the thickness of the flux tube can be ignored and the physics of the Yang-Mills theory approaches the theory of a hadronic string. This approximation can, however, only be used for long, i.e., highly excited mesons. Low-lying mesons are held together by short fat flux tubes which become spherical for the ground state. The string picture breaks down completely for these states, which look more like bags. In fact, the low-lying states of a string have a negative norm. Only in spacetime of much higher dimension than four does the norm become positive.

When theorists ran into these problems of a string approximation they abandoned the entire model. Others, who had spent a lot of effort in studying the mathematics of strings, decided to postulate the string picture to be physical representations of entirely new fundamental particles. Therefore they had to assume that we live in a spacetime with more than four dimensions, and proposed many possible consequences of which there has been no evidence so far. They even derive from this picture the existence of black mini-holes which could be produced in present-day accelerators such as the Large Hadron Collider at the European laboratory CERN in Geneva.

An important defect of the string model so far is that there exists no quantum field theory for a grand-canonical ensemble of strings. Only the first-quantized language of a single string is well developed. There are only rudimentary attempts at a second-quantized field theory of strings [14].

In order to learn how a translation between the different languages might operate, we consider here the simplified field theory in which quarks are colorless, have N flavors, and are held together by vector gluons of arbitrary mass μ . This theory incorporates several realistic features of strong interactions, for example current algebra and PCAC. Moreover, the cases $N = 1$ and $\mu = 0$ include ordinary quantum electrodynamics (QED). This will provide a good deal of intuition as well as the possibility of a detailed test of our results.

First we demonstrate how functional methods can be employed to transform the local quark-gluon theory into a new completely equivalent field theory involving only bilocal fields. The new free field quanta coincide with quark-antiquark bound states when calculated by ladder exchanges only. They may be considered as *bare mesons*. Accordingly, the transition from the local quark theory to the bilocal meson theory will be named *mesonization*. In the special case of QED, bare mesons are positronium atoms in ladder approximation.

The functional technique will ensure that bare mesons have exactly the correct interactions among each other, so that mesonization preserves the equivalence to the original quark gluon theory. It is simple to establish the connection between classes of Feynman graphs involving quarks and gluons with single graphs involving mesons. The topology of meson graphs is the same as that of dual diagrams. It is interesting to observe the appearance of a current-meson field identity for photons just as employed in phenomenological discussions of vector meson dominance. Moreover, since the theory is bilocal, this identity can be extended to bilocal currents which are measured in deeply inelastic electromagnetic and weak interactions.

The limit of a very heavy gluon mass can be mesonized most simply. Here the bilocal fields become local and describe only a few mesons with the quantum numbers of π -, ρ -, A_1 -, and σ -mesons. The Lagrange density coincides with that of the standard chirally and SU(3)-invariant σ -model which is known to account quite well for the low-energy aspects of meson physics. Here mesonization renders additional connection between quark and meson properties. It also makes transparent the relation between the very small bare quark masses (which describe the explicit breakdown of chiral symmetry) and the constituent quark masses (which include the dynamic effects due to spontaneous symmetry violations).

26.2 Abelian Quark Gluon Theory

Consider now a system of N quarks $\psi(x)$ held together by an abelian gluon field $G^\nu(x)$ of mass μ via a Lagrangian

$$\mathcal{L}(x) = \bar{\psi}(x) (i\mathcal{D} - \mathcal{M}) \psi(x) - \frac{1}{4} F_{\mu\nu}^2(x) + \frac{\mu^2}{2} G_\nu^2. \quad (26.1)$$

Here $\mathcal{D}$ is the Dirac covariant derivative $\mathcal{D} \equiv \gamma^\mu D_\mu$, in which the ordinary covariant derivatives $D_\mu \equiv \partial_\mu - igG_\mu$ associated with the gluon fields are contracted with the Dirac matrices. The tensor $F_{\mu\nu} \equiv \partial_\mu G_\nu - \partial_\nu G_\mu$ is the usual spacetime curl of G_μ . In the special case in which $N = 1$, $\mu = 0$, and $g^2 = 4\pi\alpha$, this Lagrangian describes quantum electrodynamics. In other cases it may be considered as a model field theory which illustrates many properties of strong interactions, for example approximate SU(3)-symmetry, chiral SU(3) $\times$ SU(3) current algebra, PCAC, and scaling up to small corrections. Certainly, this model will never be able to confine quarks, give symmetric baryon wave functions, and explain infinitely rising meson trajectories. For this it would have to contain an additional, exactly conserved, color symmetry with $G^\nu(x)$ being a matrix-valued vector field describing non-abelian gauge mesons. Before attempting to deal with this far more complicated situation we shall develop [21] our tools for the less realistic but much simpler model (26.1) without color.

The generating functional of all time-ordered Green function is

$$Z[\eta, \bar{\eta}, j^\nu] = \text{const} \times \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}G e^{i \int dx (\mathcal{L} + \bar{\psi}\eta + \bar{\eta}\psi + gj^\nu G_\nu)}. \quad (26.2)$$

The exponent is quadratic in $G^\nu(x)$, such that the functional integration over the gluon field can be performed [15, 16] with the help of formula (14.100). The result is

$$Z[\eta, \bar{\eta}, j^\nu] = \text{const} \times \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{i\mathcal{A}[\psi, \bar{\psi}, \eta, \bar{\eta}, j^\nu]}, \quad (26.3)$$

with an action

$$\begin{aligned} \mathcal{A}[\psi, \bar{\psi}, \eta, \bar{\eta}, j^\nu] = \int dx dy \Big\{ & \left(\mathcal{L}(x) + \bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x) \right) \delta(x-y) \\ & - \frac{i}{2} g^2 D(x-y) \left(\bar{\psi}(x)\gamma^\nu \psi(x) + j^\nu(x) \right) \left(\bar{\psi}(y)\gamma_\nu \psi(y) + j_\nu(y) \right) \Big\}. \end{aligned} \quad (26.4)$$

By employing the Fierz identity:

$$\gamma_{\alpha\beta}^\nu \otimes \gamma_{\nu\gamma\delta} = 1_{\alpha\delta} \otimes 1_{\alpha\beta} + (i\gamma_5)_{\alpha\delta} \otimes (i\gamma_5)_{\gamma\beta} - \frac{1}{2} \gamma_{\alpha\beta}^\nu \otimes \gamma_{\nu\gamma\delta} - \frac{1}{2} (\gamma^\nu \gamma_5)_{\alpha\delta} \otimes (\gamma_\nu \gamma_5)_{\gamma\beta}, \quad (26.5)$$

the four-fermion quark interaction term can be rewritten more explicitly as

$$\begin{aligned} \frac{i}{2} g^2 D(x-y) \Big\{ & \bar{\psi}(x)\psi(y)\bar{\psi}(y)\psi(x) + \bar{\psi}(x)i\gamma_5\psi(y)\bar{\psi}(y)i\gamma_5\psi(x) \\ & - \frac{1}{2} \bar{\psi}(x)\gamma^\nu \psi(y)\bar{\psi}(y)\gamma_\nu \psi(x) - \frac{1}{2} \bar{\psi}(x)\gamma^\nu \gamma_5 \psi(y)\bar{\psi}(y)\gamma_\nu \gamma_5 \psi(x) \Big\}. \end{aligned} \quad (26.6)$$

A short way of writing this is

$$\frac{i}{2} g^2 D(x-y) \bar{\psi}_\alpha(x) \psi_\delta(y) \xi_{\alpha\delta, \gamma\beta} \bar{\psi}_\gamma(y) \psi_\beta(x), \quad (26.7)$$

where the matrix $\xi_{\alpha\delta, \gamma\beta}$ denotes the right-hand side of Eq. (26.5).

This is the point where our elimination of quark fields in favor of new bilocal fields starts. The trick is to make use of the Hubbard-Stratonovich transformation introduced in Eq. (14.99). Let $S(x, y)$, $P(x, y)$, $V^\nu(x, y)$, $A^\nu(x, y)$ be a set of Hermitian auxiliary fields:

$$S(x, y) = S^*(y, x), \quad P(x, y) = P^*(y, x), \quad V^\mu(x, y) = V^{*\mu}(y, x), \quad A^\mu(x, y) = A^{*\mu}(y, x). \quad (26.8)$$

With the help of these fields, we can construct the following functional identities [20]:

$$\begin{aligned} \int \mathcal{D}S(x, y) e^{-\frac{i}{2}|S(x, y) + ig^2 D(x-y)\bar{\psi}(y)\psi(x)|^2 / ig^2 D(x-y)} &= \text{const.}, \\ \int \mathcal{D}P(x, y) e^{-\frac{i}{2}|P(x, y) + ig^2 D(x-y)\bar{\psi}(y)i\gamma_5\psi(x)|^2 / ig^2 D(x-y)} &= \text{const.}, \\ \int \mathcal{D}V(x, y) e^{i|V(x, y) - \frac{i}{2}g^2 D(x-y)\bar{\psi}(y)g^\nu \psi(x)|^2 / ig^2 D(x-y)} &= \text{const.}, \\ \int \mathcal{D}A(x, y) e^{i|A^\nu(x, y) + \frac{i}{2}g^2 D(x-y)\bar{\psi}(y)\gamma^\nu \gamma_5 \psi(x)|^2 / ig^2 D(x-y)} &= \text{const.}, \end{aligned} \quad (26.9)$$

where $\int \mathcal{D}V$ and $\int \mathcal{D}A$ are short for $\int \mathcal{D}V^\mu$ and $\int \mathcal{D}A^\mu$. These constant integrals are independent of the quark fields $\psi(x)$. If we now multiply $Z[\eta, \bar{\eta}, j^\nu]$ in (26.3) by these constants, and make use of (26.6), all four-fermion quark terms cancel. The generating functional becomes

$$Z[\eta, \bar{\eta}, j^\nu] = \text{const} \times \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}S \mathcal{D}P \mathcal{D}V \mathcal{D}A e^{i\tilde{\mathcal{A}}}, \quad (26.10)$$

where the new action $\tilde{\mathcal{A}}$ is obtained as an integral

$$\tilde{\mathcal{A}}[\psi, \bar{\psi}, S, P, V, A, \eta, \bar{\eta}, j^\nu] = \int dx dy \mathcal{L}(x, y) \quad (26.11)$$

over a bilocal Lagrange density:

$$\begin{aligned} \mathcal{L}(x, y) \equiv & \left\{ \bar{\psi}(x) (i\cancel{\partial} - \mathcal{M}) \psi(x) + \bar{\psi}(x) \eta(x) + \bar{\eta}(x) \psi(x) \right\} \delta^{(4)}(x - y) \\ & - \bar{\psi}(x) m(x, y) \psi(y) - \frac{i}{2} g^2 D(x - y) j^\nu(x) j_\nu(y) \\ & - \left\{ \frac{1}{2} |S|^2 + \frac{1}{2} |P|^2 - |V|^2 - |A|^2 \right\} \frac{1}{ig^2 D(x - y)}. \end{aligned} \quad (26.12)$$

Here $m(x, y)$ has been introduced as an abbreviation for the combined field:

$$\begin{aligned} m(x, y) \equiv & S(x, y) + P(x, y) i\gamma_5 \\ & + \left[V^\nu(x, y) + \delta^{(4)}(x - y) \int dz ig^2 D(x - z) j^\nu(z) \right] \gamma_\nu + A^\nu(x, y) \gamma_\nu \gamma_5. \end{aligned} \quad (26.13)$$

Due to (26.8), the matrix $m(x, y)$ is self-adjoint in the sense

$$\left[\overline{m(x, y)} \right]_{\alpha\beta} \equiv \gamma_{\alpha\alpha'}^0 \left[m^*(x, y)^T \right]_{\alpha'\beta'} \gamma_{\beta'\beta}^0 = m_{\alpha\beta}(y, x). \quad (26.14)$$

At this place it is worth remarking that the Lagrangian (26.12) shows its equivalence to the previous form (26.4) also quite directly. Extremizing the action we obtain the Euler-Lagrange equations for the fields S, P, V, A , which are seen to be dependent fields coinciding with the corresponding bilocal quark expressions

$$S(x, y) = -ig^2 D(x - y) \bar{\psi}(y) \psi(x), \quad (26.15)$$

$$P(x, y) = -ig^2 D(x - y) \bar{\psi}(y) i\gamma_5 \psi(x), \quad (26.16)$$

$$V^\nu(x, y) = \frac{i}{2} g^2 D(x - y) \bar{\psi}(y) \gamma^\nu \psi(x), \quad (26.17)$$

$$A^\nu(x, y) = \frac{i}{2} g^2 D(x - y) \bar{\psi}(y) \gamma^\nu \gamma_5 \psi(x), \quad (26.18)$$

if fluctuations are neglected. Inserting these relations back into (26.12), we reproduce (26.4). In the action (26.11), quark fields enter only in a quadratic form such that they can be integrated out according to formula (14.100). The functional matrix A is given by

$$L(x, y) = (-\cancel{\partial} - \mathcal{M}) \delta^{(4)}(x - y) - m(x, y). \quad (26.19)$$

Hence $L^{-1}(x, y) \equiv -iG(x, y)$ is the Green function associated with the equation

$$\int dy \left[(i\partial - \mathcal{M}) \delta^{(4)}(x - y) - m(x, y) \right] G(y, z) = i\delta^{(4)}(x - z). \quad (26.20)$$

With this notation, the quark integration brings the functional (26.10) to the form

$$Z[\eta, \bar{\eta}, j^\nu] = \text{const} \times \int \mathcal{D}m(x, y) e^{i\mathcal{A}[\eta, \bar{\eta}, j^\nu]}, \quad (26.21)$$

with

$$\begin{aligned} \mathcal{A}[m, \eta, \bar{\eta}, j^\nu] = & \int dx dy \left\{ -i \text{tr} \left(\ln iG^{-1} \right) (x, y) \delta^{(4)}(x - y) \right. \\ & - \frac{1}{2} \text{Tr} \left[m(x, y) \xi^{-1} m(y, x) \right] \frac{1}{ig^2 D(x - y)} + i\bar{\eta}(x) G(x, y) \eta(y) - ig^2 \frac{[\delta^{(4)}(x - y)]^2}{D(0)} \\ & \left. - \frac{2}{D(0)} V^\nu(x, x) D(x - y) j_\nu(y) + \int dz dz' D(z - x) D(y - z') j^\nu(z) j_\nu(z') \right\}, \end{aligned} \quad (26.22)$$

where we have introduced the short notation for the measure of functional integration

$$\mathcal{D}m(x, y) \equiv \mathcal{D}S \mathcal{D}P \mathcal{D}V \mathcal{D}V. \quad (26.23)$$

The symbol tr denotes the trace with respect to the Dirac indices. Written with a capital letter as Tr , it comprises also the functional arguments, i.e., $\text{tr} m(x, y) \equiv \sum_\alpha [m(x, y)]_{\alpha\alpha}$, $\text{Tr} m(x, y) \equiv \int dx \sum_\alpha [m(x, x)]_{\alpha\alpha}$. Note that the effect of the matrix ξ^{-1} defined in Eq. (26.6) is to divide the projections into S, P, V, A by 4, $-4, -2, 2$, respectively.¹ The new functional (26.21) is identical to the original one in Eq. (26.2). As a consequence, a quantum theory based on the action (26.22) will be completely equivalent to the original quantized quark gluon theory.

A remark is in order concerning the internal symmetry $\text{SU}(N)$ among the N quarks ($i = 1, \dots, N$) under consideration. Since the gluon is an $\text{SU}(N)$ -singlet, the interaction in Eq. (26.1) is $g \sum_{i=1}^N \bar{\psi}_i \gamma^\nu \psi_i G_\nu(x)$. In the Fierz transformed version (26.6), the indices i and j appear separately on pairs of fields:

$$\frac{i}{2} g^2 D(x - y) \left(\bar{\psi}^j(x) \psi_i(y) \right) \xi \left(\bar{\psi}^i(y) \psi_j(x) \right). \quad (26.24)$$

Hence, in the presence of N quarks, the fields $m(x, y)$ have to be thought of as matrices in $\text{SU}(N)$ space $[m(x, y)]_i^j$. This carries over to the action where the traces are extended to include, in addition, $\text{SU}(N)$ -indices.

Let us now develop a quantum theory for the new action. In general, the field $m(x, y)$ may oscillate around some constant non-zero vacuum expectation value $m_0 \delta^{(4)}(x - y)$. It is convenient to subtract such a value from $m(x, y)$ and introduce the field

$$m'(x, y) \equiv m(x, y) - m_0 \delta^{(4)}(x, y). \quad (26.25)$$

¹Since $\frac{1}{4} 1 \otimes 1, -\frac{1}{4} (i\gamma_5) \otimes (i\gamma_5), \frac{1}{4} \gamma^\nu \otimes \gamma_\nu, -\frac{1}{4} \gamma^\nu \gamma_5 \otimes \gamma_\nu \gamma_5$ are the corresponding projection matrices.

With this and the definition

$$M \equiv \mathcal{M} + m_0, \quad (26.26)$$

Eq. (26.20) can be rewritten as

$$\int dy \left[(i\not{\partial} - M) \delta^{(4)}(x - y) - m'(x, y) \right] G(y, z) = i\delta^{(4)}(x - z). \quad (26.27)$$

Now let us assume that the oscillations $m'(x, y)$ are sufficiently small as to permit a perturbation expansion for $G(x, y)$:

$$G(x, y) = G_M(x, y) - i(G_M m' G_M)(x, y) - (G_M m' G_M m' G_M)(x, y) + \dots, \quad (26.28)$$

where $G_M(x, y)$ are the usual propagators of a free fermion of mass M :

$$G_M(x, y) \equiv G_M(x - y) \equiv \int \frac{d^4 p}{(2\pi)^4} e^{-ipx} \frac{i}{\not{p} - M}.$$

Using this expansion, the action (26.22) takes the form²

$$\mathcal{A}[m', \eta, \bar{\eta}, j^\nu] = \mathcal{A}_1[m'] + \mathcal{A}_2[m'] + \mathcal{A}_{\text{int}}[m'] + \mathcal{A}_{\text{ext}}[m', \eta, \bar{\eta}, j^\nu], \quad (26.29)$$

with

$$\mathcal{A}_1[m'] \equiv \int dx dy \text{tr}_{\text{SU}(2)} \left[G_M(x - y) m'(x, y) - \xi^{-1} m'(x, y) m_0 \frac{\delta(y, x)}{ig^2 D(x - y)} \right], \quad (26.30)$$

and $\mathcal{A}_2$ being quadratic in m' :

$$\mathcal{A}_2[m'] \equiv \int dx dy \text{tr}_{\text{SU}(2)} \left[\frac{i}{2} G_M m G_M m'(x, y) - \frac{1}{2} \xi^{-1} m'(x, y) m'(y, x) \frac{1}{ig^2 D(x - y)} \right]. \quad (26.31)$$

The third action term $\mathcal{A}_{\text{int}}[m']$ collects all remaining powers in m' :

$$\mathcal{A}_{\text{int}}[m'] \equiv \int dx \text{Tr} \left[- \sum_{n=3}^{\infty} \frac{(-i)^{n+1}}{n} (G_M m')^n(x, x) \right]. \quad (26.32)$$

The last action term $\mathcal{A}_{\text{ext}}$, finally, contains all interactions with the external sources

$$\begin{aligned} \mathcal{A}_{\text{ext}}[m', \eta, \bar{\eta}, j^\nu] = & \int dx dy \left\{ i\bar{\eta}(x) G(x, y) \eta(y) \right. \\ & - \frac{i}{2} g^2 D(x - y) j^\nu(x) j_\nu(y) - \frac{2}{D(0)} V^\nu(x, x) D(x - y) j_\nu(y) \\ & \left. - ig^2 \frac{\delta^{(4)}(0) \delta^{(4)}(x - y)}{D(0)} \int dz dz' D(z - x) D(y - z') j^\nu(z) j_\nu(z') \right\}. \quad (26.33) \end{aligned}$$

For the quantization of the collective field theory, we shall adopt an interaction picture. As usual, the quadratic part of the action, $\mathcal{A}_2[m']$, serves to construct the

²A trivial additive constant has been dropped.

free-particle Hilbert space. According to the least action principle, the free equations of motion are obtained from the extremality condition $\delta \mathcal{A}_2[m']/\delta m'(x, y) = 0$, rendering

$$m'(x, y) = g^2 \xi D(x - y) (G_M m' G_M)(x, y). \quad (26.34)$$

Going to momentum space

$$m'(p_2, p_1) \equiv \int dx_2 dx_1 e^{i(x_2 p_2 - x_1 p_1)} m'(x_2, x_1),$$

and introducing relative and total momenta

$$P \equiv (p_2 + p_1)/2, \quad q \equiv (p_2 - p_1)/2,$$

together with the notation

$$m'(P|q) \equiv m'(p_2, p_1),$$

the field equation becomes

$$m'(P|q) = \xi g^2 \int \frac{d^4 P'}{(2\pi)^4} D(P' - P) G_M \left(P' + \frac{q}{2}\right) m'(P'|q) G_M \left(P' - \frac{q}{2}\right). \quad (26.35)$$

In this form we easily recognize the Bethe Salpeter equation [22] for the vertex function of quark-antiquark bound states in the ladder approximation:

$$\Gamma^H(P|q) \equiv N_H \left(P + \frac{q}{2}\right) \int dz e^{iPz} \langle 0|T\psi\left(\frac{z}{2}\right) \bar{\psi}\left(-\frac{z}{2}\right)|0\rangle G_M \left(P' - \frac{q}{2}\right), \quad (26.36)$$

where N_H is some normalization factor. As a consequence our free field $m'(x, y)$ can be expanded in a complete set of ladder bound state solutions. These are the bare quanta spanning the Hilbert space of the interaction picture. Because of their bound quark-antiquark nature, they are called *bare mesons*. In the special case of QED, the “quarks” are electrons and the bare mesons are positronium atoms.

For mathematical reasons it is convenient to solve (26.35) for *fixed* $q^2 \in (0, 4M^2)$ and all possible coupling constants g^2 , to be called $g_H^2(q^2)$, i. e.

$$\Gamma^H(P|q) = \xi g_H^2(q^2) \int \frac{d^4 P'}{(2\pi)^4} D(P - P') G_M \left(P' + \frac{q}{2}\right) \Gamma^H \left(P' - \frac{q}{2}\right). \quad (26.37)$$

A useful normalization condition is

$$-i \int \frac{d^4 P}{(2\pi)^4} \text{Tr} \left[G_M \left(P + \frac{q}{2}\right) \Gamma^H(P|q) \Gamma^{\bar{H}'}(P|q) \right] = \epsilon^H \delta^{HH'}. \quad (26.38)$$

Here we have allowed a sign factor $\epsilon^H(q)$ which cannot be absorbed in the normalization N_H of (26.36). It may take the values +1, -1, or zero. Then the

expansion of the free field $m'(x, y)$ in terms of meson creation and annihilation operators $a_H^\dagger(\mathbf{q}), a_H(\mathbf{q})$ can be written as

$$m'_{\alpha\beta}(x, y) = \int \frac{d^4 q}{(2\pi)^4} \sum_H \delta^{(+)}(g_H^2(q^2) - g^2) \int \frac{d^4 P}{(2\pi)^4} \quad (26.39)$$

$$\times \left\{ e^{-i(q(x+y)/2 + P(x-y))} \Gamma^H(P|q) n_H a_H(\mathbf{q}) + e^{-i(q(x+y)/2 - P(x-y))} \bar{\Gamma}^H(P|-q) n_H^* a_H^\dagger(\mathbf{q}) \right\},$$

where n_H are appropriate factors giving $a_H(\mathbf{q})$ the standard normalization

$$[a_H(\mathbf{q}), a_{H'}^\dagger(\mathbf{q}')] = (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{q}') 2\omega^H(\mathbf{q}) \epsilon^H(q). \quad (26.40)$$

Here the sign factor $\epsilon^H(q)$ controls the norm of the mesonic state $a_H^\dagger|0\rangle \equiv |H\rangle$. In general there will be many states with unphysical norms since the *bare mesons* are produced by ladder diagrams only and may not be directly related to physical particles. This situation presents no fundamental difficulty. There are many interactions among bare mesons which are capable of excluding unphysical states from the S -matrix. In fact, the equivalence of the mesonized theory to the healthy original quark gluon version is a guarantee for physical results (on shell).

The propagator of the free field $m'(x, y)$ can be found most directly by adding an external disturbance to the free action

$$\mathcal{A}_2[m'] \rightarrow \mathcal{A}_2[m'] - \int dx dy \text{Tr} [m'(x, y) J(y, x)]. \quad (26.41)$$

This current enters the equation of motion as

$$m'(x, y) = -\xi g^2 D(x-y) J(x, y) + \xi g^2 D(x-y) (G_M m' G_M)(x, y). \quad (26.42)$$

The propagator

$$\mathbf{G}_{\alpha\beta, \alpha'\beta'}(x, y; x', y') \equiv \overline{m'(x, y) m'(x', y')} \quad (26.43)$$

is then defined as the solution of (26.42) for the δ -function disturbance

$$J_{\alpha\beta}(x, y) = i\delta(x-x')\delta(y-y')\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \quad (26.44)$$

It satisfies the inhomogeneous Bethe-Salpeter equation

$$\mathbf{G}_{\alpha\beta, \alpha'\beta'}(x, y; x', y') = \xi_{\alpha\beta, \beta'\alpha'} g^2 D(x-y) \delta(x-x') \delta(y-y') \\ + \xi_{\alpha\beta, \alpha'\beta'} D(x-y) \int d\bar{x} d\bar{y} G_M(x-\bar{x})_{\alpha\bar{\alpha}} \mathbf{G}_{\bar{\alpha}\bar{\beta}, \alpha'\beta'}(\bar{x}, \bar{y}; x' y') G_M(\bar{y}-y)_{\bar{\beta}\beta}.$$

This expression is immediately recognized as the equation for the two-quark transition matrix in the ladder approximation [see Eq. (26A.19) in Appendix 26A].

We can now give an explicit representation of the Green function in terms of the solutions $\Gamma^H(P|q)$ of the homogeneous equation (26.37). If $\mathbf{G}_{\alpha\beta, \alpha'\beta'}(P, P'|q)$ denotes the Fourier transform

$$(2\pi)^4 \delta^{(4)}(q - q') \mathbf{G}_{\alpha\beta, \alpha'\beta'}(P, P'|q) \equiv \int dx dy dx' dy' e^{i[P(x-y) + q(x+y)/2 - P'(x'-y') - q'(x+y')/2]} \mathbf{G}_{\alpha\beta, \alpha'\beta'}(x, y; x' y'), \quad (26.45)$$

it can be written as the sum over all meson solutions:

$$\mathbf{G}_{\alpha\beta,\alpha'\beta'}(P, P'|q) = -ig \sum_H \epsilon_H(q) \frac{\Gamma_{\alpha\beta}^H(P|q) \bar{\Gamma}_{\beta'\alpha'}^H(P'|-q)}{g_H^2(q^2) - g^2}, \quad (26.46)$$

where the sum comprises possible integrals over a continuous set of solutions. If quarks and gluons were scalars, the sum would be discrete for $q^2 \in (0, 4M^2)$ since the kernel of the integral equation (26.37) would be of the Fredholm type. A more detailed discussion was given in Appendix 26A. Here we only note that a power series expansion of the denominator

$$\mathbf{G}_{\alpha\beta,\alpha'\beta'}(P, P'|q) = -i \sum_{n=1}^{\infty} \sum_H \left(\frac{g^2}{g_H^2(q^2)} \right)^n \epsilon_H(q) \Gamma_{\alpha\beta}^H(P|q) \bar{\Gamma}_{\beta'\alpha'}^H(P'|-q) \quad (26.47)$$

renders explicit the exchange of one, two, three, etc. gluons. Hence one additional gluon can be inserted (or removed) by multiplying (or dividing) (26.46) by a factor $g^2/g_H^2(q^2)$. This fact will be of use later on.

Seen microscopically in terms of quarks and gluons, the free meson propagator (26.46) is given by the sum of ladders (see Fig. 26.1). Graphically, this will be

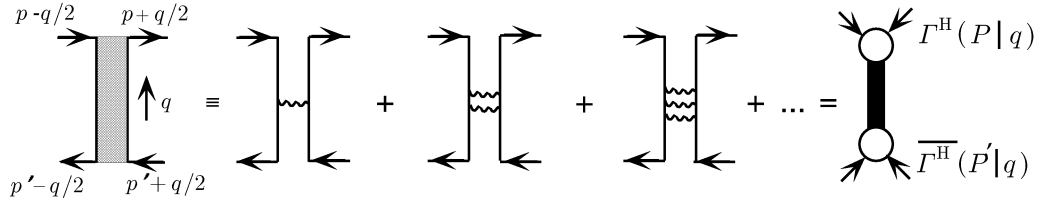


FIGURE 26.1 Ladder diagrams summed by a solution of the Bethe-Salpeter equation in Eq. (26.46).

represented by a wide band. In the last term of Fig. 26.1, we have also given a visualization of the expansion (26.46). Here, the fat line denotes the propagator

$$\Delta_H(q) = -i\epsilon_H(q) \frac{g^2}{g_H^2(q^2) - g^2}, \quad (26.48)$$

where upper and lower bubbles stand for the Bethe Salpeter vertices $\Gamma^H(P|q)$ and $\Gamma^H(P'|-q)$, respectively. This picture suggests another way of representing the new bilocal theory in terms of an *infinite-component* meson field depending only on the average position $X = (x + y)/2$. For this we simply expand the *interacting* field $m'(P|q)$ in terms of the complete set of vertex functions

$$m'(P|q) = \sum_H \Gamma^H(P|q) m_H(q). \quad (26.49)$$

Inserting this expansion into (26.29), the free action becomes directly

$$\mathcal{A}_2[m'] = \frac{1}{2} \int dX m_H(X) \left(1 - g_H^2(q^2)/g^2 \right) m_H(X), \quad (26.50)$$

implying the free propagator (26.48) for the field $m_H(X)$. With this understanding of the free part of the action we are now prepared to interpret the remaining pieces.

Consider first the linear part $\mathcal{A}_1[m']$. The first term in it can graphically be presented as shown in Fig. 26.2. When attached to other mesons it produces a tadpole correction. When interpreted within the underlying quark gluon picture,

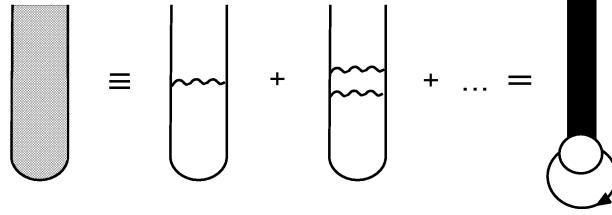


FIGURE 26.2 Ladder diagrams summed in the tadpole term $\mathcal{A}_1[m']$ of Eq. (26.46).

such a correction sums up all rainbow contributions to the quark propagator (see Fig. 26.3). The second term in $\mathcal{A}_1[m']$ has also a straight-forward graphical inter-

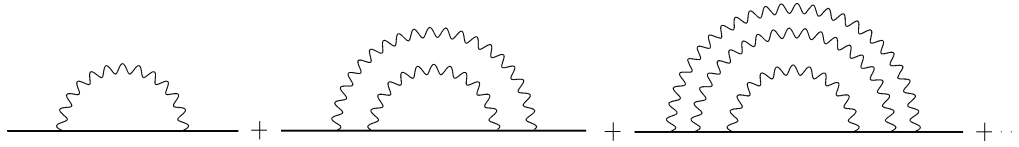


FIGURE 26.3 Rainbow diagrams in the tadpole term of the previous figure.

pretation. First of all, the division by $\xi g^2 D(x-y)$ has the effect of removing one rung from the ladder sum (such that the ladder starts with no rung, one rung, etc.). In addition, it creates two open quark legs. This can be seen directly from (26.37) and (26.46): Suppose a meson line ends at the interaction

$$-\int dxdy \text{Tr} [m'(x,y)\xi^{-1}m_0] / ig^2 D(x-y)\delta^{(4)}(x-y). \quad (26.51)$$

Then the factor $[\xi g^2 D(x-y)]^{-1}$ applied to $\mathbf{G}(P, P'|q)$ gives (omitting irrelevant indices)

$$[\xi g^2 D]^{-1} \mathbf{G} = -ig^2 \sum_H \epsilon_H \frac{[\xi g^2 D]^{-1} \Gamma^H \bar{\Gamma}^H}{g_H^2(q^2) - g^2}. \quad (26.52)$$

Due to (26.37), this is equal to

$$[\xi g^2 D]^{-1} \mathbf{G} = -ig^2 \sum_H \epsilon_H \frac{g_H^2(q^2)}{g^2} \frac{(G_M \Gamma^H G_M) \bar{\Gamma}^H}{g_H^2(q^2) - g^2}. \quad (26.53)$$

As discussed before, the factor $g_H^2(q^2)/g^2$ amounts to the removal of one rung. Multiplication by $-m_0$ and integration over $\int dP/(2\pi)^4$ yields the total contribution of this meson graph

$$i m_0 \sum_H \frac{g_H^2(q^2)}{g_H^2(q^2) - g^2} \times \int \frac{d^4 P}{(2\pi)^4} \text{Tr} \left[G_M \left(P + \frac{q}{2} \right) \Gamma^H(P|q) G_M \left(P - \frac{q}{2} \right) \right] \epsilon_H(q) \bar{\Gamma}^H(P'| - q). \quad (26.54)$$

As far as quarks and gluons are concerned, this amounts to the insertion of a mass term m_0 on top of a ladder graph with one rung removed (this being indicated by a slash in Fig. 26.4). The quark gluon picture leads us to expect that m_0 must

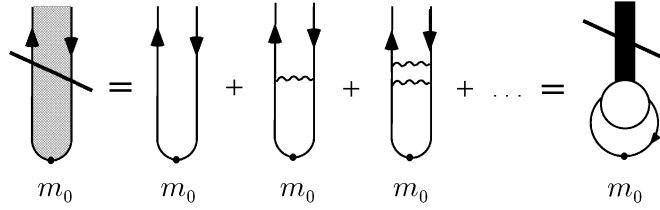


FIGURE 26.4 Ladder of gluon exchanges summed in a meson tadpole diagram marked by a slash. Compare Fig. 26.1.

be a cutoff-dependent quantity canceling the logarithmic divergence in every upper loop of the ladder sum of Fig. 26.2. Numerically, m_0 is most easily calculated by canceling the infinity contributed by $\mathcal{A}_1[m']$ to the equation of motion (26.35). If we include $\mathcal{A}_1[m']$, this equation reads

$$m_0(2\pi)^4 \delta^{(4)}(q) + m'(P|q) = \left[\xi i g^2 \int \frac{d^4 P'}{(2\pi)^4} D(P - P') G(P') \right] (2\pi)^4 \delta^{(4)}(q) + \xi g^2 \int \frac{d^4 P'}{(2\pi)^4} D(P - P') G_M \left(P' + \frac{q}{2} \right) m'(P'|q) G_M \left(P' - \frac{q}{2} \right). \quad (26.55)$$

The first term on the right-hand side is exactly the usual self-energy $\Sigma(P)(2\pi)^4 \delta^{(4)}(q)$ in second order

$$\Sigma_{\alpha\beta}(P) \equiv -\xi_{\alpha\beta,\gamma\delta} i \int \frac{d^4 P'}{(2\pi)^4} \frac{1}{(P - P')^2 - \mu^2} \frac{1}{\not{P} - M}. \quad (26.56)$$

Normalizing $\Sigma(P)$ on the mass shell, one finds the usual expression

$$\Sigma(P) = \Sigma_0 + \Sigma_1 \times (\not{P} - M) + \Sigma_R(P), \quad (26.57)$$

where Σ_R is the regularized self-energy. The cutoff dependent term

$$\Sigma_0 = \frac{3}{4\pi} \frac{g^2}{4\pi} M \left(\log \Lambda^2/M^2 + \frac{1}{2} \right) \quad (26.58)$$

must be balanced by choosing $m_0 = -\Sigma_0$ on the left-hand side of (26.55). Also, the second term Σ_1 is cutoff dependent:

$$\Sigma_1 = \frac{1}{4\pi} \frac{g^2}{4\pi} \left(\log \Lambda^2/M^2 + \frac{9}{2} + 2 \log \mu^2/M^2 \right), \quad (26.59)$$

and a renormalization is necessary to cancel this infinity. Most economic is the introduction of an appropriate wave function counter term $(Z_2 - 1) \bar{\psi}(i\partial - M)$ in the original Lagrangian (26.1). Such a term would enter Eq. (26.20) as

$$\begin{aligned} \int dy \left\{ (i\partial - \mathcal{M}) \delta^{(4)}(x - y) \right. \\ \left. + (Z_2 - 1) (i\partial - M) \delta^{(4)}(x - y) - m(x, y) \right\} G(y, x) = i\delta^{(4)}(x - y). \end{aligned} \quad (26.60)$$

Instead of (26.25), $m(x, y)$ should now be assumed to fluctuate around $[m_0 + (Z_2^{-1} - 1) (i\partial - M)] \delta^{(4)}(x - y)$. By defining a new $m'(x, y)$ via

$$m'(x, y) \equiv m(x, y) - [m_0 + (Z_2^{-1} - 1) (i\partial - M)] \delta^{(4)}(x - y), \quad (26.61)$$

the full action (26.29) is obtained exactly as before, except for the linear part $\mathcal{A}$, in which the new wave function renormalization term enters together with m_0 :

$$\begin{aligned} \mathcal{A}_1[m'] = \int dx dy \operatorname{tr}_{\text{SU}(2)} \left\{ G_M(x - y) m'(x, y) \right. \\ \left. - \xi^{-1} m'(x, y) [m_0 + (Z_2^{-1} - 1) (i\partial - M)] \frac{\delta^{(4)}(x - y)}{ig^2 D(x - y)} \right\}. \end{aligned}$$

By choosing

$$Z_2^{-1} - 1 = -\Sigma_1, \quad (26.62)$$

the cutoff dependent term Σ_1 is exactly compensated in the equation of motion (26.55). After this renormalization procedure, only the finite term $\Sigma_R(P)$ is left. The regularized action is

$$\mathcal{A}_1[m']_R = \int dx dy \Sigma_R(x - y) m'(x, y) \frac{1}{ig^2 D(x - y)}. \quad (26.63)$$

Using the expansion (26.49), this can be rewritten as

$$\mathcal{A}_1[m']_R = \sum_H \int dX f_H(-\square) m_H(X), \quad (26.64)$$

with

$$f_H(q^2) = i \int \frac{d^4 P}{(2\pi)^4} \operatorname{Tr} \left[\Sigma_R(\not{P}) G_M \left(P + \frac{q}{2} \right) \Gamma^H(P|q) G_M \left(P - \frac{q}{2} \right) \right] \frac{g_H^2(q^2)}{g^2}. \quad (26.65)$$

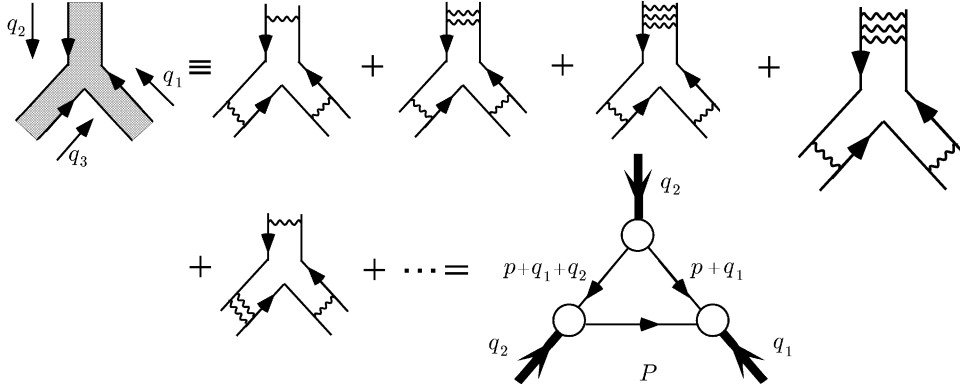


FIGURE 26.5 Gluon diagrams contained in a three-meson vertex.

By momentum conservation, the tadpole momentum always vanishes such that only $f_H(0)$ is needed eventually.

Let us now proceed to the discussion of the interaction part $\mathcal{A}_{\text{int}}[m']$ of Eq. (26.32). Take as an example the term of the third order in m' . If a meson line ends at every m' , it can be represented graphically as shown in Fig. 26.5. Employing the expansion (26.49), this interaction term can be rewritten as

$$\begin{aligned} \mathcal{A}_{\text{int}}^{\text{3hadr}}[m'] &= -\frac{1}{3} \sum_{H_1 H_2 H_3} \int \frac{d^4 q_3}{(2\pi)^4} \frac{d^4 q_2}{(2\pi)^4} \frac{d^4 q_1}{(2\pi)^4} (2\pi)^4 \delta^{(4)}(q_1 + q_2 + q_3) \\ &\times \int \frac{d^4 P}{(2\pi)^4} \text{tr}_{\text{SU}(2)} \left[\Gamma^H \left(P - \frac{q_3}{2} \middle| q_3 \right) G_M(P + q_1 q_2) \Gamma^{H_2} \left(P + q_1 + \frac{q - 2}{2} \middle| q_2 \right) \right. \\ &\quad \left. G_M(P + q_1) \Gamma^{H_1} \left(P + \frac{q_1}{2} \middle| q_1 \right) G_M(P) \right] m_{H_3}(q_3) m_{H_2}(q_2) m_{H_1}(q_1) \\ &\times \frac{1}{3} \sum_{H_1 H_2 H_3} \int dX v_{H_3 H_2 H_1} \left(i\partial_X^{H_3}, i\partial_X^{H_2}, i\partial_X^{H_1} \right) m_{H_3}(X) m_{H_2}(X) m_{H_1}(X), \quad (26.66) \end{aligned}$$

with a vertex function $v_{H_3 H_2 H_1} \left(i\partial_X^{H_3}, i\partial_X^{H_2}, i\partial_X^{H_1} \right)$ whose derivatives $\partial_X^{H_i}$ should be applied only to the argument of the corresponding hadron field $m_{H_i}(X)$. A corresponding formula holds for every power of the hadron field $m_{H_i}(X)$.

Notice that the flow of the quark lines in every interaction is anticlockwise. When drawing up mesonic Feynman graphs it may sometimes be more convenient to draw a clockwise flow. A simple identity helps to write down directly the corresponding Feynman rules. Consider a graph for a three meson interaction and cross the upper band downwards (see Fig. 26.6). The interaction appears now with the mesonic bands in anticyclic order, and the fermion lines in the meson vertex flow clockwise. This is topologically compensated by twisting every band once. Mathematically, this deformation displays the following identity of the vertex functions

$$v_{H_3 H_2 H_1}(q_3, q_2, q_1) = \eta_{H_3} \eta_{H_2} \eta_{H_1} v_{H_1 H_2 H_3}(q_1 q_2 q_3), \quad (26.67)$$

where the phase η_H denotes the charge parity of the meson H . This phase may be absorbed in the propagator characterizing the twisted band.

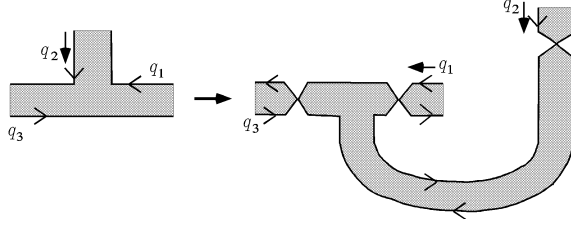


FIGURE 26.6 Three-meson vertex drawn in two alternative ways.

The proof of this identity is quite simple. Let C be the charge conjugation matrix

$$C = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}, \quad (26.68)$$

where c is the 2×2 -matrix

$$c = -i\sigma^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (26.69)$$

This matrix is the two-dimensional representation of rotation around the 2-axis by an angle π :

$$c = e^{-i\pi\sigma^2/2}, \quad (26.70)$$

as can easily be verified using

$$R_{\hat{\varphi}}(\varphi) = e^{-i\varphi \cdot \boldsymbol{\sigma}/2} = \cos \frac{\varphi}{2} - i\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\varphi}} \sin \frac{\varphi}{2}, \quad (26.71)$$

and the property $\sigma^{i2} = 1$. From the rotation property of σ^i under C it follows directly that

$$c^{-1} \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix} c = \begin{pmatrix} -\sigma^1 \\ \sigma^2 \\ -\sigma^3 \end{pmatrix}, \quad (26.72)$$

and we find

$$\begin{aligned} \begin{pmatrix} c^{-1} & 0 \\ 0 & -c^{-1} \end{pmatrix} \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix} \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} &= \begin{pmatrix} 0 & -c^{-1}\sigma^\mu c \\ -c^{-1}\tilde{\sigma}^\mu c & 0 \end{pmatrix} \\ &= (-\gamma^0, \gamma^1, -\gamma^2, \gamma^3) = -\gamma^{\mu T}, \end{aligned} \quad (26.73)$$

so that (26.68) satisfies

$$C^{-1}\gamma^\mu C = -\gamma^{\mu T}, \quad (26.74)$$

thus ensuring a sign change of the electromagnetic interaction $A_\mu \bar{\psi} \gamma^\mu \psi$. As a consequence, the vertices satisfy:

$$C \Gamma^H(P|q) C^{-1} = \eta_H \Gamma^H(-P|q)^T. \quad (26.75)$$

Inserting now CC^{-1} between all factors in (26.66) and observing $C\gamma^\mu C^{-1} = -\gamma^{\mu T}$ [recall (4.602)], one has

$$\begin{aligned} v_{H_3 H_2 H_1}(q_3, q_2, q_1) &= -\eta_{H_3} \eta_{H_2} \eta_{H_1} \times \\ &\times \int \frac{dP}{(2\pi)^4} \text{tr}_{\text{SU}(2)} \left\{ \Gamma^{H_3} \left(-P + \frac{q_3}{2} \middle| q_3 \right)^T \left(\frac{i}{-\not{P} - \not{q}_1 - \not{q}_2 - M} \right)^T \right. \\ &\left. \Gamma^{H_2} \left(-P - q_1 - \frac{q_2}{2} \middle| q_2 \right)^T \left(\frac{i}{-\not{P} - \not{q}_1 - M} \right)^T \Gamma^{H_1} \left(-P - \frac{q_1}{2} \middle| q_1 \right) \left(\frac{i}{-\not{P} - M} \right)^T \right\}. \end{aligned} \quad (26.76)$$

Taking the transpose inside the trace and changing the dummy variable P to $-P$, the vertices appear in anticyclic order and the right-hand side coincides indeed with $\eta_{H_3} \eta_{H_2} \eta_{H_1} v_{H_1 H_2 H_3}(q_1, q_2, q_3)$. Twisted propagators are physically very important. They describe the strong rearrangement collisions of quarks and certain classes of cross-over gluon lines. Fig. 26.7 shows some twisted graphs together with their quark gluon contents. Meson scattering rearrangement collisions shown in Fig. 26.7a have

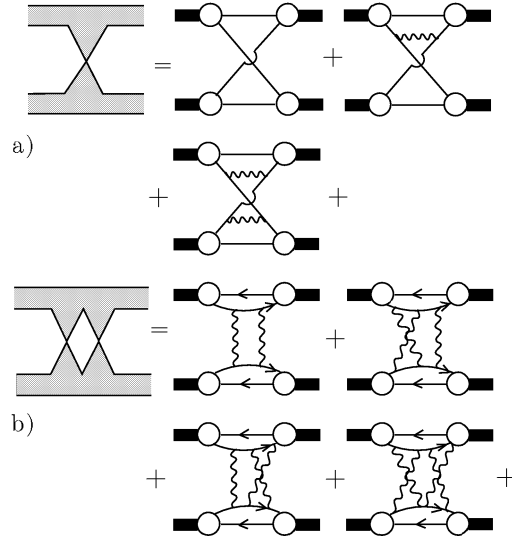


FIGURE 26.7 Quark-gluon exchanges summed in meson exchange diagrams.

roughly the same coupling strength as direct (untwisted) exchanges. In QED they are the source of the main binding forces in molecules.

The exchange of two twisted meson lines (Fig. 26.7b) seems to be an important part of diffraction scattering (Pomeron).

Two more examples are shown in Fig. 26.8. Note that, in the pseudoscalar channel, these graphs incorporate the effect of the Adler triangle anomaly.

In this connection it is worth pointing out that all fundamental meson vertices are planar graphs as far as the quark lines are concerned. Non-planar graphs are generated by building up loops involving twisted propagators. With propagator

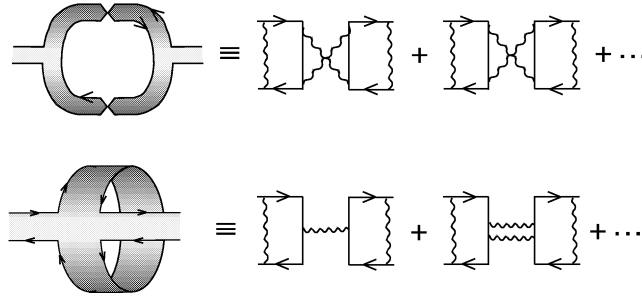


FIGURE 26.8 Quark-gluon diagrams summed in a meson loop diagram.

bands, their twisted modifications and planar fundamental meson graphs are seen to possess exactly the same topology as the graphs used in dual models [23], except for the stringent dynamical property of duality itself: In the present mesonized theory one still must sum s and t channel exchanges, and they are by no means the same. Only after introduction of color and the ensuing linearly rising mass spectra one can hope to account also for this particular aspect of strong interactions.

The similarity in topology can be exploited to study an important phenomenon of strong interactions: the Okubo, Zweig, and Iizuka rule. Obviously all meson couplings derived by mesonization exactly respect this rule. Violations will come from graphs of the so-called cylinder type [14] (for example Fig. 26.7b).

Let us finally discuss the external sources. From $\mathcal{A}_{\text{ext}}$ in (26.44) we see that external fermion lines are connected via the full propagator G which after expansion in powers of m' amounts to radiation of any number of mesons (see Fig. 26.9). These mesons interact further among each other as quantum fields. Diagrammatically, every bubble carries again a factor $\Gamma^H(P|q)$.

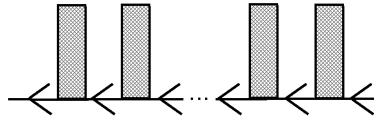


FIGURE 26.9 Multi-meson emission from a quark line.

It has to be watched out that mesons are always emitted to the right-hand side of each line. For example, the lowest order quark-quark-scattering amplitude should initially be drawn as shown in Fig. 26.10 in order to avoid phase errors due to twisted bands. Then the graphical rules yield directly the expression (26.46) as they should. Afterwards, arbitrary deformations can be performed if all twisted factors η_H are respected.

External vector fields such as photons interact with mesons according to the third term in Eq. (26.33)

$$-\frac{2}{g^2 D(0)} \int dxdy V^\nu(x, x) g^2 D(x - y) j_\nu(y). \quad (26.77)$$

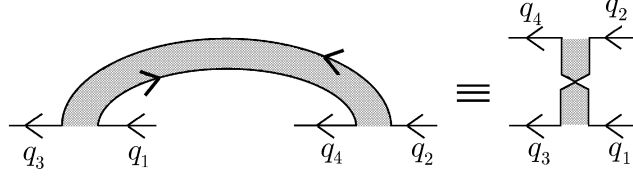


FIGURE 26.10 Twisted exchange of a meson between two quark lines.

Hence every external vector field enters the mesonic world only via an intermediate vector particle and there is a current field identity as has been postulated in phenomenological treatments of vector mesons (VMD). Here one finds a non-trivial coupling between the gluon and the vector mesons: As discussed before, the division by $g^2 D$ amounts to a removal of one rung from the ladder of the incoming meson propagator and takes care of the direct coupling of the gluon to the quarks *without* the ladder corrections. This is accounted for by a factor $g_H^2(q^2)/g^2$ in the propagator sum (26.47). Thus the direct coupling of the vector meson field $m_H(x)$ to an external vector field $A_\nu^{\text{ext}}(x)$ can be written as:

$$g \sum_H \int \frac{d^4 q}{(2\pi)^4} \int \frac{d^4 P}{(2\pi)^4} \times \text{Tr} \left\{ \gamma^\nu G_M \left(P + \frac{q}{2} \right) \Gamma^H(P|q) G_M \left(P - \frac{q}{2} \right) \right\} \frac{g_H^2(q^2)}{g^2} m_H(q) A_\nu^{\text{ext}}(-q). \quad (26.78)$$

In a mesonic graph, the removal of one rung will be indicated by a slash. As an example, the lowest order contribution to the quark gluon form factor is illustrated in Fig. 26.11. The slash guarantees the presence of the direct coupling. The free

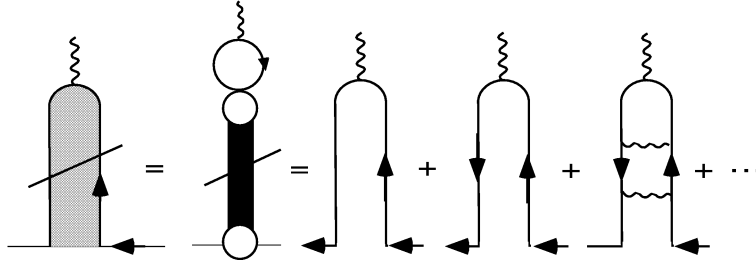


FIGURE 26.11 Vector meson dominance in the coupling of an external photon to a quark line.

propagator of an external gluon is given by the second term of Eq. (26.33). The lowest radiative corrections consist in an intermediate slashed vector meson (see Fig. 26.12). Here the slash is important to ensure the presence of one single quark loop.

The divergent last term in the external action (26.33) has no physical significance since it contributes only to the external gluon mass and can be canceled by an appropriate counter term.

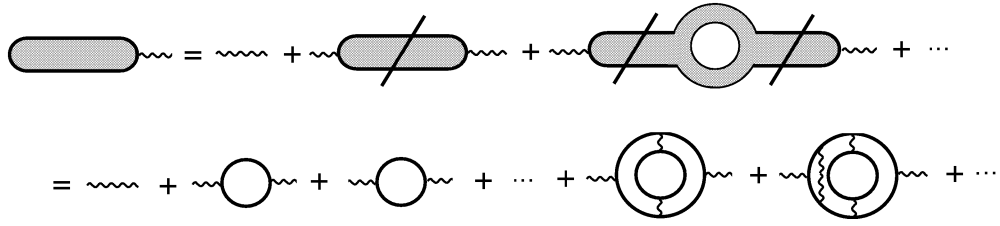


FIGURE 26.12 Vector meson dominance in a photon propagator.

A final remark concerns the bilocal currents as measured in deep inelastic electron and neutrino scattering. These are vector currents of the type

$$j^\nu(x, y) \equiv \bar{\psi}(x) \gamma^\nu \psi(y). \quad (26.79)$$

It is obvious that also for bilocal currents there is a current-field identity with the bilocal field $V^\mu(x, y)$. In fact, if one had added an external source term $C_\nu(x, y)$ with an action

$$\Delta \mathcal{A}_{\text{ext}} \equiv \int dx dy \bar{\psi}(x) \gamma^\nu \psi(y) C_\nu(x, y), \quad (26.80)$$

this would appear in the mesonized version in the form

$$\Delta \mathcal{A}_{\text{ext}} = \int dx dy \frac{1}{i g^2 D(x - y)} V^\nu(x, y) C_\nu(x, y), \quad (26.81)$$

which proves our statement. Again, a rung has to be removed in order to allow for the pure quark contribution (see Fig. 26.13).

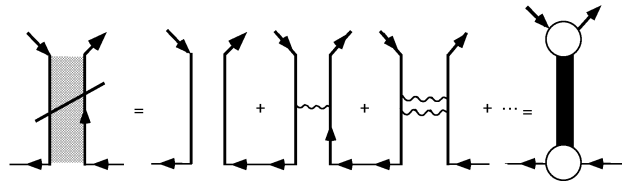


FIGURE 26.13 Gluon diagrams in a meson propagator (dashed).

Bilocal currents carry direct information on the properties of Regge trajectories [16]. Therefore the present bilocal field theory seems to be the appropriate tool for the construction of a complete field theory of Reggeons [19], which is again equivalent to the original quark gluon theory. Technically, such a construction would proceed via analytic continuation of the propagators (26.36) in the angular momentum (and the principal quantum number) of the mesons H . The result would be a “reggeonized” quark gluon theory. The corresponding Feynman graphs would be unitarity in all three scattering channels.

26.3 The Limit of Heavy Gluons

As an illustration of the mesonization procedure we now discuss in detail the limit of very heavy gluons [21, 38]. Apart from its simplicity, this limit is quite attractive on physical grounds since it may yield a reasonable approximation to low energy meson interactions. This is suggested by the following arguments:

Suppose hydrodynamics is governed by a colored quark-gluon theory. Then the color degree of freedom is very important for generating a potential between quarks rising at long distances. This would explain the observed large number of high-mass resonances. However, as far as low-energy interactions among the lowest lying mesons are concerned, color seems to be a rather superfluous luxury:

First, many fundamental aspects of strong interaction dynamics are independent of color. Examples are chiral $SU(3) \times SU(3)$ current algebra relations with PCAC (together with the low-energy theorems derived from both) and the approximate light cone algebra.

Second, there is no statistics argument concerning the symmetry of the meson wave function as there is for baryons [22].

Third, high-lying resonances are known to contribute very little in most dispersion relations of low-energy amplitudes. For example, the low-energy value of the isospin odd $\pi\pi$ -scattering amplitude is given by a dispersion integral over the mesons ρ and σ with $\approx 90\%$ accuracy [23]. Similarly, $\pi\rho$ -scattering is saturated by the intermediate mesons π and A_1 . By looking at all scattering combinations, we can easily convince ourselves that the resonances π , ρ , A_1 , σ form an approximately closed “subworld” of mesons as far as dispersion relations are concerned. As a consequence, it would not at all be astonishing if the neglect of color in a quark gluon theory would not change the dynamics when restricting the attention to this mesonic “subworld”.³ The point is now that, in the limit of a large gluon mass $\mu \rightarrow \infty$, exactly this restricted set of mesons appears as particles in the mesonized quark gluon theory (26.1) *without* color. Thus it might be considered as some approximation to the low-energy aspects of the colored version. Indeed, we shall see that the mesonized theory coincides exactly with the well-known chirally invariant σ -model. In the past, this model has proven to be an appropriate tool for a rough description of low-energy meson physics [27]. Our derivation of the σ model via mesonization will render several new relations between meson and quark properties [21]. We shall at first confine ourselves to $SU(2)$ quarks only, such that symmetry breaking may be neglected. The extension to broken $SU(3)$ will be performed afterwards.

³There exists a simple estimate of the electromagnetic decay of $\pi^0 \rightarrow \gamma\gamma$ based on short-distance arguments, which therefore depend on color [25]. However, the same decay can be estimated also via intermediate distance arguments, using the coupling $\rho\omega\pi$ and vector meson dominance. Then color does not enter the argument.

In order to start with the derivation observe that, in the limit $\mu \rightarrow \infty$, the gluon propagator approaches a δ -function:

$$iD(x-y) \rightarrow \frac{1}{\mu^2} \delta^{(4)}(x-y). \quad (26.82)$$

The interaction (26.6) takes the four-fermion local form

$$\begin{aligned} \frac{1}{2}G \left\{ \bar{\psi}(x)\psi(y)\bar{\psi}(y)\psi(x) + \bar{\psi}(x)i\gamma_5\psi(y)\bar{\psi}(y)i\gamma_5\psi(x) \right. \\ \left. - \frac{1}{2}\bar{\psi}(x)\gamma^\nu\psi(y)\bar{\psi}(y)\gamma_\nu\psi(x) - \frac{1}{2}\bar{\psi}(x)\gamma^\nu\gamma_5\psi(y)\bar{\psi}(y)\gamma_\nu\gamma_5\psi(x) \right\}. \end{aligned} \quad (26.83)$$

with the Fermi-like coupling constant

$$G \equiv \frac{g^2}{\mu^2}. \quad (26.84)$$

The equation of motion (26.34) forces $m'(x, y)$ to become a local field $m'(x)$:

$$m'(x, y) \rightarrow m'(x)\delta^{(4)}(x-y), \quad (26.85)$$

which satisfies the free field equation

$$m'(x) = -i\frac{g^2}{\mu^2}\xi \int dy G_M(x-y)m'(y)G_M(y-x). \quad (26.86)$$

In the local limit, the action without external sources takes the form

$$\begin{aligned} \mathcal{A}[m'] = \int dx \operatorname{tr}_{\text{SU}(2)} \left\{ G_M(x, x)m'(x) - \frac{1}{2} (G_M m' G_M m') (x, x) \right. \\ \left. + \sum_{n=3}^{\infty} \frac{(-i)^{n-1}}{n} (G_M m')^n (x, x) - \frac{\mu^2}{g^2} \frac{1}{2\xi} m'(x)^2 - \frac{1}{\xi} m'(x)m_0 \right\}, \end{aligned} \quad (26.87)$$

where $(G_M m' G_M m') (x, x)$ is short for $\int dy G_M(x-y)m'(y)G_M(x-y)$ etc. As discussed earlier, the constant m_0 is determined by the vanishing of the tadpole parts in (26.87). This amounts to balancing the constant contributions in the wave equation. Due to the singularity of $G_M(x-y)$ for $x \rightarrow y$, this condition has a meaning only if a cutoff is introduced such that $G_M(0)$ is finite:

$$\begin{aligned} [G_M(0)]_{\alpha\beta} &= \int \frac{d^4 P}{(2\pi)^4} \left[\frac{i}{\not{P} - M} \right]_{\alpha\beta} = M \int_0^\Lambda \frac{d^4 P_E}{(2\pi)^4} (P_E^2 + M^2)^{-1} \delta_{\alpha\beta} \\ &= M \frac{\pi^2}{(2\pi)^4} (\Lambda^2 - M^2 \log \Lambda^2/M^2) \delta_{\alpha\beta} \equiv MQ \delta_{\alpha\beta}. \end{aligned} \quad (26.88)$$

Here the dP^0 integration has been Wick-rotated by 90° such that the momentum $P^\mu = (P^0, \mathbf{P})$ becomes $(iP^4, \mathbf{P})$ with $P^4 \in (-\infty, \infty)$ along the integration path. The new real momentum $(P^4, \mathbf{P})$ has been denoted by P_E^μ , and its euclidean scalar

product by $P_E^\mu = P^{42} + \mathbf{P}^2 = -P^2$. The tadpoles can now be canceled by satisfying the equation

$$G_M(0) = \frac{1}{\xi} m_0. \quad (26.89)$$

For the scalar part of the matrix $[G_M(0)]_{\alpha\beta}$, this implies the *gap equation*

$$m_0 = 4 \frac{g^2}{\mu^2} QM. \quad (26.90)$$

Remembering the relation to the bare quark mass $m_0 = M - \mathcal{M}$, this determines the connection between the “true” quark mass M and the bare mass $\mathcal{M}$ contained in the Lagrangian:

$$M = \mathcal{M} + 4 \frac{g^2}{\mu^2} QM. \quad (26.91)$$

Equation (26.90) is called *gap equation* because of its analogous appearance in the theory of superconductivity (see Eq. (23.115) in Chapter 23, and Chapter 3 in the textbook Ref. [17]. See also [18]).

Consider now the free part $\mathcal{A}_2[m']$ of the action. Performing again a decomposition of the type (26.13), but with the local field $m'(x)$, it can be written in the form

$$\mathcal{A}_2[m'] = \int dx \operatorname{tr}_{\operatorname{SU}(2)} \left\{ \frac{1}{2} m'_i(x) J_{ij}(i\partial) m_j(x) - \frac{\mu^2}{2g^2} [S^2(x) + P^2(x) - 2V^2(x) - 2A^2(x)] \right\}, \quad (26.92)$$

where $m'_i(x) (i = 1, 2, 3, 4)$ is short for the fields⁴ $S(x)$, $P(x)$, $V(x)$, $A(x)$ and the trace runs only over internal SU(2) indices. The coefficients $J_{ij}(q)$ are given by the integrals

$$J_{ij}(q) \equiv -4 \int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P + q/2)_E^2 + M^2} \frac{1}{(P - q/2)_E^2 + M^2} t_{ij}(P|q), \quad (26.93)$$

where $t_{ij}(P|q)$ denotes the Dirac traces

$$t_{ij}(P|q) \equiv \frac{1}{4} \operatorname{tr}_{\operatorname{Dirac}} \left\{ \Gamma_i \left(\not{P} + \frac{\not{q}}{2} + M \right) \Gamma_j \left(\not{P} - \frac{\not{q}}{2} + M \right) \right\}, \quad (26.94)$$

with $\Gamma_i (i = 1, 2, 3, 4)$ abbreviating the standard Dirac covariants $1, i\gamma_5, \gamma^\nu, \gamma^\nu\gamma_5$. The traces are displayed in Eqs. (26A.32)–(26A.35) of Appendix A. Some of them grow quadratically in P . The corresponding integrals $J_{ij}(q)$ are quadratically divergent for large cutoffs. The others diverge logarithmically. If one introduces the basic integral

$$L \equiv \int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^2} = \frac{\pi^2}{(2\pi)^4} \left(\log \frac{\Lambda^2}{M^2} - 1 \right), \quad (26.95)$$

⁴The Lorentz indices of V^ν and A^ν fields are suppressed.

the divergent parts of J_{ij} are (see Appendix 26B)

$$J_{SS}(q) = Q + L \left(\frac{q^2}{2} - 2M^2 \right), \quad (26.96)$$

$$J_{PP}(q) = Q + L \frac{q^2}{2}; \quad J_{PA^\nu} = -iLMq^\nu, \quad (26.97)$$

$$J_{V^\mu V^\nu}(q) = -\frac{1}{3} (q^2 g^{\mu\nu} - q^\mu q^\nu) L, \quad (26.98)$$

$$J_{A^\mu A^\nu}(q) = -\frac{1}{3} [(q^2 g^{\mu\nu} - q^\mu q^\nu) - 6M^2 g^{\mu\nu}] L, \quad (26.99)$$

$$J_{A^\mu P}(q) = iLMq^\mu, \quad (26.100)$$

with all other integrals vanishing.

If we neglect the finite contributions as compared with these divergent ones, the action $\mathcal{A}_2[m']$ is seen to correspond to the local Lagrangian⁵

$$\begin{aligned} \mathcal{L}(x) = & \text{tr}_{\text{SU}(2)} \left\{ \frac{1}{2} S'(x) \left[4Q - 2(\square + 4M^2) L - \frac{\mu^2}{g^2} \right] S'(x) \right. \\ & + \frac{1}{2} P(x) \left[4Q - 2\square L - \frac{\mu^2}{g^2} \right] P(x) \\ & + \frac{1}{2} V_\mu(x) \left[\frac{4}{3} (\square g^{\mu\nu} - J^\mu \partial^\nu) L + \frac{2\mu^2}{g^2} \right] V_\nu(x) \\ & + \frac{1}{2} A_\mu(x) \left[\frac{4}{3} (\square g^{\mu\nu} - \partial^\mu \partial^\nu) L + 8M^2 g^{\mu\nu} L + \frac{2\mu^2}{g^2} \right] A_\nu(x) \\ & \left. + 2ML [\partial_\mu P(x) A^\mu(x) + A^\mu(x) \partial_\mu P(x)] \right\}. \end{aligned} \quad (26.101)$$

If we insert the gap equation (26.91) in this Lagrangian, the quadratically divergent terms Q can be eliminated. The mixed terms may be removed by introducing a new field $\tilde{A}^\mu(x)$ via

$$A^\mu(x) = \tilde{A}^\mu(x) + \lambda \partial^\mu P, \quad (26.102)$$

and fixing λ as

$$\lambda = -3M/m_A^2, \quad (26.103)$$

where m_A^2 is short for

$$m_A^2 = m_V^2 + 6M^2, \quad (26.104)$$

with

$$m_V^2 = 3\mu^2/(2g^2 L). \quad (26.105)$$

⁵Since $m(x)$ and $m'(x)$ differ only by a Dirac scalar constant $m_0 1_{\alpha,\beta}$, there is no difference between primed and unprimed fields except for $S'(x) = S(x) - m_0$.

This substitution produces additional kinetic terms for the pseudoscalar fields which now appear with a factor

$$-\text{tr}_{\text{SU}(2)}(P(x)\square P(x))\left(1+\frac{2}{3}m_A^2\lambda^2+4M_\lambda\right)L=\text{tr}_{\text{SU}(2)}(\partial_\mu P(x)\partial^\mu P(x))Z_P^{-1}L. \quad (26.106)$$

Using (26.103), the renormalization constant Z_P becomes

$$Z_P^{-1}=1-6M^2/m_A^2. \quad (26.107)$$

After this diagonalization, the quadratic part of the collective Lagrangian reads

$$\begin{aligned} \mathcal{L}(x) = \text{tr}_{\text{SU}(2)} \bigg\{ & \partial_\mu S' \partial^\mu S' - \left(4M^2 + \frac{1}{3}m_V^2\mathcal{M}/M\right) S'^2 \\ & - \partial_\mu P \partial^\mu P Z_P^{-1} - \frac{1}{3}m_V^2\mathcal{M}/MP^2 \\ & - \frac{1}{3}F_V^{\mu\nu}F_{\mu\nu}^V + \frac{2}{3}m_V^2V_\mu^2 \\ & - \frac{1}{3}F_{\tilde{A}}^{\mu\nu}F_{\mu\nu}^{\tilde{A}} + \frac{2}{3}m_A^2\tilde{A}_\mu^2 \bigg\} \times L, \end{aligned} \quad (26.108)$$

where $F_{V,\tilde{A}}^{\mu\nu}$ are the usual field tensors of vector and axial vector fields. The particle content of this free Lagrangian is now obvious. There are vector mesons of mass m_V^2 , axial-vector mesons of mass m_A^2 , and scalar and pseudoscalar mesons of mass

$$m_S^2 = 4M^2 + \frac{1}{3}m_V^2\frac{\mathcal{M}}{M}, \quad (26.109)$$

$$m_P^2 = \frac{1}{3}m_V^2\frac{\mathcal{M}}{M}Z_P. \quad (26.110)$$

With (26.105), the constant (26.107) can also be written as

$$Z_P^{-1} = \frac{m_V^2}{m_A^2}. \quad (26.111)$$

As we have argued before, there is a good chance that the fields P, V, S, A describe approximately the lowest lying mesons π, ρ, σ, A_1 . Let us test this hypothesis as far as the masses are concerned. Since experimentally $m_{A_1}^2 \approx 2m_\rho^2$, the factor Z_π becomes ≈ 2 . Furthermore, Eq. (26.104) determines the quark mass by

$$6M^2 = m_{A_1}^2 - m_\rho^2, \quad M \approx 310\text{MeV}, \quad (26.112)$$

in good agreement with other estimates [29]. The small pion mass yields, via (26.110),

$$\mathcal{M} \approx 15\text{MeV}. \quad (26.113)$$

Thus the bare quark mass has to be extremely small. Also this result has been obtained by many authors [30]. It is common to all models in which the smallness

of the pion mass is related to the approximate conservation of the axial current (PCAC).

The scalar meson finally is predicted from (26.109) to have a mass

$$m_S \approx 2M \sim 620 \text{ MeV}. \quad (26.114)$$

This agrees well with the observed broad resonance in $\pi\pi$ -scattering [31] [23].

One disagreement with experiment appears in connection with the SU(2)-singlet pseudoscalar mass (the η -meson). According to (26.110), it should be degenerate with the pion. The resolution of this problem will be discussed later, when the theory has been extended to SU(3).

After these first encouraging results we shall rename the fields P, S, V, S, A by their corresponding particle symbols

$$\sqrt{L}P \equiv \pi, \quad -\sqrt{L}S' \equiv \sigma', \quad -\sqrt{\frac{2}{3}}LV^\mu \equiv \rho^\mu, \quad -\sqrt{\frac{2}{3}}LA^\mu \equiv A_1^\mu, \quad (26.115)$$

where a normalization factor has been introduced in order to bring the kinetic terms in the Lagrangian to a conventional form.

A comment is in order concerning the appearance of a quadratic divergence in equations (26.91), (26.96). Such a strong divergence indicates that the limiting procedure $\mu \rightarrow \infty$ of Eq. (26.82) has been performed too carelessly. In fact, if one inserts (26.82) into the action (26.4), the theory is of the four-fermion type with an interaction $(\bar{\psi}\psi)^2$, and thus non-renormalizable. If we want to maintain renormalizability, we have to deal with a large but finite gluon mass $\mu^2 \gg \Lambda^2$. Then the quadratic divergence becomes actually one of the logarithmic type (compare (26.56)):

$$\begin{aligned} Q &= \int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{P_E^2 + M^2} \frac{1}{P_E^2 + \mu^2} \\ &= \frac{\pi^2}{\mu^2 - M^2} \left[\mu^2 \log \left(\frac{\Lambda^2}{\mu^2} + 1 \right) - M^2 \log \left(\frac{\Lambda^2}{M^2} + 1 \right) \right], \end{aligned} \quad (26.116)$$

(which, in the careless limit $\mu^2 \rightarrow \infty$, reduces again to (26.88)). The logarithmic divergence (26.95), in turn, becomes in a more careful treatment of the integral independent of the cutoff. At a finite gluon mass, it is replaced by

$$\begin{aligned} L &= \int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^2} \frac{1}{(P_E^2 + \mu^2)} \\ &\times \frac{\pi^2}{(2\pi)^4} \frac{\mu^2}{(\mu^2 - M^2)^2} \left[\mu^2 \log \frac{\mu^2}{M} + M^2 - \mu^2 \right] \approx \frac{\pi^2}{(2\pi)^4} \log \frac{\mu^2}{M^2}. \end{aligned} \quad (26.117)$$

Hence all our results refer to a renormalizable theory if one reads both Q and L as logarithmic expressions, once in the cutoff Λ and once in the gluon mass μ , respectively.

Let us now proceed to study the interaction terms. The n 'th order contribution to the action is given by

$$\mathcal{A}_n[m'] = \frac{(-i)^{n-1}}{n} \int dx \text{Tr} (G_M m')^n. \quad (26.118)$$

In momentum space this can be written as the one loop integral

$$\begin{aligned} \mathcal{A}_n[m'] &= 4 \frac{(-1)^{n-1}}{n} \int \frac{d^4 q_n}{(2\pi)^4} \cdots \frac{d^4 q_1}{(2\pi)^4} (2\pi)^4 \delta^{(4)}(q_n + \cdots + q_1) \\ &\times \int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P + q_n + \cdots + q_1)_E^2 + M^2} \cdots \frac{1}{(P + q_1)_E^2 + M^2} \\ &\times t_{i_n \dots i_1} (P | q_{n-1}, \dots, q_1) \text{tr}_{\text{SU}(2)} [m'_{i_n}(q_n) \cdots m'_{i_1}(q_1)], \end{aligned} \quad (26.119)$$

where $t_{i_n \dots i_1} (P | q_{n-1}, \dots, q_1)$ is the generalization of the tensor (26.94):

$$\begin{aligned} t_{i_n \dots i_1} (P | q_{n-1}, \dots, q_1) &\equiv \\ &\frac{1}{4} \text{Tr} [\Gamma_{i_n} (\not{P} + \not{q}_{n-1} + \cdots + \not{q}_1 + M) \Gamma_{i_{n-1}} \cdots \Gamma_{i_2} (\not{P} + \not{q}_1 + M) \Gamma_{i_1} (\not{P} + M)]. \end{aligned} \quad (26.120)$$

The result is hard to evaluate in general (except in a $1+1$ dimensional space). With the approximation of a large cutoff one may, however, neglect again all contributions which do not diverge. This considerably simplifies the results. Since $t_{i_n \dots i_1} (P | q_{n-1}, \dots, q_1)$ are polynomials in P of order n , the integral is seen to converge for $n > 4$. For $n = 4$ there is a logarithmic divergence with only the leading momentum behavior of $t_{i_n \dots i_1}$ contributing. For $n \leq 3$ also lower powers in momentum P of $t_{i_n \dots i_1} (P | q_{n-1}, \dots, q_1)$ diverge logarithmically. A simple but somewhat tedious calculation of all integrals (see Appendix 26B) yields the remaining terms in the Lagrangian. They can be written down in a most symmetric fashion by employing the unshifted fields $S(x) \equiv M + S'(x)$ rather than S' , or in a renormalized form⁶

$$\sigma(x) = -\sqrt{L}M + \sigma'(x). \quad (26.121)$$

Then the Lagrangian reads

$$\begin{aligned} \mathcal{L}(x) &= \text{Tr}_{\text{SU}(2)} \left\{ \left[(D_\mu \sigma)^2 + (D_\mu \pi)^2 \right] + M_0^2 (\sigma^2 + \pi^2) \right. \\ &\quad - \frac{2}{3} \gamma^2 [\sigma^4 + \pi^4 - 2\sigma\pi\sigma\pi] - \frac{1}{2} F_{\mu\nu}^2 - \frac{1}{2} F_{\mu\nu}^{A^2} \\ &\quad \left. + m_V^2 (V_\mu^2 + A_\mu^2) - \frac{2}{3} m_V^2 \sqrt{L} \mathcal{M} \right\}. \end{aligned} \quad (26.122)$$

Here $D_\mu \sigma$ and $D_\mu \pi$ are the usual covariant derivatives:

$$\begin{aligned} D_\mu \sigma &= \partial_\mu \sigma - i\gamma [V_\mu, \sigma] - \gamma \{A_\mu, \pi\}, \\ D_\mu \pi &= \partial_\mu \pi - i\gamma [V_\mu, \pi] + \gamma \{A_\mu, \sigma\}, \end{aligned} \quad (26.123)$$

⁶Note that with this notation $m(x) = m_0 + m'(x) = (M - \mathcal{M}) + m'(x) = -\mathcal{M} + S + P_i \gamma_5 + V^\mu \gamma_\mu + A^\mu \gamma_\mu \gamma_5$.

and $F_{\mu\nu}^V$, $F_{\mu\nu}^A$ are the covariant curls

$$\begin{aligned} F_{\mu\nu}^V &= \partial_\mu V_\nu - \partial_\nu V_\mu - i\gamma [V_\mu, V_\nu] - i\gamma [A_\mu, A_\nu], \\ F_{\mu\nu}^A &= \partial_\mu A_\nu - \partial_\nu A_\mu - i\gamma [V_\mu, A_\nu] - i\gamma [A_\mu, V_\nu]. \end{aligned} \quad (26.124)$$

The constant γ is

$$\gamma = \sqrt{\frac{3}{2L}}. \quad (26.125)$$

It describes the direct coupling of the vector mesons to the currents, i.e., it coincides with the coupling conventionally denoted by γ_ρ . Here γ has its origin in the renormalization of the fields. The mass term is short for

$$2M_0^2 \equiv 2M^2 - \frac{1}{3}m_V^2 \mathcal{M}/M. \quad (26.126)$$

Actually, the so-defined mass quantity has an intrinsic significance. This can be seen by deriving the Lagrangian in a different fashion from the beginning. Consider the tadpole terms of the action

$$\mathcal{A}_1[m_1] = \int dx \operatorname{tr}_{\text{SU}(2)} \left\{ G_M(x, x) m'(x) - \frac{1}{\xi} m'(x) m_0 \right\}. \quad (26.127)$$

In the former treatment we have eliminated m_0 completely by giving the quarks a mass M satisfying the gap equation

$$M - \mathcal{M} \equiv m_0 = 4 \frac{g^2}{\mu^2} Q M. \quad (26.128)$$

Instead, we could have introduced an auxiliary mass M_0 satisfying the equation

$$M_0 = 4 \frac{g^2}{\mu^2} Q_0 M_0, \quad (26.129)$$

where Q_0 is the same function of M_0 as Q is of M . The connection between this M_0 and the other masses is obtained by inserting $M = M_0 \delta M$ into Q :

$$Q = Q_0 - 2M_0 \delta M (1 + \delta M/2M_0) L, \quad (26.130)$$

which holds exactly in δM with only small corrections for large cutoffs (notice that at this accuracy $L_0 = L$). Inserting this into (26.128), we find

$$\mathcal{M} = 4 \frac{g^2}{\mu^2} L 2M_0 M (1 + \delta M/2M_0) \delta M \quad (26.131)$$

and, using m_V^2 from (26.105),

$$\mathcal{M} = \frac{12}{m_V^2} M_0 M (1 + \delta M/2M_0) \delta M. \quad (26.132)$$

If $m(x)$ is split in a different fashion

$$m(x) = \tilde{m}_0 + m''(x) \quad (26.133)$$

with a new $\tilde{m}_0 = M_0 - \mathcal{M}$, then the propagator $G(x, y)$ would have an expansion

$$G(x, y) = G_{M_0}(x - y) - i (G_{M_0} m'' G_{M_0})(x, y) + \dots \quad (26.134)$$

For this reason, the derivation of all Lagrangian terms yields exactly the same results as before, only with m'' , M_0 , L_0 , and Q_0 occurring instead of m' , M , L and Q , respectively. There are only two differences: First, due to the gap equation (26.129), the scalar and pseudoscalar mass terms become $4M_0^2$ and zero, rather than (26.109), (26.110). Second, the tadpole terms in this derivation do *not* cancel completely. Instead one finds from (26.127)

$$\begin{aligned} \mathcal{A}_1[m'] &= \int dx \operatorname{tr}_{\mathrm{SU}(2)} \left\{ \left(4Q_0 M_0 - \frac{M_0 - \mathcal{M}}{g^2/\mu^2} \right) m''(x) \right\} \\ &= \int dx \frac{\mu^2}{g^2} \operatorname{tr}_{\mathrm{SU}(2)} \{ \mathcal{M} m''(x) \} = \frac{2}{3} m_x^2 \int dx \operatorname{tr}_{\mathrm{SU}(2)} \{ \mathcal{M} m''(x) \}. \end{aligned} \quad (26.135)$$

These tadpole terms provide exactly the necessary additional shifts in the fields which are needed in order to bring the scalar and pseudoscalar masses from $4M_0^2$ and O to their correct values m_σ^2 and m_π^2 . The symmetric form (26.122) of the Lagrangian is again reached by introducing the original unprimed fields

$$S(x) \equiv M_0 + S''(x), \quad \sigma = -\sqrt{L} M_0 + \sigma''. \quad (26.136)$$

Then the mass term appears as an $SU(3) \times SU(3)$ invariant⁷

$$2M_0^2 (\sigma^2 + \pi^2).$$

Note that this coincides exactly with a former calculation that rendered

$$\left(2M^2 - \frac{1}{3} m_V^2 \mathcal{M}/M \right) (\sigma^2 + \pi^2). \quad (26.137)$$

Indeed, by inserting here $M = M_0 + \delta M$ and (26.132), we see that

$$\begin{aligned} 2M^2 - \frac{1}{3} m_V^2 \mathcal{M}/M &= 2M_0^2 + 4M_0 \delta M + 2(\delta M)^2 - 4M_0 \left(1 + \frac{\delta M}{M_0} \right) \delta M \\ &= 2M_0^2. \end{aligned} \quad (26.138)$$

Hence the $SU(3)$ symmetric mass M_0 defined by the gap equations (26.129) coincides with the mass M_0 introduced as an abbreviation to the mass combination (26.126).

⁷With this substitution, the unprimed field S really coincides with the formerly introduced field S since now $m(x) = (M_0 - \mathcal{M}) + S''(x) + P(x)i\gamma_5 + \dots = -\mathcal{M} + S(x) + P(x)i\gamma_5 + \dots$, whereas before $m(x) = (M - \mathcal{M}) + S'(x) + P(x)i\gamma_5 + \dots = -\mathcal{M} + S(x) + P(x)i\gamma_5 + \dots$.

The Lagrangian (26.122) is recognized as the standard chirally invariant σ model. Its symmetry transformations are for isospin

$$\begin{aligned}\delta\sigma &= i[\alpha, \sigma]; & \delta\pi &= i[\alpha, \pi], \\ \delta V^\mu &= i[\alpha, V^\mu] + \frac{1}{\gamma}\partial^\mu\alpha; & \delta A^\mu &= i[\alpha, A^\mu].\end{aligned}\quad (26.139)$$

For axial transformations the fields change according to

$$\begin{aligned}\bar{\delta}\sigma &= -\{\bar{\alpha}, \pi\}; & \bar{\delta}\pi &= \{\bar{\alpha}, \sigma\}, \\ \bar{\delta}V^\mu &= i[\bar{\alpha}, A^\mu]; & \bar{\delta}A^\mu &= i[\bar{\alpha}, V^\mu] + \frac{1}{\gamma}\partial^\mu\bar{\alpha}.\end{aligned}\quad (26.140)$$

The only term in the Lagrangian which is not invariant is the last linear term. In fact, from

$$\bar{\delta}\mathcal{L} = i\frac{2}{3}m_V^2\mathcal{M}\sqrt{L}\{\bar{\alpha}, \pi\} \equiv i\{\bar{\alpha}, \partial A\} \quad (26.141)$$

one finds

$$\partial A(x) = f_\pi m_\pi^2 Z_\pi^{-1/2} \pi(x). \quad (26.142)$$

Introducing the conventional *pion decay constant* via

$$\partial A(x) \equiv f_\pi m_\pi^2 Z_\pi^{-1/2} \pi(x), \quad (26.143)$$

one can read off

$$f_\pi m_\pi^2 = Z_\pi^{1/2} \frac{2}{3} m_V^2 \sqrt{L} \mathcal{M}. \quad (26.144)$$

Inserting m_π^2 from (26.110) this gives

$$f_\pi = Z_\pi^{-1/2} 2M\sqrt{L}. \quad (26.145)$$

By squaring this and using $\gamma = \sqrt{3/2L}$, one obtains

$$f_\pi^2 = \frac{6M^2}{Z_\pi} \frac{1}{\gamma^2} = \frac{m_\rho^2 m_A^2 - m_\rho^2}{\gamma^2 m_A^2}, \quad (26.146)$$

which, for $m_A^2 \approx 2m_\rho^2$, renders the so-called KSFR relation, that relates properties of the ρ -meson to the pion decay constant [26]. Apart from that, the model has the usual predictions

$$g_{\rho\pi\pi} = \gamma_\rho \left(1 - \frac{m_A^2 - m_\rho^2}{2m_A^2}\right) \approx \frac{3}{4}\gamma_\rho, \quad (26.147)$$

and

$$g_{A_1\rho\pi} = \frac{1}{2m_\rho}\gamma^2 Z_\pi f_\pi \approx \frac{m_\rho}{2f_\pi} \approx 4, \quad h_{A_1\rho\pi} = 0, \quad (26.148)$$

$$g_{A_1\sigma\pi} = \gamma Z_\pi^{1/2} \approx \frac{m_\rho}{f_\pi} \approx 8, \quad (26.149)$$

$$g_{\sigma\pi\pi} = \frac{2}{m_\sigma} \frac{1}{3} \gamma^2 f_\pi Z_\pi^{3/2} \approx \frac{m_\sigma}{f_\pi} \sqrt{2} \approx 9. \quad (26.150)$$

When compared with experiment, the only real discrepancy consists in the theoretical prediction that the d-wave coupling of the vertex $A_1\rho\pi$, i.e., the coupling constant $h_{A_1\rho\pi}$, is supposed to be zero. Additional chirally invariant terms are needed in the Lagrangian, for example, the so-called δ -term:

$$\delta \text{Tr} \left[(F_{\mu\nu}^A + F_{\mu\nu}^V) D^\mu (\sigma + i\pi) D^\nu (\sigma - i\pi) - (V \rightarrow -V, \pi \rightarrow -\pi) \right]. \quad (26.151)$$

Such terms appear in our derivation if the approximation of large μ^2 is improved by terms which do not grow logarithmically in μ .

Let us now determine the couplings of π , σ , ρ and A_1 to external quark fields. The external propagation proceeds via

$$i\bar{\eta}G\eta = i\bar{\eta}G_{M_0}\eta + \bar{\eta}G_{M_0}m''G_{M_0}m''G_{M_0}\mu - \dots \quad (26.152)$$

If we define the couplings by the interaction Lagrangian

$$\mathcal{L} \equiv g_{\pi QQ} \bar{\psi} i\gamma_5 \tau_a \psi \pi^a + g_{\sigma QQ} \bar{\psi} \tau_a \psi \sigma^a + g_{V QQ} \bar{\Psi} \gamma^\mu \frac{\tau_a}{2} \Psi V_\mu^a + g_{A QQ} \bar{\Psi} \gamma^\mu \gamma_5 \frac{\tau_a}{2} \Psi A_\mu^a, \quad (26.153)$$

we can read off

$$g_{\pi QQ} = \frac{1}{2\sqrt{L}} Z_\pi^{1/2} = \frac{M}{f_\pi}; \quad g_{\sigma QQ} = \frac{1}{2\sqrt{L}} = \frac{M}{f_\pi Z_\pi^{1/2}}, \quad g_{\rho QQ} = g_{A_1 QQ} = \gamma. \quad (26.154)$$

We see that the vector coupling to quark-antiquark pairs shows vector-meson dominance. Due to PCAC, also the Goldberger-Treiman relation is respected

$$g_{\pi QQ} = g_A \frac{M}{f_\pi}, \quad (26.155)$$

since the axial charge of the quark is $g_A = 1$. With the quark mass being roughly $M \approx m_N/3$, the pionic coupling to quarks is considerably smaller than that to nucleons. Numerically this implies that

$$\frac{g_{\pi QQ}^2}{4\pi} \approx \frac{1}{17} \frac{g_{\pi NN}^2}{4\pi} \approx 0.86. \quad (26.156)$$

The σ -meson couples like

$$\frac{g_{\sigma QQ}^2}{4\pi} \approx 0.43.$$

Vector- and axial-vector mesons, on the other hand, couple as strongly to quarks as to nucleons:

$$\frac{g_{\rho QQ}^2}{4\pi} = \frac{g_{AQQ}^2}{4\pi} = \frac{\gamma^2}{4\pi} \approx 2.6 \left(\approx \frac{g_{\rho NN}^2}{4\pi} \right). \quad (26.157)$$

We are now ready to extend our consideration to SU(3) (and higher groups). In this case the explicit symmetry breaking in the Lagrangian is too large to be neglected. Thus the bare masses $\mathcal{M}$ of the quarks have to be considered as a matrix

$$\mathcal{M} \approx \begin{pmatrix} \mathcal{M}^n & & \\ & \mathcal{M}^d & \\ & & \mathcal{M}^s \end{pmatrix}. \quad (26.158)$$

The derivation of the Lagrangian presented above [via the gap equation (26.129)] has shown complete SU(3) symmetry of M_0^2 . Hence when extending from SU(2) to SU(3), no change occurs except in the last symmetry breaking term of (26.122). As a consequence, the mass expressions for m_p^2 and m_s^2 remain as they are, only that the renormalization constants Z_p become more complicated SU(3)-dependent quantities, due to the involved mixing of pseudoscalar and axialvector mesons. For a complete discussion of this SU(3) $\times$ SU(3) invariant chiral Lagrangian the reader is referred to the review articles [27]. Here we only give a few results:

A best fit to the masses of π - and K -meson requires the current masses⁸

$$\mathcal{M} \approx \begin{pmatrix} 15 & & \\ & 15 & \\ & & 435 \end{pmatrix} \text{ MeV}. \quad (26.159)$$

Thus the explicit symmetry breakdown of SU(3) caused by the bare masses is quite large. The standard parameter C [32] that characterizes this is

$$C \equiv \frac{\mathcal{M}^8}{\mathcal{M}^0} = \frac{\frac{1}{\sqrt{3}}(\mathcal{M}^n + \mathcal{M}^d - 2\mathcal{M}^s)}{\sqrt{\frac{2}{3}}(\mathcal{M}^n + \mathcal{M}^d + \mathcal{M}^s)} \approx -1.28 (\approx -\sqrt{2}). \quad (26.160)$$

Comparing (26.159) with (26.132), we find the shifts in the quark masses caused by dynamics

$$\delta M = \begin{pmatrix} 7 & & \\ & 7 & \\ & & 127 \end{pmatrix} \text{ MeV}, \quad (26.161)$$

and hence for the “physical” quark masses

$$M \approx \begin{pmatrix} 3/2 & & \\ & 3/2 & \\ & & 432 \end{pmatrix} \text{ MeV}. \quad (26.162)$$

⁸For other determinations of $\mathcal{M}^{u,d,s}$, see Ref. [30].

Thus contrary to the large explicit SU(3) violation in the bare masses $\mathcal{M}$, the physical quark masses M show only the moderate violation:

$$C' \equiv \frac{M^8}{M^0} = \frac{\frac{1}{\sqrt{3}}(M^n + M^d - 2M^s)}{\sqrt{\frac{2}{3}}(M^n + M^d + M^s)} \approx -16\%. \quad (26.163)$$

Since the quark masses M are produced almost completely by dynamical effects, we expect some symmetry breakdown to appear also in the vacuum. A measure of this is provided by the expectation values of the scalar quark densities

$$\langle 0|\tilde{U}^a|0\rangle \equiv \langle 0|\bar{\psi}(x)\frac{\lambda^a}{2}\psi(x)|0\rangle. \quad (26.164)$$

In the mesonized theory, the scalar densities are identical with the scalar fields, up to a factor:

$$S_j^i(x) = -\frac{g^2}{\mu^2}\bar{\psi}^i(x)\psi_j(x), \quad (26.165)$$

as can be seen most easily by considering the equations of constraint (26.15) following from the Lagrangian (26.12) in the large $-\mu$ limit. Hence

$$\langle 0|\tilde{u}^a|0\rangle = -\frac{\mu^2}{g^2}\sum_{i,j}\lambda_i^{aj}\langle 0|S_j^i|0\rangle = -\frac{\mu^2}{2g^2}\text{tr}_{\text{SU}(2)}(\mathcal{M}\lambda^a) = -\frac{\mu^2}{2g^2}M^a. \quad (26.166)$$

Inserting (26.105) and (26.145), the factor becomes simply

$$\frac{\mu^2}{2g^2} = \frac{1}{3}\frac{1}{\frac{2}{3}\frac{g^2}{\mu^2}L}L = \frac{1}{3}m_V^2Z_\pi\frac{f_\pi^2}{4M^2} \approx f_\pi^2,$$

so that

$$\langle 0|\tilde{u}^0|0\rangle \approx f_\pi^2M^0 = -f_\pi^2\sqrt{\frac{2}{3}}(M^n + M^d + M^s) \approx -8 \times 10^{-3}\text{GeV}^3, \quad (26.167)$$

$$\langle 0|\tilde{u}^8|0\rangle \approx -f_\pi^2M^8 = c'\langle 0|\tilde{u}^0|0\rangle. \quad (26.168)$$

This shows that the SU(3)-violation in the vacuum equals that in the quark masses with an accuracy of $\approx -16\%$.⁹ Notice that the three results (26.110), (26.132) and (26.165) are in complete agreement with what one obtains by very general considerations using only chiral symmetry and PCAC (see Appendix 26C).

The extension of the Lagrangian to SU(3) produces additional defects which are well known from general discussions of chiral $SU(3) \times SU(3)$ symmetry [27]. For example the vector mesons ω and φ are not mixed (almost) ideally as they should, but φ remains close to an SU(3) singlet. In general discussions, additional terms

⁹In Ref. [34], the breaking of SU(3)-symmetry in the vacuum was neglected. For a more general discussion and earlier references see Ref. [33].

have been added to the chiral Lagrangian in order to account for this. On the one hand, one needs so-called “current mixing terms”:

$$\text{Tr} \left\{ \left(F_{\mu\nu}^V + F_{\mu\nu}^A \right)^2 (\sigma + i\pi)(\sigma - i\pi) + (A \rightarrow -A, \pi \rightarrow -\pi) \right\}. \quad (26.169)$$

Further one needs “mass mixing terms”

$$\text{Tr} \left\{ (V^\mu + A^\mu)^2 (\sigma + i\pi)(\sigma - i\pi) + (V^\mu - A^\mu)^2 (\sigma - i\pi)(\sigma + i\pi) \right\}. \quad (26.170)$$

In our derivation these arise as a next correction to the $\mu^2 \rightarrow \infty$ limit. Another problem is the degeneracy of the ideally mixed isosinglet pseudoscalar meson μ'_{ideal} with the pion. In order to account for the fact that the $\eta'(\Xi_0)$ meson is almost a pure SU(3) singlet and much heavier than the other pseudoscalar mesons, one needs some chirally symmetric term

$$\det(\sigma + i\pi) + \det(\sigma - i\pi). \quad (26.171)$$

Such a term breaks PCAC for the ninth component of the axial vector current. It is well known [34] that the quark gluon triangle anomaly operates in the singlet channel. It might be capable of producing such a PCAC violation. In fact, if this was not true, quantum electrodynamics would possess an exactly massless Goldstone boson [35] with η quantum numbers. The term (26.171) will also appear in the effective Lagrangian when μ is no longer very large.

It is obvious that corrections to the $\mu^2 \rightarrow \infty$ approximation will become even more important if one tries to extend the consideration to SU(4) since then vector and pseudoscalar masses are quite heavy. In addition, the narrow width of the SU(4) vector meson ψ/J seems to indicate that short-distance parts of the gluon propagator are probed. Thus the colorless quark gluon theory itself cannot be considered any more a realistic approximation to the colored theory.

At this place we should remark that standard explanations of electromagnetic mass differences require also a breakdown of SU(2)-symmetry in $\mathcal{M}$ [36]. This is conventionally parametrized by

$$d \equiv \frac{\mathcal{M}^3}{\mathcal{M}^0} = \frac{\mathcal{M}^n - \mathcal{M}^d}{\sqrt{\frac{2}{3}}(\mathcal{M}^n + \mathcal{M}^d + \mathcal{M}^s)}. \quad (26.172)$$

From meson masses (as well as from the electromagnetic $\eta \rightarrow 3\pi$ decay) one finds [37]

$$d \approx -3\%. \quad (26.173)$$

This amounts to the bare quark masses

$$\mathcal{M} \approx \begin{pmatrix} 10 & & \\ & 20 & \\ & & 435 \end{pmatrix} \text{ MeV}, \quad (26.174)$$

giving the “true” masses

$$M \approx \begin{pmatrix} 310 & & \\ & 315 & \\ & & 432 \end{pmatrix} \text{ MeV.} \quad (26.175)$$

Thus the SU(2) breaking of the vacuum is very small:

$$d' \equiv \frac{\langle 0 | \tilde{u}^3 | 0 \rangle}{\langle 0 | \tilde{u}^0 | 0 \rangle} = \frac{M^3}{M^0} \approx -0.6\%. \quad (26.176)$$

With all parameters fixed numerically we should finally check whether the approximation of a large gluon mass is self-consistent. From (26.145) we have

$$L \approx \frac{1}{2} \frac{f_\pi^2}{M^2} \approx 0.046. \quad (26.177)$$

Inserting this into (26.117), we calculate

$$\log \frac{\mu^2}{M^2} \sim (4\pi)^2 \times 0.046 \approx 7.3, \quad (26.178)$$

and hence

$$\mu^2 \approx 1500 M^2 \gg M^2, \quad (26.179)$$

or

$$\mu \approx 12 \text{ BeV}. \quad (26.180)$$

It is gratifying to note that this value is much larger than the mass of the vector mesons. In this way it is assured that higher powers of $q^2 / (P_E^2 + M^2)$ which were neglected in the derivation of the Lagrangian remain really small as compared to unity for *all* mesons of the theory (see Appendix 26B).

We should point out that the quark gluon theory in the limit $\mu^2 \rightarrow \infty$ coincides with the well-known Nambu–Jona-Lasinio model which [28] has proven in the past to be a convenient tool for studying the spontaneous breakdown of chiral symmetry and the dynamical generation of PCAC. Those authors have demonstrated the close analogy of the dynamic structure of this model with that of superconductivity. As we have mentioned before, the equation (26.128) removing the tadpoles in the action is analogous to the gap equation for superconductors.

A similar analogy to superconductors exists also for the hadronized theory. The classical version of it corresponds exactly to the classical Ginzburg-Landau equation for type II superconductors in which the gap is allowed to be spacetime-dependent. In fact, the classical mesonized theory can be derived alternatively by assuming such a dependence in the gap equation (26.88) [28, 38]. The advantage of our functional derivation is that the mesonized theory is not merely some classical approximation

but becomes, upon quantization, completely equivalent to the original quark gluon theory.

A final comment concerns the Okubo-Zweig-Iizuka rule. As argued in the general section, the meson Lagrangian exactly respects this rule. This can be checked directly for all interaction terms in (26.122). Violations of this rule are all coming from meson loops whose calculations allow to estimate their size.

26.4 More Quarks

Of course the set of quarks to be treated has to be extended by all those flavors which have been left out in the short discussion presented in this chapter. The quarks which have been discovered over the years are listed in Table 24.4 with their properties. The reader is referred to the textbook [39] for a more detailed discussion.

Most important will be a better way of dealing with the non-renormalizability of the theory [40, 41, 42, 43, 44, 45]. Promising are the insights gained on the various mass scales and composite particle spectra which are relevant in strong four-fermion interactions [46].

The four-fermion interactions of the Nambu–Jona-Lasinio type have three distinct range of dynamics, depending on the strength of their couplings. In the very weak coupling regime, two-particle scattering occurs and chiral symmetry is preserved. This is not a fixed point of the theory, and no renormalizable field theory can be realized. In the intermediate coupling regime, chiral symmetry is broken and fermion masses are generated at the electroweak scale, when there exists an infrared fixed point. There is possible to set up effectively a renormalizable field theory with fundamental particles which make up the famous Standard Model (SM) of fundamental particles. In the very strong coupling limit, the chiral symmetry is restored and realized by massive composite bosons, with fermions being composed by the elementary particles of the Standard Model. At the ultraviolet-stable fixed point, one finds effectively a renormalizable quantum field theory involving massive composite particles which preserve the chiral gauge symmetries of the Standard Model [47].

The experimentally found masses deviate somewhat from those which fit the data of the model. This is no surprise considering the roughness of the model. The orders of magnitude of the various quark masses have been estimated with the help of the gap equation (26.90) or (26.91). Ignoring the bare mass $\mathcal{M}$ for the heaviest quark T , we estimate the mass of the top quark from the gap equation

$$M_t \approx 4 \frac{g}{\mu^2} Q M_t = 4 \frac{g}{\mu^2} \int \frac{d^4 P_E}{(2\pi)^4} (P_E^2 + M_t^2)^{-1}, \quad (26.181)$$

which amounts to the estimate of the top mass [41]:

$$M_t \approx 4 \frac{g}{\mu^2} \frac{\pi^2}{(2\pi)^4} (\Lambda^2 - M_t^2 \log \Lambda^2 / M_t^2) \approx G \frac{1}{4\pi^2} (\Lambda^2 - M_t^2 \log \Lambda^2 / M_t^2). \quad (26.182)$$

The right-hand side has one multiplied with a factor N_c which counts the number of colors of the quarks.

26.5 Summary

In this chapter we have shown that, in the absence of color, quark gluon theories can successfully be mesonized. The resulting quantum field theory incorporates correctly many features of strong interactions. Its basic fields are bilocal and the Feynman rules are topologically similar to dual diagrams. Our considerations have to take place at a rather formal level. Certainly, there are many problems which have been left open. For example, there is need for an understanding of the non-trivial gauge properties of the bilocal theory. Also, a better way of dealing with the non-renormalizability of the theory will have to be developed.

The inclusion of color is the challenging problem left open by this investigation. If the color quark gluon theory is really equivalent to some kind of dual model, the corresponding mesonization program should not produce bilocal but multilocal fields which are characterized by the position of a whole string rather than just its end points. A field theory should be constructed for gauge invariant objects like

$$\bar{\psi}(x) \exp \left(ig \int_x^y G^\nu(z) dz_\nu \right) \psi(y), \quad (26.183)$$

which depend on the whole path from x to y .

The difficulty in a direct generalization of the previous procedure is the self-interaction of the gluons. Only after the infrared behavior of gluon propagators will be known, bare mesons can be constructed inside the corresponding potential well and the “mesonization” methods can serve for the determination of the complete residual interactions.

It is hoped that mesonic Feynman rules in the presence of color will follow a pattern similar to that found here for the non-abelian theory.

Let us finally mention that an interesting field of applications of our methods lies in solid-state physics. Semi-conductors in which conduction and valence band have only small separations may show a phase transition to what is called excitonic insulator. The critical phenomena taking place inside such an exciton system will find their most appropriate description by making use of the scaling properties of the bilocal field theory.

26.6 Baryons

So far we have discussed only the generation of the mesons in strong interactions (“mesonization” as a special case of “hadronization”). The procedure has been extended to describe also baryons, and thus to nuclear physics in general. Here the Faddeev equation of three-body bound states comes in [48] to replace the Bethe-Salpeter equation governing pairs of quarks. Examples can be seen in the papers [49].

Appendix 26A Remarks on the Bethe-Salpeter Equation

Consider the four-fermion Green function

$$G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') \equiv \langle 0 | T (\psi_\alpha(x) \bar{\psi}_\beta(y) \bar{\psi}_{\alpha'}(x') \psi_{\beta'}(y')) | 0 \rangle, \quad (26A.1)$$

which becomes in the interaction picture

$$G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') \equiv \left[\langle 0 | T e^{ig \int d^4 z \bar{\psi}(z) \gamma^\mu \psi(z) G_\mu(z)} | 0 \rangle \right]^{-1} \times \langle 0 | T \left(e^{ig \int d^4 z \bar{\psi}(z) \gamma^{\mu A} \psi(z) G_\mu(z)} \psi_\alpha(x) \bar{\psi}_\beta(y) \psi_{\alpha'}(x') \psi_{\beta'}(y') \right) | 0 \rangle. \quad (26A.2)$$

Expanding the exponential and keeping only the ladder exchanges corresponding to the Feynman graph in Fig. 26.14, we obtain

$$\begin{aligned} G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') &= G_{\alpha\alpha'}(x - x') G_{\beta'\beta}(y' - y) + \\ &g^2 \int dx_1 dy_1 G_{\alpha\alpha_1}(x - x_1) \gamma_{\alpha_1\alpha'_1}^\mu G_{\alpha'_1\alpha'}(x_1 - x') G_{\beta'\beta'_1}(y' - y_1) \gamma_{\mu\beta'_1\beta_1} G_{\beta_1\beta}(y_1 - y) D(x - y) + \\ &g^4 \int dx_1 dy_1 dx_2 dy_2 G_{\alpha\alpha_1}(x - x_1) \gamma_{\alpha_1\alpha'_1}^{\mu_1} G_{\alpha'_1\alpha'_2}(x_1 - x_2) \gamma_{\alpha'_2\alpha'_2}^{\mu_2} G_{\alpha'_2\alpha'}(x_2 - x') \times \\ &D(x_1 - y_1) D(x_2 - y_2) G_{\beta'\beta'_2}(y' - y_2) \gamma_{\mu_2\beta'_2\beta_2} G_{\beta_2\beta'_1}(y_2 - y_1) \gamma_{\mu_1\beta'_1\beta_1} G_{\beta_1\beta}(y_1 - y). \end{aligned} \quad (26A.3)$$

The series can be summed to form an integral equation

$$\begin{aligned} G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') &= G_{\alpha\alpha'}(x - x') G_{\beta'\beta}(y' - y) + g^2 \int dx_1 dy_1 \\ &\times G_{\alpha\alpha_1}(x - x_1) \gamma_{\alpha_1\alpha'_1}^\mu G_{\alpha'_1\beta'_1,\alpha'\beta'}^{(4)}(x, y_1; x', y') \gamma_{\mu\beta'_1\beta_1} G_{\beta_1\beta}(y_1 - y) D(x_1 - y_1). \end{aligned} \quad (26A.4)$$

With the abbreviation

$$\begin{aligned} \xi_{\alpha_1\beta_1,\beta'_1\alpha'_1} &= \gamma_{\alpha_1\alpha'_1}^\mu \gamma_{\mu\beta'_1\beta_1} = 1_{\alpha_1\beta_1} 1_{\beta'_1\alpha'_1} + (i\gamma_5)_{\alpha_1\beta_1} (i\gamma_5)_{\beta'_1\alpha'_1} \\ &- \frac{1}{2} \gamma_{\alpha_1\beta_1}^\mu \gamma_{\mu\beta'_1\alpha'_1} - \frac{1}{2} (\gamma^\mu \gamma_5)_{\alpha_1\beta_1} (\gamma_\mu \gamma_5)_{\beta'_1\alpha'_1}, \end{aligned} \quad (26A.5)$$

this can be written as

$$\begin{aligned} G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') &= G_{\alpha\alpha'}(x - x') G_{\beta'\beta}(y' - y) + \\ &g^2 \int dx_1 dy_1 G_{\alpha\alpha_1}(x - x_1) \xi_{\alpha_1\beta_1,\beta'_1\alpha'_1} D(x_1 - y_1) G_{\alpha'_1\beta'_1,\alpha'\beta'}^{(4)} G_{\beta_1\beta}(y_1 - y), \end{aligned} \quad (26A.6)$$

or, symbolically, as

$$G^{(4)} = GG^T + GG^T \xi g^2 DG^{(4)}. \quad (26A.7)$$

The transition matrix T is defined by removing the external particle poles in the connected part of $G^{(4)}$:

$$\begin{aligned} G_{\alpha\beta,\alpha'\beta'}^{(4)}(x, y; x', y') &\equiv G_{\alpha\alpha'}(x - x') G_{\beta'\beta}(y' - y) + \int dx_1 dy_1 dx_2 dy_2 \\ &\times G_{\alpha\alpha_1}(x - x_1) G_{\beta'\beta_2}(y' - y_2) T_{\alpha_1\beta_1,\alpha_2\beta_2}(x_1, y_1; x_2, y_2) G_{\alpha_1\alpha}(x_2 - x') G_{\beta_1\beta}(y_1 - y), \end{aligned} \quad (26A.8)$$

which may be abbreviated by

$$G^{(4)} = GG^T + GG^T TGG^T. \quad (26A.9)$$

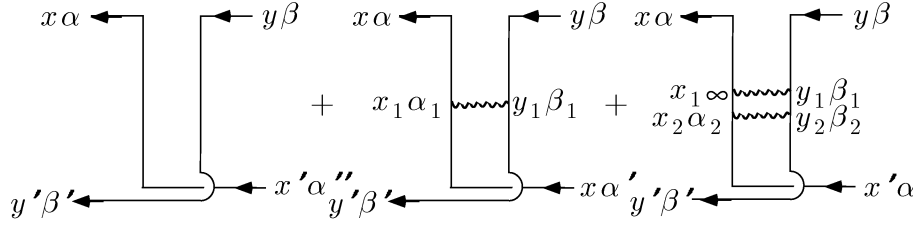


FIGURE 26.14 Diagrams in the Bethe-Salpeter equation.

From (26A.6) and (26A.8), the transition matrix satisfies the integral equation

$$T_{\alpha_1\beta_1,\alpha_2\beta_2}(x_1, y_1; x_2, y_2) = \xi_{\alpha_1\beta_1,\beta_2\alpha_2} g^2 D(x_1 - y_1) \delta(x_1 - y_1) \delta(x_2 - y_2) \quad (26A.10)$$

$$+ \xi_{\alpha_1\beta_1,\beta_1\alpha_1} D(x_1 - y_1) \int dx'_1 dy'_1 G_{\alpha_1\alpha'_1}(x_1 - x'_1) T_{\alpha'_1\beta_1,\alpha_2\beta_2}(x'_1, y'_1; x_2, y_2) G_{\beta'\beta_1}(y'_1 - y_2),$$

which is seen to coincide with the equation (26.45) for the propagator of the bilocal field. In a short notation, this equation can be written as

$$T = \xi g^2 D + \xi g^2 D G G^T T. \quad (26A.11)$$

The perturbation expansion

$$T = \xi g^2 D + \xi g^2 D G G^T \xi g^2 D + \dots \quad (26A.12)$$

reveals the one, two etc. photon exchanges of the ladder diagrams. In momentum space, the four-particle Green function is defined by

$$(2\pi)^4 \delta^4(q' - q) G_{\alpha\beta,\alpha'\beta'}^{(4)}(P, P'|q)$$

$$= \int dx dy dx' dy' e^{i[(P+\frac{q}{2})x + (P'-\frac{q}{2})y - (P-\frac{q}{2})y - (P'+\frac{q}{2})x]} G_{\alpha\beta\alpha'\beta'}^{(4)}(xy, x'y'). \quad (26A.13)$$

The momenta are indicated in Fig. 26.15. The corresponding scattering matrix $T(P, P'|q)$ satisfies

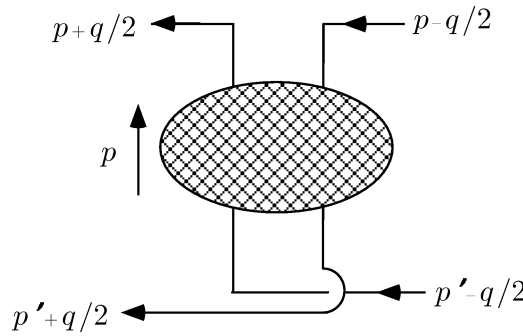


FIGURE 26.15 Momenta in the integral equation 26A.14.

the integral equation

$$T(P, P'|q) = \xi g^2 D(P - P') \quad (26A.14)$$

$$+ \xi g^2 \int \frac{dP''}{(2\pi)^4} D(P - P'') G\left(P'' + \frac{q}{2}\right) T(P'', P'|q) G\left(P'' - \frac{q}{2}\right).$$

The ladder exchange is, in general, expected to produce quark-antiquark bound states. Suppose $|H(\mathbf{q})\rangle$ is one of them. Inserting it into (26A.1) as an intermediate state, gives for $x_0, y_0 > x'_0, y'_0$ a contribution

$$G_{\alpha\beta, \alpha'\beta'}^{(4)}(x, y; x' y') = \int \frac{d^3 q}{2E_q (2\pi)^3} \Theta \left(R_0 - R'_0 - \frac{1}{2}(|z_0| + |z'_0|) \right) \\ \times \langle 0 | T(\psi_\alpha(x) \bar{\psi}_\beta(y)) | H(\mathbf{q}) \rangle \langle H(\mathbf{q}) | T(\bar{\psi}_{\alpha'}(x') \psi_{\beta'}(y')) | 0 \rangle,$$

where $R \equiv (x + y)/2$ and $z = x - y$. The Heaviside function Θ is non-zero if

$$\min(x_0, y_0) > \max(x'_0, y'_0).$$

Using the standard integral representation of the Heaviside function,

$$\Theta(x_0) = \frac{i}{2\pi} \int da e^{-q_0 x_0} \frac{1}{q_0 + i\epsilon},$$

we may write

$$\Theta \left(R_0 - R'_0 - \frac{1}{2}(|z_0| + |z'_0|) \right) = \frac{i}{2\pi} \int dq_0 \frac{e^{-i(q_0 - E_q)(R_0 - R'_0)} e^{i(q_0 - E_q)\frac{1}{2}(|z_0| + |z'_0|)}}{q_0 - E_q + i\eta}. \quad (26A.15)$$

Inserting now the Bethe-Salpeter wave functions

$$\begin{aligned} \phi_{\alpha\beta}(x, y|q) &\equiv \langle 0 | T(\psi_\alpha(x) \bar{\psi}_\beta(y)) | H(\mathbf{q}) \rangle, \\ \bar{\phi}_{\beta'\alpha'}(y' x' | -q) &\equiv \langle H(\mathbf{q}) | T(\psi_{\beta'}(y') \bar{\psi}_{\alpha'}(x')) | 0 \rangle, \end{aligned} \quad (26A.16)$$

and their momentum space versions

$$\phi_{\alpha\beta}(x, y|q) = e^{-i(E_1 R_0 - \mathbf{q}\mathbf{R})} \int \frac{d^4 P}{(2\pi)^4} e^{-iP(x-y)} \phi_{\alpha\beta}(P|q), \quad (26A.17)$$

$$\bar{\phi}_{\beta'\alpha'}(x', y' | -q) = e^{i(E_1 R'_0 - \mathbf{q}\mathbf{R}')} \int \frac{d^4 P'}{(2\pi)^4} e^{-iP'(x'-y')} \phi_{\alpha'\beta'}(P' | -q), \quad (26A.18)$$

the four-particle Green function in momentum space is seen to exhibit a pole at $q_0 \approx E_q$:

$$G_{\alpha\beta\alpha'\beta'}^{(4)}(P, P'|q) \approx \frac{-i}{2E_q(q_0 - E_q + i\epsilon)} \phi_{\alpha\beta}(P|q) \bar{\phi}_{\beta'\alpha'}(P' | -q). \quad (26A.19)$$

The opposite time ordering $x_0, y_0 < x'_0, y'_0$ contributes a pole at $q_0 = -E_q$. Both poles can be collected in a single expression by exchanging the pole term in (26A.19) by

$$-\frac{i}{q^2 - M_H^2 + i\epsilon}.$$

This factorization is consistent with the integral equation only for a specific normalization of the Bethe-Salpeter wave functions. In order to see this, we write (26A.7) in the form

$$\begin{aligned} G^{(4)} &= GG^T + GG^T \xi g^2 DG^{(4)} = (1 - GG^T \xi g^2 D)^{-1} GG^T \\ &= GG^T (1 - \xi g^2 DGG^T)^{-1}. \end{aligned} \quad (26A.20)$$

Suppose now that a solution is found for different values of the coupling constant g^2 . Then the variation of $G^{(4)}$ for small changes of g^2 is

$$\begin{aligned} \frac{\partial G^{(4)}}{\partial g^2} &= (1 - GG^T \xi g^2 D)^{-1} GG^T \xi D \times GG^T (1 - \xi g^2 D)^{-1} \\ &= G^{(4)} \xi D G^{(4)}. \end{aligned} \quad (26A.21)$$

If one remains in the vicinity of the pole at $q^2 = M_H^2(g^2)$, this becomes

$$\begin{aligned} -\frac{\partial}{\partial g^2} \frac{i}{s - M_H^2(g^2)} \phi_H^g(P|q) \bar{\phi}_H^g(P| - q) &= \frac{i}{s - M_H^2(g^2)} \phi_H^g(P|q) \\ &\times \int \frac{d\bar{P} d\bar{P}'}{(2\pi)^8} \bar{\phi}_H^g(\bar{P}| - q) \xi D(\bar{P} - \bar{P}') \phi_H^g(\bar{P}'|q) \bar{\phi}_H^g(\bar{P}'| - q) \frac{i}{s - M_H^2(g^2)}. \end{aligned} \quad (26A.22)$$

This can be true at $q^2 = M_H^2(g^2)$ only if

$$\frac{\partial M_H^2(g^2)}{\partial g^2} = -i \int \frac{dP dP'}{(2\pi)^4 (2\pi)^4} \phi_H(P|q) \xi D(P - P') \bar{\phi}_H(P'| - q). \quad (26A.23)$$

If we go over to the Bethe Salpeter vertex function (26.36):

$$\begin{aligned} \Gamma^H(P|q) &= N_H G_M^{-1} \left(P + \frac{q}{2} \right) \phi^H(P|q) G_M^{-1} \left(P - \frac{q}{2} \right), \\ \Gamma^H(P| - q) &= N_H^* G_M^{-1} \left(P - \frac{q}{2} \right) \bar{\phi}^H(P| - q) G_M^{-1} \left(P + \frac{q}{2} \right), \end{aligned} \quad (26A.24)$$

we obtain

$$\begin{aligned} g_V^2(q^2) \frac{\partial M_H^2(g^2)}{\partial g^2} &= i |N_H|^2 \int \frac{dP dP'}{(2\pi)^4 (2\pi)^4} \text{Tr} \left\{ G_M \left(P + \frac{q}{2} \right) \Gamma^H(P|q) G_M \left(P - \frac{q}{2} \right) \right. \\ &\quad \times g_H^2(q^2) D(P - P') G_M \left(P' - \frac{q}{2} \right) \bar{\Gamma}^H(P'| - q) G_M \left(P' + \frac{q}{2} \right) \left. \right\}. \end{aligned} \quad (26A.25)$$

Using now the integral equation (26.37), we find the normalization condition

$$\begin{aligned} \frac{g_H^2(q^2)}{\frac{\partial g_H^2(q^2)}{\partial q^2}} &= -i |N_H|^2 \int \frac{d^4 P}{(2\pi)^4} \\ &\times \text{Tr} \left[G_M \left(P + \frac{q}{2} \right) \Gamma^H(P|q) G_M \left(P - \frac{q}{2} \right) \bar{\Gamma}^H(P| - q) \right], \end{aligned} \quad (26A.26)$$

which determines $|N_H|^2$ to be

$$|N_H|^2 = \frac{g_H^2(q^2)}{\frac{\partial g_H^2(q^2)}{\partial q^2}}. \quad (26A.27)$$

Note that the normalization is defined for all q^2 with some $N_H(q^2)$. For real $\Gamma(P|q)$, we may choose a real $N_H(q^2)$, so that

$$\bar{\Gamma}(P| - q) = \Gamma(P| - q).$$

Both satisfy the same integral equation.

The orthogonality of $\Gamma^H(P|q)$ and $\bar{\Gamma}^{H'}(P| - q)$ for different mesons is proved, as usual, by considering (26.37), once for $(\xi g^2 D)^{-1} \Gamma^H$ and once for $(\xi g^2 D)^{-1} \bar{\Gamma}^{H'}$, multiplying the first by $\bar{\Gamma}^{H'}$ and the second by Γ^H , taking the trace and subtracting the results from each other [assuming no degeneracy of $g_H(q^2)$ and $g_{H'}(q^2)$]. The normalization (26A.27) is seen to be consistent with the expansion of the T -matrix given in (26.46):

$$T_{\alpha\beta, \alpha'\beta'}(P, P'|q) = -ig^2 \sum_H \frac{\Gamma_{\alpha\beta}^H(P|q) \bar{\Gamma}_{\beta'\alpha'}^H(P'| - q)}{g_H^2(q^2) - g^2}. \quad (26A.28)$$

If q^2 runs into a pole M_H^2 , this expression is singular as

$$T_{\alpha\beta,\alpha'\beta'}(P, P'|q) \approx -ig^2 \frac{1}{(q^2 - M_H^2) \frac{\partial g_H^2(q^2)}{\partial q^2}} \Gamma_{\alpha\beta}^H(P|q) \bar{\Gamma}_{\beta'\alpha'}^H(P'| - q). \quad (26A.29)$$

According to (26A.9) this produces a singularity in $G^{(4)}$ (in short notation)

$$\begin{aligned} G^{(4)} &\approx -i \frac{g^2}{\frac{\partial g_H^2(q^2)}{\partial q^2}} \frac{1}{q^2 - M_H^2} (G \Gamma^H G) (G \bar{\Gamma}^H G) \\ &= -i \frac{g^2}{\frac{\partial g_H^2(q^2)}{\partial q^2}} \frac{1}{q^2 - M_H^2} |N_J|^2 \phi^H \bar{\phi}^H, \end{aligned} \quad (26A.30)$$

which coincides with (26A.19) by virtue of (26A.27).

For completeness we now give the Bethe-Salpeter equation (26.34) the form projected into the different covariants:

$$m'(P|q) = S(P|q) + P(P|q)i\gamma_5 + V^\mu(P|q)\gamma_\mu + A^\mu(P|q)\gamma_\mu\gamma_5.$$

If $m_i(P|q)$ ($i = 1, 2, 3, 4$) abbreviates S, P, V, A , one has

$$\begin{aligned} m_i(P|q) &= -4\xi_i g^2 \sum_{j=1}^4 \frac{d^4 P'}{(2\pi)^4} \frac{1}{(P - P')_E^2 + \mu^2} \frac{1}{(P' + \frac{q}{2})_E^2 + M^2} \\ &\times \frac{1}{(P' - \frac{q}{2})_E^2 + M^2} t_{ij}(P'|q) m_j(P'|q), \end{aligned} \quad (26A.31)$$

with $t_{ij}(P|q)$ being the traces defined in (26.94) and $\xi_i = (4, +4, -2, -2)$. Explicitly, one finds

$$t_{SS}(P|q) = P^2 - \frac{q^2}{4} + M^4, \quad t_{SV}(P|q) = t_{VS} = 2MP^\mu, \quad (26A.32)$$

$$t_{PP}(P|q) = P^2 - \frac{q^2}{4} - M^2, \quad t_{PA^\mu}(P|q) = -t_{A^\mu P} = iMq^\mu, \quad (26A.33)$$

$$t_{V^\mu V^\nu}(P|q) = -\left(P^2 - \frac{q^2}{4} - M^2\right) g^{\mu\nu} + 2P^\mu P^\nu - \frac{1}{2}q^\mu q^\nu, \quad (26A.34)$$

$$t_{A^\mu A^\nu}(P|q) = -\left(P^2 - \frac{q^2}{4} - M^2\right) g^{\mu\nu} + 2P^\mu P^\nu - \frac{1}{2}q^\mu q^\nu - 2M^2 g^{\mu\nu}, \quad (26A.35)$$

with all other traces vanishing. Notice that, in the Bethe-Salpeter equation for $m'(P|q)$, there is no tensor contribution due to the absence of such a term in the Fierz transform of $\gamma^\mu \otimes \gamma_\mu$. The integrals in (26A.31) go directly over into (26.93) for a large gluon mass μ .

Appendix 26B Vertices for Heavy Gluons

Here we present the calculation of the vertices $\mathcal{A}_2, \mathcal{A}_3, \mathcal{A}_4$ for large μ . As discussed in the text, all higher vertices remain finite when the cutoff and μ goes to infinity like $\Lambda^2 \gg \mu^2 \gg M^2$, and will consequently be neglected.

Consider first $\mathcal{A}_2$ as described in (26.94) and (26A.32). The integrals $J_{ij}(q)$ are evaluated by expanding

$$\begin{aligned} &\left[\left(P + \frac{q}{2}\right)_E^2 + M^2\right]^{-1} \left[\left(P - \frac{q}{2}\right)_E^2 + M^2\right]^{-1} \left[\left(P - \frac{q}{2}\right)_E^2 + M^2\right]^{-1} = \\ &\left[P_E^2 + M^2\right]^{-2} \left\{ 1 + \frac{q^2/2}{P_E^2 + M^2} + \frac{(P_q)^2}{(P_E^2 + M^2)^2} + \mathcal{O}\left(\frac{M^4}{(P_E^2 + M^2)^2} \frac{q^4}{(P_E^2 + M^2)^2}\right) \right\}. \end{aligned} \quad (26B.1)$$

Since $t_{ij}(P|q)$ grows at most like P_E^2 [see (26A.32)], the terms $\mathcal{O}(M^4/E^4, q^4/P_E^4)$ contribute finite amounts upon integration, and will be neglected. At this place we have assumed q^2 to remain of the same order of M^2 . Actually, this is not true for vector- and axialvector meson fields¹⁰ but, since $m_\rho^2, m_{A_1}^2 \lesssim \mu^2/100$, the neglected terms are indeed very small.

The following integrals are needed, in addition to (26.88), (26.95) (neglecting finite amounts):

$$\int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^2} P^2 = -(Q - M^2 L), \quad (26B.2)$$

$$\int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^2} P_\mu P_\nu = -(Q - M^2 L) \frac{g_{\mu\nu}}{4}, \quad (26B.3)$$

$$\int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)} P_\mu P_\nu = -L \frac{g_{\mu\nu}}{4}, \quad (26B.4)$$

$$\int \frac{d^4 P_E}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^4} P_\mu P_\nu P_\lambda P_\kappa = \frac{L}{24} (g_{\mu\nu} g_{\lambda\kappa} + g_{\mu\lambda} g_{\nu\kappa} + g_{\mu\kappa} g_{\nu\lambda}). \quad (26B.5)$$

The results have been used in Eq. (26.96).

There is one subtlety connected with gauge invariance when evaluating the integrals $J_W(q)$ and $J_{AA}(q)$. In fact, the first of these integrals coincides with the standard photon self-energy graph in quantum electro-dynamics. There the cutoff procedure is known to produce a non-gauge invariant result. The cutoff calculation yields:

$$J_{V^\mu V^\nu}(q) = -\frac{1}{3} (q^2 g_{\mu\nu} - q_\mu q_\nu) L - \frac{1}{2} (Q + M^2 L) g_{\mu\nu}, \quad (26B.6)$$

$$J_{A^\mu A^\nu} = -\frac{1}{3} [(q^2 - 6M^2) g_{\mu\nu} - q_\mu q_\nu] L - \frac{1}{2} (Q + M^2 L) g_{\mu\nu}. \quad (26B.7)$$

There are many equivalent ways to enforce gauge invariance. The simplest of these proceeds via dimensional regularization. If one evaluates the integrals Q and L in $D = 4 - \epsilon$ dimensions with a small $\epsilon > 0$, then

$$\begin{aligned} L &= \int \frac{d^D p}{(2\pi)^4} \frac{1}{(P_E^2 + M^2)^2} = \frac{\pi^{D/2}}{(2\pi)^4} \frac{1}{(M^2)^{2-(D/2)}} \frac{\Gamma(2 - \frac{D}{2})}{\Gamma(2)} \\ &= \frac{\pi^2}{(2\pi)^4} \frac{2}{\epsilon} + \mathcal{O}(\epsilon), \end{aligned} \quad (26B.8)$$

$$\begin{aligned} Q &= \int \frac{d^D P_E}{(2\pi)^4} \frac{1}{P_E^2 + M^2} = \frac{\pi^{D/2}}{(2\pi)^4} \frac{1}{(M^2)^{1-(D/2)}} \frac{\Gamma(1 - \frac{D}{2})}{\Gamma(2)} \\ &= \frac{\pi^2}{(2\pi)^4} M^2 \left(-\frac{2}{\epsilon} \right) + \mathcal{O}(\epsilon). \end{aligned} \quad (26B.9)$$

Hence at the pole at $\epsilon = 0$, Q and L become related, for instance as $Q + M^2 L = 0$, canceling the last terms in (26B.6). Notice that, when dealing with the renormalizable theory with large gluon mass $\mu^2 \ll \Lambda^2$, this cancellation is still present while the other Q integrals in $J_{ij}(q)$ become unrelated with the L integrals, the first being essentially $\mu^2 \log \Lambda^2 / \mu^2$, the other $\log \mu^2 / M^2$.

Consider now the interaction terms $\mathcal{A}_3$. Here the traces grow at most as P_E^2 . Thus, as far as the divergent contributions are concerned, the denominators in the integrals (26.115) can be approximated as

$$\begin{aligned} &\frac{1}{(P + q_2 + q_1)_E^2 + M^2} \frac{1}{(P + q_1)_E^2 + M^2} \frac{1}{P_E^2 + M^2} = \\ &\frac{1}{(P_E^2 + M^2)^3} \left\{ 1 + \frac{P(2q_1 + q_2)}{P_E^2 + M^2} + \mathcal{O} \left(\frac{M^2}{P_E^2 + M^2}, \frac{q_1^2}{P_E^2 + M^2} \right) \right\}. \end{aligned} \quad (26B.10)$$

¹⁰ $m_\rho^2 = 6M^2$; $m_{A_1}^2 \approx 12M^2$; $\mu^2 \approx 144\text{GeV}^2$.

Since this expression decreases at least as $1/p_E^6$, the traces have to be known only with respect to their leading P_E^2 and P_E^2 behaviors. These are

$$\begin{aligned}
t_{SSS}(P|q_2q_1) &\simeq 3P^2M \simeq t_{SPP}(P|q_2q_1), \\
t_{SPA^\mu}(P|q_2q_1) &\simeq iP^2P^\mu + 2iP^\mu[P(q_1+q_2)] - iP^2q_2^\mu, \\
t_{SA^\mu P}(P|q_2q_1) &\simeq -iP^2P^\mu - iP^2(2q_1+q_2)^\mu, \\
t_{SSV^\mu}(P|q_2q_1) &\simeq P^2P^\mu - P^2q_2^\mu + 2P^\mu[P(q_1+q_2)] \simeq t_{PPV^\mu}(P|q_2q_1), \\
t_{SV^\mu S}(P|q_2q_1) &\simeq P^2P^\mu + P^2(2q_1+q_2)^\mu \simeq t_{PV^\mu P}(P|q_2q_1), \\
t_{SV^\mu V^\nu}(P|q_2q_1) &\simeq 4MP^\mu P^\nu - MP^2g^{\mu\nu}, \\
t_{SA^\mu A^\nu}(P|q_2q_1) &\simeq 4MP^\mu P^\nu - 3MP^2g^{\mu\nu}, \\
t_{V^\mu V^\lambda V^\kappa}(P|q_1q_2) &\simeq 4P^\mu P^\lambda P^\kappa - P^2(P^\mu g^{\lambda\kappa} + P^\lambda g^{\mu\kappa} + P^\kappa g^{\mu\lambda}) \\
&\quad + 2P^\mu P^\lambda q_1^\kappa + 2P^\lambda P^\kappa(q_1+q_2)^\mu + 2P^\mu P^\kappa(2q_1+q_2)^\lambda \\
&\quad - 2P^\kappa P(q_1+q_2)g^{\mu\lambda} - 2P^\mu Pq_1g^{\lambda\kappa} \\
&\quad - P^2[-g^{\mu\lambda}q_2 + g^{\lambda\kappa}q_2 + g^{\mu\kappa}(2q_1+q_2)].
\end{aligned} \tag{26B.11}$$

Using (26B.2) one obtains exactly the third order terms in the Lagrangian Eq. (26.117) (if this is written in the σ' -form).

The fourth-order couplings in $\mathcal{A}_4$ are the simplest to evaluate. Here only the leading P^4 behavior of $t_{ij}(P|q_3q_2q_1)$ contributes proportional to L and the propagator can directly be used in the form $(P_E^2 + M^2)^{-4}$:

$$t_{SSSS}(P|q_3q_2q_1) \simeq t_{SSPP} \simeq t_{PPPP} \simeq P^4, \tag{26B.13}$$

$$t_{SSV^\mu V^\nu}(P|q_3q_2q_1) \simeq t_{PPV^\mu V^\nu} \simeq t_{SSA^\mu A^\nu}, \tag{26B.14}$$

$$\simeq t_{PPA^\mu A^\nu} \simeq -it_{SPA^\mu V^\nu} \simeq -it_{PSA^\mu V^\nu}, \tag{26B.15}$$

$$\simeq 2P^2P^\mu P^\nu - P^4g^{\mu\nu}. \tag{26B.16}$$

Appendix 26C Some Algebra

Here we want to compare some of our results with traditional derivations [32, 33], obtained by purely algebraic considerations together with PCAC.

The vector and axial-vector currents

$$V_\mu^a(x) = \bar{\psi}(x)\gamma_\mu^a \frac{\lambda^a}{2}\psi(x), \quad A_\mu^a(x) = \bar{\psi}(x)\gamma_\mu\gamma_5 \frac{\lambda^a}{2}\psi(x) \tag{26C.1}$$

generate chiral $SU(3) \times SU(3)$, under which the quark gluon Lagrangian transforms as

$$\mathcal{L} = \mathcal{L}_{\text{chirally invariant}} - u^0 - cu^8 - du^3, \tag{26C.2}$$

where

$$\begin{aligned}
u^0 + cu^8 + du^3 &= \bar{\psi}\mathcal{M}\psi \equiv \sum_a \mathcal{M}^a \bar{\psi} \frac{\lambda^a}{2} \psi \\
&= \sqrt{\frac{2}{3}} (\mathcal{M}^u + \mathcal{M}^d + \mathcal{M}^s) \bar{\psi} \frac{\lambda^0}{2} \psi \\
&\quad + \frac{1}{\sqrt{3}} (\mathcal{M}^u + \mathcal{M}^d - 2\mathcal{M}^s) \bar{\psi} \frac{\lambda^8}{2} \psi + (\mathcal{M}^u - \mathcal{M}^d) \bar{\psi} \frac{\lambda^3}{2} \psi.
\end{aligned} \tag{26C.3}$$

By identifying

$$u^a \equiv \mathcal{M}^0 \bar{\psi} \frac{\lambda^a}{2} \psi, \tag{26C.4}$$

we see that the coefficients in (26C.2) are

$$c \equiv \frac{\mathcal{M}^8}{\mathcal{M}^0}, \quad d = \frac{\mathcal{M}^3}{\mathcal{M}^0}. \quad (26C.5)$$

After defining also the pseudoscalar densities

$$v^a \equiv \mathcal{M}^0 \bar{\psi} i \gamma_5 \frac{\lambda^a}{2} \psi, \quad (26C.6)$$

we verify that u^a and v^a transform like a $(\bar{3}, 3) \pm (3, \bar{3})$ -representation of the group $SU(3) \times SU(3)$ since the commutation relations are:

$$[Q_5^a, u^a] = i d^{abc} v^c, \quad [Q_5^a, v^b] = -i d^{abc} u^c. \quad (26C.7)$$

From the equation of motion one finds the conservation law

$$\begin{aligned} \partial^\mu V_\mu^a(x) &= \partial^\mu \bar{\psi} \gamma_\mu \frac{\lambda^a}{2} \psi = \bar{\psi} \left[\frac{\lambda^a}{2} \mathcal{M} \right] \psi \\ &= i f^{abc} \mathcal{M}^b \bar{\psi} \frac{\lambda^c}{2} \psi \quad a = 0, 1, \dots, 8, \\ \partial^\mu A_\mu^a(x) &= \partial^\mu \bar{\psi} \gamma_\mu \gamma_5 \frac{\lambda^a}{2} \psi = -\bar{\psi} \left[\frac{\lambda^a}{2} \mathcal{M} \right] \gamma_5 \psi \\ &= i d^{abc} \mathcal{M}^b \bar{\psi} i \gamma_5 \frac{\lambda^c}{2} \psi \quad a = 1, \dots, 8. \end{aligned} \quad (26C.8)$$

Let us neglect $SU(2)$ breaking in $\mathcal{M}$. By taking (26C.8) between vacuum and pseudoscalar meson states we find

$$\begin{aligned} f_\pi m_\pi^2 &= \frac{1}{\sqrt{3}} \left(\sqrt{2} \mathcal{M}^0 + \mathcal{M}^8 \right) \frac{m_V^2}{3} \sqrt{L} Z_\pi^{1/2}, \\ f_K m_K^2 &= \frac{1}{\sqrt{3}} \left(\sqrt{2} \mathcal{M}^0 + \mathcal{M}^8 \right) \frac{m_V^2}{3} \sqrt{L} Z_K^{1/2}. \end{aligned} \quad (26C.9)$$

Similar equations hold for the other members of the multiplet. We have used the definitions [see the pseudoscalar version of (26.165)]:

$$\begin{aligned} \langle 0 | \partial^\mu A_\mu^a | \pi \rangle &\equiv f_\pi m_\pi^2, \\ \langle 0 | \bar{\psi} i \gamma_5 \frac{\lambda^a}{2} \psi | \pi \rangle &= \frac{\mu^2}{2g^2} \frac{1}{2g^2} \frac{1}{\sqrt{L}} \langle 0 | \pi | \pi \rangle = \frac{\mu^2}{2g^2} \frac{Z_\pi^{1/2}}{\sqrt{L}} = \frac{m_V^2}{3} \sqrt{L} Z_\pi^{1/2}. \end{aligned}$$

If we write the matrix $\mathcal{M}$ in the form

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}^u & & \\ & \mathcal{M}^d & \\ & & \mathcal{M}^s \end{pmatrix} = \frac{1}{2\sqrt{3}} \begin{pmatrix} \sqrt{2}\mathcal{M}^0 + \mathcal{M}^8 & & \\ & \sqrt{2}\mathcal{M}^0 + \mathcal{M}^8 & \\ & & \sqrt{2}\mathcal{M}^0 - 2\mathcal{M}^8 \end{pmatrix}, \quad (26C.10)$$

then Eqa. (26C.9) take the form

$$\begin{aligned} f_\pi^2 m_\pi^2 &= \frac{\mathcal{M}^u + \mathcal{M}^d}{2} Z_\pi^{1/2} \frac{2}{3} m_V^2 \sqrt{L}, \\ f_K^2 m_K^2 &= \frac{\mathcal{M}^u + \mathcal{M}^s}{2} Z_\pi^{1/2} \frac{2}{3} m_V^2 \sqrt{L}, \end{aligned} \quad (26C.11)$$

which agrees with (26.144).

By evaluating (26C.7) between vacuum states and saturating the commutator with a pseudoscalar intermediate state, one finds

$$f_\pi \mathcal{M}_0 \frac{\mu^2}{2g^2} \frac{Z_\pi^{1/2}}{\sqrt{L}} = \frac{1}{\sqrt{3}} \left(\sqrt{2} \langle 0|u^0|0 \rangle + \langle 0|u^8|0 \rangle \right), \quad (26C.12)$$

$$f_K \mathcal{M}_0 \frac{\mu^2}{2g^2} \frac{Z_K^{1/2}}{\sqrt{L}} = \frac{1}{\sqrt{3}} \left(\sqrt{2} \langle 0|u^0|0 \rangle - \frac{1}{2} \langle 0|u^8|0 \rangle \right), \quad (26C.13)$$

and similar for the other partners of the multiplet. Inserting the result of Eq. (26.165),

$$\langle 0|u^a|0 \rangle = \mathcal{M}^0 \langle 0|\tilde{u}^a|0 \rangle = \frac{1}{2} \frac{\mu^2}{g^2} \mathcal{M}^0 M^a, \quad (26C.14)$$

and writing M in the same way as $\mathcal{M}$ in (26C.10), brings (26C.12) and (26C.13) to the form

$$f_\pi Z_\pi^{1/2} = \sqrt{L} (M^u + M^d), \quad (26C.15)$$

$$f_K Z_K^{1/2} = \sqrt{L} (M^u + M^s), \quad (26C.16)$$

which agrees exactly with (26.144) (written there in the SU(3)-matrix form). Considerations of this type have led to the determination [32, 33, 37]

$$c \approx -1.28, \quad (26C.17)$$

or

$$\frac{(\mathcal{M}^u + \mathcal{M}^d)/2}{\mathcal{M}^s} \approx \frac{1}{29}.$$

Including also SU(2)-violation in such a consideration, gives [37]

$$d \approx -0.03, \quad (26C.18)$$

or

$$\frac{\mathcal{M}_u - \mathcal{M}_d}{\mathcal{M}_u + \mathcal{M}_d} \approx -\frac{1}{4}.$$

There are numerous extensions to SU(4), but they have to be viewed with caution, since it is hard to see how the large pseudoscalar and vector masses occurring there can dominate the divergence of the axial current and the vector current, respectively.

Notes and References

This chapter is based on a lecture at the 1974 Erice Summer School:

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*People who have no weaknesses are terrible;
there is no way of taking advantage of them.*
ANATOLE FRANCE (1844–1924)

27

Weak Interactions

The decay of nuclei proceeds via α -, β -, γ -emission, or by fission. The first is governed by nuclear forces, the third by electromagnetic interactions. The β -emission has an entirely different origin. It is caused by *weak interactions*. Initially, such processes posed a serious puzzle: The observed emerging particles, electrons or positrons, did not come out with a definite energy equal to the mass difference between initial and final nuclei. Instead, they had an energy *distribution* with a maximal energy at the expected value. This led Nils Bohr to speculate that energy conservation could possibly be violated in quantum physics. In 1939, however, Wolfgang Pauli suggested in a historic letter to colleagues [1] meeting in Tübingen, that the missing energy was carried off by a neutral particle, now called *neutrino*. Its spin had to be $1/2$, to preserve angular momentum.

The simplest nuclear particle which shows β -decay is the neutron itself which decays, after about 900 seconds, as follows:

$$n \rightarrow p + e^- + \bar{\nu}_e, \quad (27.1)$$

where $\bar{\nu}_e$ denotes a right-handed version of Pauli's particle, which is nowadays referred to as an antineutrino associated with the electron.

As time went on, many more particles were discovered that arose from similar interactions. All of them are now called leptons. Recall the classification in Section 24.1.

27.1 Fermi Theory

In 1934, Fermi made a first theoretical attempt to describe β -decay in lowest-order perturbation theory [2]. He suggested that the interaction is due to a local current-current interaction with a Lagrangian density of the form

$$\mathcal{L} = C \bar{p}(x) \gamma^\mu n(x) \bar{e}(x) \gamma_\mu \nu(x) + \text{c.c.} \quad (27.2)$$

In accordance with the standard short notation for the fields, we have denoted $\psi_e(x)$ by $e(x)$ and $\psi_p(x)$ by $p(x)$, etc. This interaction looks similar to the electric

interaction in Eq. (12.85), except that the Coulomb potential describing the electric long-range interaction is replaced by a short-range δ -function potential. Fermi also realized that Lorentz invariance and locality allow a more general Lagrangian density of the form

$$\begin{aligned}\mathcal{L} = & C_S \bar{p}(x)n(x) \bar{e}(x)\nu(x) + C_P \bar{p}(x)i\gamma_5 n(x) \bar{e}(x)i\gamma_5 \nu(x) \\ & + C_V \bar{p}(x)\gamma^\mu n(x) \bar{e}(x)\gamma_\mu \nu(x) + C_A \bar{p}(x)\gamma^\mu \gamma_5 n(x) \bar{e}(x)\gamma_\mu \gamma_5 \nu(x) \\ & + \tfrac{1}{2}C_T \bar{p}(x)\sigma^{\lambda\kappa} n(x) \bar{e}(x)\sigma_{\lambda\kappa} \nu(x) + \text{c.c.} .\end{aligned}\quad (27.3)$$

Fermi postulated the validity of time-reversal invariance, which to our present knowledge is fulfilled to a high degree of accuracy. A tiny violation of this is observable only in very few particularly sensitive processes. Hence the coefficients C_i in (27.3) have to be real, with only very small imaginary parts. If Γ_i denotes the five Dirac matrices $1, i\gamma_5, \gamma^\mu, \gamma^\mu \gamma_5$, and $\sigma^{\mu\nu}/\sqrt{2}$, one may write the interaction (27.3) short as

$$\mathcal{L} = \sum_{i=S,P,V,A,T} C_i \bar{p}(x)\Gamma_i n(x) \bar{e}(x)\Gamma_i \nu(x) + \text{c.c.} . \quad (27.4)$$

The decay of an initial nucleus at rest $|\Psi_i\rangle$ into a final nucleus $|\Psi_f\rangle$ is governed by the matrix elements

$$\langle \Psi_f | \bar{p}(x)\Gamma_i n(x) | \Psi_i \rangle. \quad (27.5)$$

Due to the small energy differences involved, the final state will be almost at rest (since the decaying nucleus is usually big enough), and one may use the nonrelativistic limit for the matrix elements between nucleons. Taking the Dirac matrices in Dirac's original representations, one can use the direct-product expressions (27.6),

$$\gamma_D^0 = \sigma^3 \times 1, \quad \gamma_D = i\sigma^2 \times \boldsymbol{\sigma}, \quad \gamma_D^5 = \sigma^1 \times 1, \quad (27.6)$$

to rewrite the matrix elements of $\bar{p}(x)\Gamma_i n(x)$ as follows:

$$\begin{aligned}S : \quad & \bar{p}(x)n(x) \approx p^\dagger(x)n(x), \\ P : \quad & \bar{p}(x)i\gamma_D^5 n(x) \approx -p^\dagger(x)\sigma^2 \times 1 n(x) \approx 0, \\ V : \quad & \bar{p}(x)\gamma_D^0 n(x) \approx p^\dagger(x)n(x), \\ & \bar{p}(x)\gamma_D^i n(x) \approx -p^\dagger(x)\sigma^1 \times \sigma^i n(x) \approx 0, \\ A : \quad & \bar{p}(x)\gamma_D^0 \gamma_D^5 n(x) \approx p^\dagger(x)\sigma^1 \times 1 n(x) \approx 0, \\ & \bar{p}(x)\gamma_D^i \gamma_D^5 n(x) \approx p^\dagger(x)1 \times \sigma^i n(x), \\ T : \quad & \bar{p}(x)\sigma^{0i} n(x) \approx -p^\dagger(x)\sigma^2 \times \sigma^i n(x) \approx 0, \\ & \bar{p}(x)\sigma^{ij} n(x) \approx \epsilon_{ijk} p^\dagger(x)1 \times \sigma^k n(x).\end{aligned}\quad (27.7)$$

The lines containing mixtures of upper and lower components are very small for small momenta, and can be omitted. Thus we are left with only two types of nuclear matrix elements:

$$\begin{aligned}\langle \Psi_f | p^\dagger(x)n(x) | \Psi_i \rangle &\equiv \langle \mathbf{1} \rangle, \\ \langle \Psi_f | p^\dagger(x)\boldsymbol{\sigma} n(x) | \Psi_i \rangle &\equiv \langle \boldsymbol{\sigma} \rangle,\end{aligned}\quad (27.8)$$

where σ in front of a Dirac spinor acts only upon the spin label.

The S -matrix elements are then approximately given by

$$S = 1 - 2\pi i \delta(E_f + E_e + E_{\bar{\nu}} - E_i) T, \quad (27.9)$$

with the T -matrix [recall (9.293)]

$$T = \frac{\sqrt{2m_{\nu}}}{V} \left\{ \langle \mathbf{1} \rangle \left[C_S \bar{u}(\mathbf{p}_e) v(\mathbf{p}_{\bar{\nu}}) + C_V \bar{u}(\mathbf{p}_e) \gamma^0 v(\mathbf{p}_{\bar{\nu}}) \right] \right. \\ \left. + \langle \sigma \rangle \left[\frac{1}{2} C_T \bar{u}(\mathbf{p}_e) \sigma v(\mathbf{p}_{\bar{\nu}}) + C_A \bar{u}(\mathbf{p}_e) \gamma \gamma_5 v(\mathbf{p}_{\bar{\nu}}) \right] \right\}. \quad (27.10)$$

The spin labels s_3 for the electron and antineutrino have been omitted, for brevity. We have also normalized the antineutrino states in the same way as photon states like

$$\langle \mathbf{p}'_{\bar{\nu}} | \mathbf{p}_{\bar{\nu}} \rangle = 2p_{\bar{\nu}}^0 \delta^{(3)}(\mathbf{p}'_{\bar{\nu}} - \mathbf{p}_{\bar{\nu}}), \quad (27.11)$$

to allow a smooth limit as $m_{\nu} \rightarrow 0$.

When calculating decay rates, we may sum over the antineutrino polarizations which are hard to measure. The polarization sum yields

$$\sqrt{2m_{\nu}} \sum_{\text{spin pol}} \bar{v}(\mathbf{p}_{\bar{\nu}}) v(\mathbf{p}_{\bar{\nu}}) = \not{p}_{\bar{\nu}} - m_{\nu}, \quad (27.12)$$

and m_{ν} is set equal to zero at the end. For unpolarized nuclei, we have

$$\langle \sigma^i \sigma^j \rangle = \frac{1}{3} |\sigma|^2, \quad \langle \sigma^i \mathbf{1} \rangle = 0. \quad (27.13)$$

If also the electrons are unpolarized, we obtain

$$\sum_{\text{spin pol}} |T|^2 = \frac{1}{2m_e V^2} \left[C_S^2 |\langle \mathbf{1} \rangle|^2 \text{tr}(\not{p}_{\bar{\nu}} \not{p}_e) + |C_V|^2 |\langle \mathbf{1} \rangle|^2 \text{tr}(\gamma_0 \not{p}_{\bar{\nu}} \gamma_0 \not{p}_e) \right. \\ + \frac{1}{3} C_A^2 |\langle \sigma \rangle|^2 \text{tr}(\gamma^i \gamma_5 \not{p}_{\bar{\nu}} \gamma_5 \gamma^i \not{p}_e) + \frac{1}{12} C_T^2 |\langle \sigma \rangle|^2 \text{tr}(\sigma^i \not{p}_{\bar{\nu}} \gamma_5 \sigma^i \not{p}_e) \\ \left. + 2C_S C_V |\langle \mathbf{1} \rangle|^2 m_e \text{tr}(\not{p}_{\bar{\nu}} \gamma_0) + \frac{1}{3} C_S C_V |\langle \sigma \rangle|^2 m_e \text{tr}(\sigma^i \not{p}_{\bar{\nu}} \gamma_0 \not{p}_e) \right], \quad (27.14)$$

or more explicitly

$$\sum_{\text{spin pol}} |T|^2 = \frac{4E_{\nu} E_{\bar{\nu}}}{2m_e V^2} \left[C_S^2 |\langle \mathbf{1} \rangle|^2 \left(1 - \frac{\mathbf{p}_e \mathbf{p}_{\bar{\nu}}}{E_e E_{\bar{\nu}}} \right) + |C_V|^2 |\langle \mathbf{1} \rangle|^2 \left(1 + \frac{\mathbf{p}_e \mathbf{p}_{\bar{\nu}}}{E_e E_{\bar{\nu}}} \right) \right. \\ + C_A^2 |\langle \sigma \rangle|^2 \left(1 - \frac{1}{3} \frac{\mathbf{p}_e \mathbf{p}_{\bar{\nu}}}{E_e E_{\bar{\nu}}} \right) + \frac{1}{4} C_T^2 |\langle \sigma \rangle|^2 \left(1 + \frac{1}{3} \frac{\mathbf{p}_e \mathbf{p}_{\bar{\nu}}}{E_e E_{\bar{\nu}}} \right) \\ \left. + 2C_S C_V |\langle \mathbf{1} \rangle|^2 m_e \frac{2m_e}{E_e} - C_A C_T |\langle \sigma \rangle|^2 \frac{m_e}{E_e} \right]. \quad (27.15)$$

The interference terms $C_S C_V$ and $C_T C_A$ show a strong threshold-dependence proportional to $1/E_e$. Since this is not observed experimentally, one concludes that

$$C_S C_V \approx 0, \quad C_T C_A \approx 0. \quad (27.16)$$

One distinguishes now *Gamow-Teller transitions*, by for which $|\langle \boldsymbol{\sigma} \rangle|^2 \neq 0$, and *Fermi transitions*, for which $|\langle \mathbf{1} \rangle|^2 \neq 0$ (both without nuclear parity change). For transitions in which initial and final nuclear spins are the same, only C_S^2 and C_V^2 contribute. These are distinguishable by the electron-antineutrino correlation in momentum space. In the first case, electron and antineutrino come out preferably in opposite direction ($\mathbf{p}_e \mathbf{p}_{\bar{\nu}} < 0$), in the second case in the same direction ($\mathbf{p}_e \mathbf{p}_{\bar{\nu}} > 0$). Experiments done for the decay

$$\text{Ne}^{19} \rightarrow \text{F}^{19} + e + \bar{\nu}, \quad (27.17)$$

in which the nuclear spin is 1/2 before and after the decay show that the latter is true. Thus we can approximate $C_S \approx 0$.

Transitions which change the nuclear spin by one unit are sensitive to C_A^2 and C_T^2 , with similar momentum correlations. The decay

$$\text{He}^6 \rightarrow \text{Li}^6 + e + \bar{\nu} \quad (27.18)$$

involves a change from nuclear spin 0 to 1. The electron and the neutrino emerge antiparallel, from which one deduces that $C_T^2 \approx 0$. Thus only C_V and C_A are appreciable.

The antineutrinos which appear in these decays have been found to interact with matter extremely weakly. Only many years later, in 1953, was it possible to detect them directly via the inverse reaction

$$\bar{\nu}_e + p \rightarrow n + e^+, \quad (27.19)$$

using a prolific antineutrino source of a large nuclear reactor filled with a high density of thermal neutrons.

After many precise measurements of angular correlations and electron and nuclear polarizations, the coefficients of the general interaction (27.3) have been quite well determined and led to

$$\mathcal{L} = -\frac{G_W}{\sqrt{2}} \left[\bar{p} \gamma^\lambda \left(1 - \frac{g_A}{g_V} \gamma_5 \right) n \right] \left[\bar{e} \gamma_\lambda (1 - \gamma_5) \nu \right] + \text{c.c.}, \quad (27.20)$$

with the weak-interaction coupling constant

$$G_W = (1.14730 \pm 0.000641) \times 10^{-5} \text{GeV}^{-2}, \quad (27.21)$$

and the ratio

$$g_A/g_V = 1.255 \pm 0.006. \quad (27.22)$$

The $\bar{e}\nu$ -part of the interaction violates space reflection symmetry in the maximal possible way. Under a parity transformation, the left-helicity field $(1 - \gamma_0)\nu(x)$ that possesses nonzero components only in the first two entries is multiplied by

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

This moves the nonzero entries to the lower two components producing a right-helicity field $(1 + \gamma_5)\gamma_0\nu$. However, such a field is not present in the Lagrangian density (27.20). This maximal parity violation is responsible for the asymmetry of the decay electrons with respect to the neutron spin as observed in Madame Wu's experiment [3].

The ratio g_A/g_V can be measured in neutron decay via the up-down asymmetry by analogy with Madame Wu's experiment. The expectation $\langle \mathbf{s}_n \cdot \mathbf{p}_e \rangle$ is proportional to

$$|C_A|^2 + \text{Re } C_V C_A^* \propto (1 - g_A/g_V). \quad (27.23)$$

The deviation of the ratio g_A/g_V from unity can be explained by strong interactions. This possibility was first suggested by the weak decay of the 1937 discovered muon (initially mistaken for a pion). The muon decays weakly as follows

$$\mu^- \rightarrow e^- + \bar{\nu}_e + \nu_\mu. \quad (27.24)$$

27.2 Lepton-Number Conservation

In 1962, a Brookhaven experiment showed that the antineutrino emerging in the decay had to be distinguished from that emerging in the β -decay of the muon. The two neutrinos are now referred to as muon neutrino $\bar{\nu}_\mu$ and electron antineutrino $\bar{\nu}_e$, respectively. With this assignment, the total number of electrons plus the associated electron neutrinos, and the total number of muons plus the associated muon neutrinos, are both separately conserved if antiparticles are counted negatively. These laws are called *lepton-number conservation laws*. The muon has no strong interaction and its decay is described by the Lagrangian density

$$\mathcal{L}_\mu = \frac{G_\mu}{\sqrt{2}} [\bar{\nu}_\mu \gamma^\lambda (1 - \gamma_5) \mu] [\bar{e} \gamma_\lambda (1 - \gamma_5) \nu_e(x)] + \text{c.c.} \quad (27.25)$$

The value of G_μ is given by

$$G_\mu = 1.16637(1) \times 10^{-5} \text{GeV}^{-2}. \quad (27.26)$$

It is 2% larger than G_W of the β -decay in Eq. (27.21).

The parameter G_μ is defined as the *Fermi constant*. There are two reasons for choosing it rather than G_W . First, the experimental value of the lifetime of μ^- is extremely well measured:

$$\tau_\mu = 2.197035(40) \times 10^{-6} \text{s}^{-1}. \quad (27.27)$$

Second, this lifetime determines G_μ via a very reliable theoretical relation that follows from QED [4]:

$$\tau_\mu^{-1} = \frac{G_\mu^2 m_\mu^5}{192\pi^3} f\left(\frac{m_e^2}{m_\mu^2}\right) (1 + \text{R.C.}) \left(1 + \frac{3}{5} \frac{m_\mu^2}{m_W^2} + \dots\right). \quad (27.28)$$

The abbreviation R.C. denotes radiative corrections

$$\begin{aligned} \text{R.C.} = & \frac{\alpha}{2\pi} \left(\frac{25}{4} - \pi^2 \right) \left[1 + \frac{\alpha}{\pi} \left(\frac{2}{3} \log \frac{m_\mu}{m_e} - 3.7 \right) \right. \\ & \left. + \left(\frac{\alpha}{\pi} \right)^2 \left(\frac{4}{9} \log^2 \frac{m_\mu}{m_e} - 2.0 \log \frac{m_\mu}{m_e} + C \right) + \dots \right]. \end{aligned} \quad (27.29)$$

These can be calculated with great accuracy by solving the renormalization group equation

$$(m_e \partial_{m_e} + \beta(\alpha) \partial_\alpha) \text{R.C.} = 0, \quad \beta(\alpha) = \frac{2}{3} \frac{\alpha^2}{\pi} + \frac{1}{2} \frac{\alpha^3}{\pi^2} + \dots, \quad (27.30)$$

where $\beta(\alpha)$ is the beta-function that governs the change of the interaction strength upon a change in the scale of the theory. It was defined in (20.31) for a scalar field theory with ϕ^4 -interaction. For QED it was first introduced by Stückelberg and Petermann [5], and soon after that by Gell-Mann and Low [6].

27.3 Cabibbo Angle

In order to explain why G_W is smaller than G_μ , Nicola Cabibbo, in 1964, put forward the hypothesis that the reduction is due to a simple geometric property of the weak [7]. Studying the β -decay the strange particles

$$\begin{aligned} \Lambda & \rightarrow p + e^- + \bar{\nu}_e, \\ \Sigma^+ & \rightarrow \Lambda + e^+ + \nu_e, \end{aligned} \quad (27.31)$$

he observed that their weak coupling constant G_W^{strange} was considerably smaller than that of neutrons. Moreover, he was able to fit the three decays (27.1), (27.24), and (27.31), quite well by assuming that the weak coupling constant defined as in (27.20) for the ordinary β -decay, and a similar G_W^{strange} for the decays (27.31) can be parametrized by setting

$$G_W = \cos \theta_c G_\mu, \quad (27.32)$$

$$G_W^{\text{strange}} = \sin \theta_c G_\mu, \quad (27.33)$$

where G_μ is the weak coupling constant (27.26) of the leptonic decay, if one chooses the value

$$\theta_c = 0.21 \quad (27.34)$$

for the so-called *Cabibbo angle*.

Nowadays it is believed that weak interactions of all hadrons proceed via the decay of quarks inside their wave functions. The non-strange hadrons decay via the elementary transitions

$$\begin{aligned} d & \rightarrow u + e^- + \nu_e, \\ d & \rightarrow u + \mu^- + \nu_\mu, \\ u & \rightarrow d + e^+ + \bar{\nu}_e, \\ u & \rightarrow d + \mu^+ + \bar{\nu}_\mu. \end{aligned} \quad (27.35)$$

The strange hadrons decay by similar transitions, with the down quarks d getting replaced by a strange quark s . Cabibbo's hypothesis amounts to the ansatz for the interaction Lagrangian density

$$\begin{aligned}\mathcal{L} &= -\frac{G_\mu}{\sqrt{2}} \bar{u} \gamma^\lambda (1 - \gamma_5) (\cos \theta_c d + \sin \theta_c s) \cdot [\bar{e} \gamma_\lambda (1 - \gamma_5) \nu] + \text{h.c.} \\ &= -\frac{G_\mu}{\sqrt{2}} \left\{ \cos \theta_c [\bar{u} \gamma^\lambda (1 - \gamma_5) d] + \sin \theta_c [\bar{u} \gamma^\lambda (1 - \gamma_5) s] \right\} \cdot [\bar{e} \gamma_\lambda (1 - \gamma_5) \nu] + \text{h.c.} \quad (27.36)\end{aligned}$$

The first expression implies that the weak interactions couple only to an isospin-rotated combination of down and strange quarks. Moreover, they appear only in a special combination of vector and axial vector currents, which were previously found to be conserved Noether currents of QCD (or partially conserved in the axial vector case). In fact we can write

$$\begin{aligned}\bar{u} \gamma^\lambda d &= \sqrt{2} j_{(1+i2)/\sqrt{2}}^\lambda \equiv \sqrt{2} j_{\pi^+}^\lambda, \\ \bar{u} \gamma^\lambda \gamma_5 d &= \sqrt{2} j_{5(1+i2)/\sqrt{2}}^\lambda = \sqrt{2} j_{5\pi^+}^\lambda, \\ \bar{u} \gamma^\lambda s &= \sqrt{2} j_{(4+i5)/\sqrt{2}}^\lambda = \sqrt{2} j_{K^+}^\lambda, \\ \bar{u} \gamma^\lambda \gamma_5^d &= \sqrt{2} j_{5(4+i5)/\sqrt{2}}^\lambda = \sqrt{2} j_{5K^+}^\lambda, \quad (27.37)\end{aligned}$$

where the subscripts π^+, K^+ indicate the SU(3)-quantum numbers which can be created by these currents. In terms of these currents, we can rewrite (27.36) as

$$\mathcal{L} = -G_\mu \left\{ \cos \theta_c [j_{\pi^+}^\lambda - j_{5\pi^+}^\lambda] + \sin \theta_c [j_{K^+}^\lambda - j_{5K^+}^\lambda] \right\} [\bar{e} \gamma_\lambda (1 - \gamma_5) \nu] + \text{h.c.} \quad (27.38)$$

27.4 Cabibbo Mass Matrix

The Cabibbo theory can be phrased in a different way. The combination of quarks $d_\theta \equiv \cos \theta_c d + \sin \theta_c s$ entering the interaction Lagrangian density (27.36) may be thought of as a result of a diagonalization of a nondiagonal mass matrix of down and strange quarks:

$$(d', u') \mathcal{M} \begin{pmatrix} d' \\ u' \end{pmatrix} = (d', u') \begin{pmatrix} m_d & m_{ds} \\ m_{ds} & m_s \end{pmatrix} \begin{pmatrix} d' \\ u' \end{pmatrix}. \quad (27.39)$$

This matrix is diagonalized by the physical down and strange quarks

$$\begin{pmatrix} d \\ s \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} \\ -V_{us} & V_{ud} \end{pmatrix} \begin{pmatrix} d' \\ s' \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} d' \\ s' \end{pmatrix}, \quad (27.40)$$

with a Cabibbo angle solving the equation

$$\tan \theta = \frac{m_{ds}}{m_s - \bar{m}} = \frac{m_d - \bar{m}}{m_{ds}}, \quad (27.41)$$

where

$$\bar{m} = \frac{1}{2} \left[(m_d + m_s) + \sqrt{(m_d + m_s)^2 + 4m_{ds}^2} \right]. \quad (27.42)$$

The weak interactions involve only the Cabibbo-rotated *bare quark* field $d' = d_\theta$. This means that the weak quark current entering the Lagrangian density (27.36) has the form

$$\bar{u}\gamma^\lambda(1 - \gamma_5)d_\theta, \quad (27.43)$$

so that Lagrangian reads

$$\mathcal{L} = -\frac{G_\mu}{\sqrt{2}} \bar{u}\gamma^\lambda(1 - \gamma_5) d_\theta \cdot [\bar{e}\gamma_\lambda(1 - \gamma_5) \nu] + \text{h.c.} \quad (27.44)$$

27.5 Heavy Vector Bosons

Historically, the fact that the coupling constant of weak interactions carries a dimension of an inverse square mass was a great obstacle in calculating higher-order corrections to weak processes: Up to that point, the only successful field theory of fundamental interactions, quantum electrodynamics, had only a three-particle interaction, with the photon mediating the interactions: This led to the hypothesis that weak interactions could be due to a similar coupling of a massive charged vector meson called W . As we shall see later in the analysis of perturbation theory, this can generate a weak coupling of the same type as in (27.20), but with G_W replaced by

$$G_W(q^2) = -\frac{e_W^2}{q^2 - M_W^2}, \quad (27.45)$$

where q is the momentum carried off by the leptons in the decay, and e_W is the coupling strength of the heavy vector meson W to the leptons and quarks. If M_W is much larger than 1 BeV, the q -dependence can be ignored and one can approximate

$$G_W(0) \approx \frac{e_W^2}{M_W^2}. \quad (27.46)$$

Since e_W is dimensionless, it was suggestive to assume it to be equal to the coupling strength of the photons. Then weak interactions would carry only one additional parameter, the mass of the vector meson. Using

$$e^2 = 4\pi\alpha, \quad (27.47)$$

this requires as mass

$$M_W = \sqrt{\frac{4\pi\alpha}{G}} \approx 90\text{GeV}. \quad (27.48)$$

A charged meson which has the desired properties was found near this predicted mass in 1983 [8]. Its experimental value is

$$M_W = 80.423 \pm 0.039 \text{ GeV}. \quad (27.49)$$

With the usual weak decays carrying off a non-zero charge via a lepton, the question has been raised whether weak interactions could also lead to a decay into $\nu_e \bar{\nu}_e$, $\nu_\mu \bar{\nu}_\mu$, $e \bar{e}$, or $\mu \bar{\mu}$. The first two could have easily escaped experimental detection, the last two would be hard to find since they would hide under the similar but much larger electromagnetic interaction. Such decays would come from couplings such as

$$\mathcal{L} = G^0 [\bar{u} \gamma^\mu (1 - \gamma_5) u] \{ [e \gamma_\mu e + \bar{\nu}_e (1 - \gamma_5) \nu] + [e \rightarrow \mu] \}. \quad (27.50)$$

The field combinations $\bar{u} \gamma_\mu (1 - \gamma_5) u$, $\bar{e} \gamma_\mu (1 - \gamma_5) e$ contained in (27.50) do not change the charge of the decaying particles and are called *neutral currents*. They appear in the same combination $V^\mu - A^\mu$ of vector and axial vector currents as in the interaction (27.38).

Experimental evidence for such neutral currents has been observed in 1973 in a purely leptonic reaction

$$\bar{\nu}_\mu + e^- \leftarrow \bar{\nu}_\mu + e^-, \quad (27.51)$$

as well as in similar reactions involving quarks

$$\begin{aligned} \nu_\mu + \begin{pmatrix} u \\ d \end{pmatrix} &\rightarrow \nu_\mu + \begin{pmatrix} u \\ d \end{pmatrix}, \\ \bar{\nu}_\mu + \begin{pmatrix} u \\ d \end{pmatrix} &\rightarrow \bar{\nu}_\mu + \begin{pmatrix} u \\ d \end{pmatrix}. \end{aligned} \quad (27.52)$$

Also a heavy neutral vector meson has been found which, by analogy with W , mediates the neutral weak interactions. It is called Z -boson and its mass is given by [11]

$$M_Z = 92.9 \pm 1.6 \text{ GeV}. \quad (27.53)$$

27.6 Standard Model of Electroweak Interactions

All these interactions, plus the electromagnetic interactions, were unified in one field theory by Glashow, Weinberg, and Salam [9] in the *standard model of electromagnetic and weak interactions* (the combination being also called *electroweak interactions*). We shall briefly review this theory here in a reduced version in which the only leptons involved are electrons and electron-neutrinos [10]. All terms involving these leptons will have to be extended by similar terms involving the other two families of leptons discovered so far:

$$\begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}, \quad \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}. \quad (27.54)$$

The charged lepton masses are well known:

$$m_e = 0.511 \text{ MeV}, \quad m_\mu = 105.7 \text{ MeV}, \quad m_\tau = 1777 \text{ MeV}. \quad (27.55)$$

The free lepton Lagrangian density for the electron part is

$$\mathcal{L} = (\bar{\nu}_{eL}, \bar{e}_L) \not{\partial} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} + \bar{e}_R i \not{\partial} e_R. \quad (27.56)$$

It is invariant under the rotation group $\text{SU}_L(2)$ of the left-handed leptons, and a trivial group $\text{U}_R(1)$ of the right-handed leptons. In the latter, the neutrino ν_R is absent. This Lagrangian density is made locally $\text{SU}_L(2) \times \text{U}_R(1)$ -invariant by means of two types of gauge fields. For the $\text{SU}_L(2)$ -symmetry of the left-handed particles one uses a 2×2 -matrix gauge field

$$\mathbf{W}_\mu = W_\mu^a \frac{\tau_a}{2}, \quad (27.57)$$

in which τ_a acts on the two $\text{SU}_L(2)$ -isospin indices. Since these are mathematically equivalent to isospin, one speaks of a *weak isospin*. For the $\text{U}_R(1)$ -symmetry of the right-handed electrons one uses a single vector field B_μ . In the Lagrangian, the ordinary derivatives are replaced by the covariant derivatives

$$\begin{aligned} D_\mu &= \partial_\mu + ig \mathbf{W}_\mu, \\ D_\mu &= \partial_\mu + ie B_\mu. \end{aligned} \quad (27.58)$$

After this, one adds dynamics to the gauge fields themselves via the Lagrangian density

$$\mathcal{L}_{\text{GF}} = -\frac{1}{4} \text{tr} (\mathbf{W}_{\mu\nu} \mathbf{W}^{\mu\nu}) - \frac{1}{4} B_{\mu\nu}^2, \quad (27.59)$$

where

$$\mathbf{W}_{\mu\nu} = \partial_\mu \mathbf{W}_\nu - \partial_\nu \mathbf{W}_\mu + ig [\mathbf{W}_\mu, \mathbf{W}_\nu] \quad (27.60)$$

is the covariant curl of the $\text{SU}(2)_L$ -gauge field, and

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu \quad (27.61)$$

the usual abelian curl of the $\text{U}(1)_R$ -gauge field.

Instead of the 2×2 matrix notation (27.60), one can use the vector notation of Eq. (27.57), and write the covariant curl in (27.60) as

$$\mathbf{W}_{\mu\nu}^a = \partial_\mu \mathbf{W}_\nu^a - \partial_\nu \mathbf{W}_\mu^a - g (\mathbf{W}_\mu \times \mathbf{W}_\nu)^a. \quad (27.62)$$

The Lagrangian density (27.59) becomes

$$\mathcal{L}_{\text{GF}} = -\frac{1}{4} (\mathbf{W}_{\mu\nu}^a)^2 - \frac{1}{4} B_{\mu\nu}^2. \quad (27.63)$$

We now introduce the charged W -boson fields

$$W_\mu^\pm = \frac{1}{\sqrt{2}} (W_\mu^1 \pm iW_\mu^2), \quad (27.64)$$

and rewrite the interactions as

$$\begin{aligned} \mathcal{L}_{\text{int}} &= -g(\bar{\nu}_{eL} \bar{e}_L) \gamma^\lambda W_\lambda^a \frac{\tau_a}{2} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} - g' \bar{e}_R \gamma^\lambda B_\lambda e_R \\ &= -g(\bar{\nu}_{eL} \bar{e}_L) \gamma^\lambda \begin{pmatrix} W_\lambda^3/2 & W_\lambda^-/\sqrt{2} \\ W_\lambda^+/\sqrt{2} & -W_\lambda^3/2 \end{pmatrix} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} - g' \bar{e}_R \gamma^\lambda B_\lambda e_R. \end{aligned} \quad (27.65)$$

Actually, there is some freedom in choosing the coupling to the vector meson B_ν , since we can always absorb an equal coupling to (ν_{eL}, e_L) into the term involving the field W^3 . Hence we may choose, instead of $-g' \bar{e}_R \gamma^\lambda B_\lambda e_R$, the interaction

$$g'(\bar{\nu}_{eL}, \bar{e}_L, e_R) \gamma^\lambda Y \begin{pmatrix} \nu_{eL} \\ e_L \\ e_R \end{pmatrix}, \quad (27.66)$$

where the 3×3 -matrix Y is called the *weak hypercharge* and has the form

$$Y = \begin{pmatrix} y_L & & \\ & y_L & \\ & & y_R \end{pmatrix}. \quad (27.67)$$

The parameter y_L can be chosen at will since it can be absorbed into g , for instance

$$y_L = 1. \quad (27.68)$$

Then the interaction reads

$$\begin{aligned} \mathcal{L}_{\text{int}} &= -\frac{g}{\sqrt{2}} (W_\lambda^+ \bar{\nu}_{eL} \gamma^\lambda e_L + \text{c.c.}) \\ &\quad -\frac{1}{2} (gW^3 - g'B_\lambda) \bar{\nu}_{eL} \gamma^\lambda \nu_{eL} \\ &\quad +\frac{1}{2} (gW_\lambda^3 + g'B_\lambda) \bar{e}_L \gamma^\lambda e_L - \frac{g'}{2} y_R B_\lambda \bar{e}_R \gamma^\lambda e_R. \end{aligned} \quad (27.69)$$

Now we observe that the two fields W_λ^3 and B_λ are initially both massless and allow for arbitrary linear mixing. One combination of them remains massless after the mixing. This may be identified as the physical photon field:

$$A_\mu = \cos \theta_W B_\mu + \sin \theta_W W_\mu^3. \quad (27.70)$$

The masslessness fixes the mixing angle θ_W to satisfy

$$\sin \theta_W = \frac{g'}{\sqrt{g^2 + g'^2}}, \quad \cos \theta_W = \frac{g}{\sqrt{g^2 + g'^2}}. \quad (27.71)$$

The mixing angle θ_W is also called *weak angle* or *Weinberg angle* [9]. The orthogonal linear combination

$$Z_\mu = \sin \theta_W B_\mu - \cos \theta_W W_\mu^3 \quad (27.72)$$

has a mass

$$M_Z = \frac{v}{2} \sqrt{g^2 + g'^2}. \quad (27.73)$$

The exchange of the Z_μ -field gives rise to another contribution to the weak interactions with no charge transfer, a so-called $\Delta Q = 0$ -weak interaction.

If we choose the other coupling in (27.68) to be $y_R = -1$ and require that the photon field couples to the electron via the usual electromagnetic current density, which consists of a sum of a right-handed and left-handed part:

$$j_{\text{em}}^\mu = \bar{e}_L \gamma^\mu e_L + \bar{e}_R \gamma^\mu e_R. \quad (27.74)$$

This is possible if we set

$$e = \frac{gg'}{\sqrt{g^2 + g'^2}}, \quad (27.75)$$

and the interaction density (27.69) becomes

$$\begin{aligned} \mathcal{L}_{\text{int}} = & -\frac{g}{2\sqrt{2}} (\bar{\nu}_{eL} \gamma^\lambda e_L W_\lambda^+ + \text{c.c.}) - e j_{\text{em}}^\lambda A_\lambda \\ & - \frac{e}{2} [\tan \theta_W (2\bar{e}_R \gamma^\lambda e_R + \bar{e}_L \gamma^\lambda e_L + \bar{\nu}_{eL} \gamma^\lambda \nu_{eL}) - \cot \theta_W (\bar{e}_L \gamma^\lambda e_L - \bar{\nu}_{eL} \gamma^\lambda \nu_{eL})] Z_\mu. \end{aligned} \quad (27.76)$$

This can be decomposed into three terms: the desired contribution from the electromagnetic current (27.74), a contribution from the left-handed weak currents written as vectors in *weak isospace*

$$j_L^{\pm\mu} = \frac{1}{\sqrt{2}} (\nu_{eL} e_L) \gamma^\mu \tau^\pm \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} = \begin{Bmatrix} \bar{\nu}_{eL} \gamma^\mu e_L \\ \bar{e}_L \gamma^\mu \nu_{eL} \end{Bmatrix}, \quad (27.77)$$

$$j_L^{3\mu} = (\nu_{eL}, \bar{e}_L) \gamma^\mu \frac{\tau^3}{2} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} = \frac{1}{2} (\nu_{eL} \gamma^\mu \nu_{eL} - \bar{e}_L \gamma^\mu e_L), \quad (27.78)$$

and a contribution from the weak *neutral current*:

$$j_{\text{nc}} = j_L^3 + \sin^2 \theta_W j_{\text{em}}. \quad (27.79)$$

The total interaction (27.76) may then be written as

$$\mathcal{L}_{\text{int}} = e \left[j_{\text{em}}^\mu A_\mu - \frac{1}{\sin \theta_W} (j_+^\mu W_\mu^+ + \text{c.c.}) + \frac{1}{\sin \theta_W} j_{\text{nc}}^\mu Z_\mu \right]. \quad (27.80)$$

The weak angle θ_W parametrizes the admixture of the ordinary electric current to the neutral weak isospin current.

Up to this point, the model had been constructed at the phenomenological level by Glashow in 1961. To explain the weakness of the interaction, he had added to the Lagrangian suitable mass terms for the W and the Z meson

$$\frac{M_W^2}{2} (W^{+2} + W^{-2}) + \frac{M_Z^2}{2} Z^2, \quad (27.81)$$

choosing the value for M_W to achieve the correct weak coupling constant. At that time he did not know what value he should choose for M_Z . In this way he obtained a model which parametrized the known weak interactions, while predicting unknown neutral currents.

27.7 Masses from Meissner-Ochsenfeld-Higgs Effect

The theory constructed so far had an important drawback: It did not permit the calculation of higher-order corrections to weak interaction processes. The masses of $W^\pm$ - and Z -bosons in (27.81) gave rise to divergencies in the higher-order Feynman diagrams which could not be removed by a redefinition of couplings, masses, and field normalization. The theory was *not* renormalizable.

This defect was corrected by generating the masses m_W and m_Z by a mechanism that had been discovered in 1950 to explain the finite range of the magnetic field observed in a superconductor. It is known as the Meissner-Ochsenfeld effect discussed in Section 17.2. In contrast to the superconductor, however, the theory needed more degrees of freedom. The single complex field of the Ginzburg-Landau Lagrangian (17.9) was not sufficient. An extension was needed that contained at least a doublet of complex fields, one charged and one uncharged:

$$\varphi(x) = \begin{pmatrix} \varphi^+ \\ \varphi^0 \end{pmatrix}. \quad (27.82)$$

Their dynamics is governed by a generalization of the Ginzburg-Landau Lagrangian (17.9), the so-called *Higgs model*:

$$\mathcal{A}_{\text{se}}[\varphi, \varphi^*, A] = \int d^D x \left\{ \frac{1}{2} D_\mu^* \varphi^* D^\mu \varphi - \frac{m^2}{2} |\varphi|^2 - \frac{g}{4} |\varphi|^4 - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right\}. \quad (27.83)$$

The nongradient part involving the scalar field is now invariant under $\text{SU}_R(2) \times \text{U}_L(1)$ -rotations of the two complex fields φ^+ and φ^0 :

$$\varphi(x) \rightarrow e^{-i\alpha(x) \cdot \tau/2} \times e^{-i\gamma(x)/2} \varphi(x). \quad (27.84)$$

The gradient term $|\partial_\mu \varphi|^2$ is not invariant under (27.84), but picks up extra gradient terms of $\alpha(x)$ and $\gamma(x)$. These can be compensated by gauge fields of $\text{SU}_L(2) \times \text{U}_R(1)$ -rotations: a singlet vector field $B^\mu(x)$ for the $\text{U}_R(1)$ transformations $e^{-i\gamma(x)/2}$, and an $\text{SU}_L(2)$ -triplet vector field $\mathbf{W}^\mu(x)$ for the $\text{SU}_L(2)$ transformations $e^{-i\alpha(x) \cdot \tau/2}$. For this purpose one defines a covariant derivative

$$D_\mu \varphi(x) = \partial_\mu \varphi(x) + i \frac{g'}{2} B_\mu \varphi(x) + i \frac{g}{2} \mathbf{W}_\mu \cdot \boldsymbol{\tau} \varphi(x). \quad (27.85)$$

The extra gradients can be absorbed by the gauge transformations

$$B_\mu(x) \rightarrow B_\mu(x) + \frac{1}{ig'} e^{-i\gamma(x)/2} \partial_\mu e^{i\gamma(x)/2} = B_\mu(x) + \frac{1}{2g'} \partial_\mu \gamma(x), \quad (27.86)$$

$$\mathbf{W}_\mu(x) \rightarrow e^{-i\alpha(x)\cdot\tau/2} \mathbf{W}_\mu e^{i\alpha(x)\cdot\tau/2} + \frac{1}{ig} e^{-i\alpha(x)\cdot\tau/2} \partial_\mu e^{i\alpha(x)\cdot\tau/2}. \quad (27.87)$$

The term $F_{\mu\nu}F^{\mu\nu}$ is a gauge-invariant Lagrangian density of the gauge fields themselves. It contains the field strength of the B_μ -field and the field strength of the $\mathbf{W}_\mu$ -field

$$-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}\text{tr}(\mathbf{W}_{\mu\nu}\mathbf{W}^{\mu\nu}), \quad (27.88)$$

where $B_{\mu\nu}B^{\mu\nu}$ is the square of the ordinary curl of the vector potential $B_\mu(x)$:

$$B_{\mu\nu}(x) = \partial_\mu B_\nu(x) - \partial_\nu B_\mu(x), \quad (27.89)$$

and $\text{tr}(\mathbf{W}_{\mu\nu}\mathbf{W}^{\mu\nu})$ the nonabelian generalization of it associated with $\mathbf{W}_\mu^a(x)$ [recall (27.62)]

$$\mathbf{W}_{\mu\nu}^a(x) = \partial_\mu \mathbf{W}_\nu^a(x) - \partial_\nu \mathbf{W}_\mu^a(x) - g(\mathbf{W}_\mu(x) \times \mathbf{W}_\nu(x))^a. \quad (27.90)$$

Just as the finite penetration depth in a superconductor, nonzero masses of the vector bosons are now assumed to be the results of a nonzero expectation value of the φ -field:

$$\langle \varphi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}. \quad (27.91)$$

Allowing for a spacetime dependence of the neutral components of the φ -field by setting

$$\varphi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + \rho(x) \end{pmatrix}, \quad (27.92)$$

the Lagrangian density of the scalar field in (27.83) takes then the form

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}[\partial_\mu \rho(x)]^2 + \frac{1}{8}[v + \rho(x)]^2[g'B_\mu - gW^3]^2 + g^2(W_\mu^1 W^{1\mu} + W_\mu^2 W^{2\mu}) \\ &- \frac{m^2}{2}[v + \rho(x)]^2 - \frac{g}{8}[v + \rho(x)]^4. \end{aligned} \quad (27.93)$$

By diagonalizing the quadratic terms in the vector fields W_μ^1 and W_μ^2 , we observe the generation of a charged field

$$W^\pm = \frac{1}{\sqrt{2}}(W_\mu^1 \pm W_\mu^2) \quad (27.94)$$

of mass

$$M_W = \frac{vg}{2}. \quad (27.95)$$

The quadratic terms in the neutral field W_μ^3 and B_μ are diagonalized by the two mixed fields

$$A_\mu = \frac{1}{\sqrt{g^2 + g'^2}}(gB_\mu + g'W_\mu^3), \quad (27.96)$$

$$Z_\mu = \frac{1}{\sqrt{g^2 + g'^2}}(g'W_\mu^3 - gB_\mu). \quad (27.97)$$

These are precisely the field combinations (27.70) and (27.72) introduced by Weinberg. The first remains massless and can be identified as the photon field. The second is massive and heavier than the W -boson:

$$M_Z = \frac{v}{2}\sqrt{g^2 + g'^2} > M_W. \quad (27.98)$$

The mass of the ρ -field is determined by

$$m_\rho^2 = \frac{-2m^2}{2}. \quad (27.99)$$

This is the relation anticipated in Eq. (17.37).

27.8 Lepton Masses

Thus we have found an explanation for the masses of the vector bosons by the spontaneous breakdown of a continuous symmetry. The nonzero ground-state expectation value of a scalar field v sets the mass scale of m_W in Eq. (27.95) and of m_Z in Eq. (27.73). It is now suggestive that also the fermion masses are due a similar mechanism. Thus we assume the leptons to start life as massless fermi fields whose mass is generated by the simplest possible coupling to the scalar field via a Lagrangian density

$$\mathcal{L} = -G_e \varphi^0 (\bar{e}_R e_L + \bar{e}_L e_R) + (e \rightarrow \mu). \quad (27.100)$$

Inserting the scalar field (27.92), we see that the spontaneous breakdown gives to the initially massless electrons and muons the new masses

$$m_e = G_e v / \sqrt{2}, \quad m_\mu = G_\mu v / \sqrt{2}. \quad (27.101)$$

27.9 More Leptons

Apart from electrons and muons, more leptons have been discovered experimentally. They are listed in Table 27.1. Their weak interactions proceed in the same way as those of electrons and their neutrinos by the coupling to the vector bosons $W^\pm$ and Z^0 .

TABLE 27.1 List of leptons and their properties taken from the Particle Data Group [22].

Lepton	Charge	Mass (MeV)
ν_e	0	$< 2 \cdot 10^{-6}$
ν_μ	0	< 0.19
ν_τ	0	< 18.2
e	-1	0.510998928(11)
μ	-1	105.6583715(35)
τ	-1	1776.82 ± 0.16

27.10 Weak Interaction of Hadrons

In order to accommodate also the weak interactions of hadrons, the above Lagrangian density (27.80) is extended by a term involving the quarks

$$\begin{aligned} \mathcal{L}_{\text{int}} = & \frac{g}{2\sqrt{2}} (W_\mu^+ j_h^{\mu+} + \text{c.c.}) + e A^\mu j_\mu^{\text{em}} \\ & - \sqrt{g^2 + g'^2} Z^\mu \left(\bar{q}_L \frac{\tau_3}{2} \gamma_\mu q_L - \sin^2 \theta_W j_{\mu h}^{\text{em}} \right), \end{aligned} \quad (27.102)$$

where

$$j_h^{\mu+} = \bar{u}_L \gamma^\mu d_{\theta L}, \quad (27.103)$$

$$j_{\mu h}^{\text{em}} = \frac{2}{3} \bar{u} \gamma_\mu u - \frac{1}{3} (\bar{d} \gamma_\mu d + \bar{s} \gamma_\mu s). \quad (27.104)$$

with

$$d_\theta = d \cos \theta_c + s \sin \theta_c. \quad (27.105)$$

When the theory arrived at this stage it was realized that it contained an unpleasant contradiction with experiments. The neutral vector meson Z was coupled to a quark current

$$\begin{aligned} \bar{q}_L \gamma^\mu \tau_3 q_L = & \bar{u}_L \gamma^\mu u_L - \cos^2 \theta_c \bar{d}_L \gamma^\mu d_L, \\ & - i \sin \theta_c \cos \theta_c (\bar{d}_L \gamma^\mu s_L + \bar{s}_L \gamma^\mu d_c) - i \sin^2 \theta_c \bar{q}_L \gamma^\mu c_L. \end{aligned} \quad (27.106)$$

The third term changed the strangeness by one unit. However, processes with a strangeness-changing neutral current were known to be strongly suppressed in nature. Otherwise one would have observed particle decays

$$\begin{aligned} K^\pm & \rightarrow \pi^\pm \nu \bar{\nu}, \\ K^0 & \rightarrow \mu^+ \mu^-, \end{aligned} \quad (27.107)$$

with a much larger branching ratio than the experimentally observed 6×10^{-7} , 10^{-8} , respectively (see Fig. 27.1).

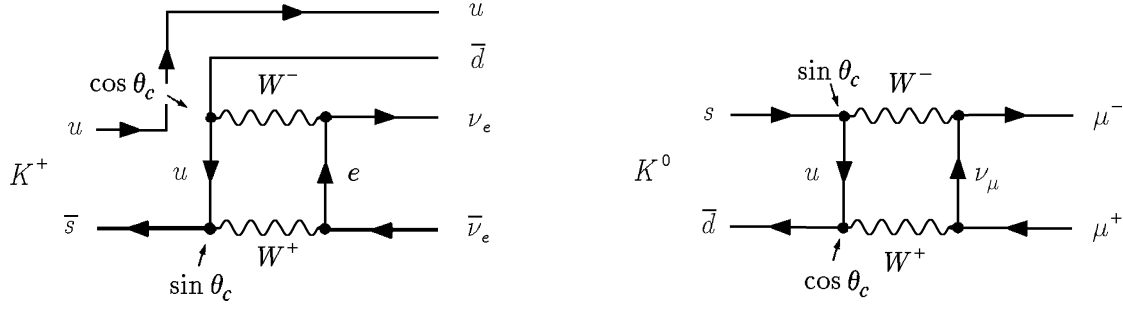


FIGURE 27.1 Quark diagrams for K^+ and K^0 decays involving strangeness changing neutral currents.

In order to achieve the desired suppression, Glashow, Iliopoulos, and Maiani [12] postulated the existence of a further quark, called *charmed* quark, denoted by c , which was supposed to form a weak isodoublet with s in the same way as u does with d . Then they considered the two doublets

$$\begin{pmatrix} u \\ d_\theta \end{pmatrix}_L, \begin{pmatrix} c \\ s_\theta \end{pmatrix}_L \quad (27.108)$$

with

$$s_\theta = -u \sin \theta_c + s \cos \theta_c \quad (27.109)$$

as two families of the same sort, both with weak hypercharge $1/3$, and wrote the left-handed neutral current as

$$(\bar{u}, \bar{d}_\theta) \frac{\tau_3}{2} \gamma^\mu \begin{pmatrix} u \\ d_\theta \end{pmatrix}_L + (\bar{c}, \bar{s}_\theta) \frac{\tau_2}{2} \gamma^\mu \begin{pmatrix} c \\ s_\theta \end{pmatrix}_L - i \sin^2 \theta_W j_{\text{em}}^\mu. \quad (27.110)$$

After this, the strangeness changing currents cancel exactly. The cancellation in the K^0 decays goes as follows. Take, for instance the decay $K^0 \rightarrow \mu^+ \mu^-$. The compensating diagrams are shown in Fig. 27.2.

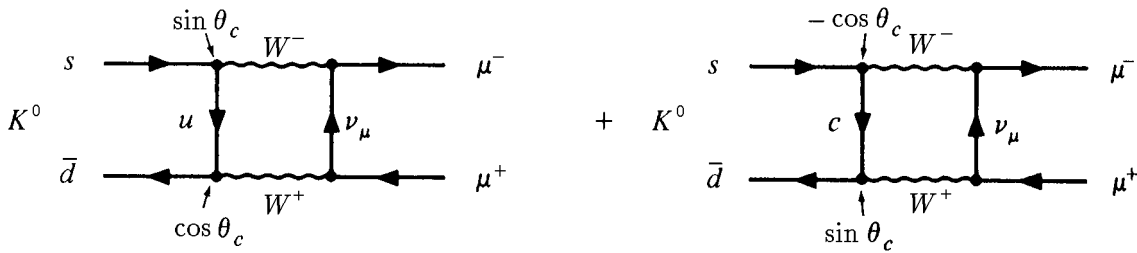


FIGURE 27.2 Diagrams for the $K^0 \rightarrow \mu^+ \mu^-$ decay with compensating strangeness-changing neutral currents.

In addition to the previous electromagnetic current (27.104), the charmed quark contributes an extra term

$$\Delta j_{\mu h}^{\text{em}} = \frac{2}{3} \bar{c} \gamma^\mu c. \quad (27.111)$$

The cancellation of the strangeness-changing neutral currents in weak interactions is named after the authors [12] as GIM mechanism. The GIM mechanism needed in the space of all leptons to suppress the strangeness-changing neutral currents is discussed in Ref. [23].

27.11 Quantum Oscillations

The standard model of weak interactions explains some interesting novel phenomena in particle physics. The nature of a fundamental particle is sometimes not fixed but can oscillate as a function of time. The first particles, where this phenomenon was observed, was the system of neutral kaons, where the K -mesons K^0 and $\bar{K}^0$ oscillate between each other.

27.11.1 Oscillations between Neutral Kaons

In our discussion of the $SU(3)$ -symmetry of strong interactions in Section 24.4, we mentioned that the mesons K^0 and $\bar{K}^0$ have strangeness -1 and $+1$, respectively. It is believed that strong interactions strictly conserve these quantum numbers. The weak interactions described by the standard model, however, conserve the symmetry CP . If we want to describe the weak decay of the strongly produced K^0 and $\bar{K}^0$ mesons, we must decompose them into eigenstates of CP . These are the states

$$|K_1^0\rangle \equiv \frac{1}{\sqrt{2}} (|K^0\rangle + |\bar{K}^0\rangle), \quad |K_2^0\rangle \equiv \frac{1}{\sqrt{2}} (|K^0\rangle - |\bar{K}^0\rangle). \quad (27.112)$$

They have different decay channels. At rest, the first state is even under CP (recall Subsections 7.1.6 and 7.1.6), the second is odd. Hence the first state can decay into two pions, while the second cannot. The lifetime of K_1^0 is $0.8922 \pm 0.0020 \times 10^{-10}$ sec, producing almost exclusively $\pi^+ \pi^-$ and $\pi^0 \pi^0$ at a ratio 2:1.

The CP -odd state K_2^0 must at least decay into three pions and has therefore a much longer lifetime. This is why K_1^0 and K_2^0 are also called K_S^0 and K_L^0 .

Let m_S , m_L be their masses and Γ_S , Γ_L their decay rates. A beam of K^0 produced in a strong-interaction process will then evolve in its rest frame as an oscillating superposition of K_S and K_L :

$$|K^0\rangle = \frac{1}{\sqrt{2}} \left[e^{-(im_S + \Gamma_S/2)\tau} |K_S\rangle + e^{-(im_L + \Gamma_L/2)\tau} |K_L\rangle \right], \quad (27.113)$$

where τ is the proper time. Since the two components decay at a different rate, the beam will contain oscillating admixtures of $\bar{K}^0$. These can be detected if the beam is directed towards a strongly interacting target, say a slab of copper. In it the forward scattering amplitude for K^0 is smaller than for $\bar{K}^0$. Thus, if one changes the thickness of the slab, the outgoing beam will have different admixtures of the short-lived component K_S^0 . In this way, one is able to regenerate K_S^0 from a beam which had turned almost completely into K_L^0 by the decay into $\pi^+ \pi^-$ or $\pi^0 \pi^0$.

The process was analyzed in 1957 [14], and the experiment showed clearly the regeneration effect [15, 16].

When experimentalists tried to set an upper limit to the decay of K_L^0 into two pions they found that this decay was not completely forbidden [17]. This implied that the weak decay of K^0 -mesons contains a small term violating CP -symmetry. Thus the correct mixtures of short- and long-lived K^0 mesons should really be slightly different from (27.112):

$$|K_S^0\rangle \equiv \frac{1}{\sqrt{2(1+\epsilon^2)}} \left[(1+\epsilon)|K^0\rangle + (1-\epsilon)|\bar{K}^0\rangle \right], \quad (27.114)$$

$$|K_L^0\rangle \equiv \frac{1}{\sqrt{2(1+\epsilon^2)}} \left[(1-\epsilon)|K^0\rangle - (1+\epsilon)|\bar{K}^0\rangle \right], \quad (27.115)$$

where ϵ is of the order of 10^{-3} .

The parameter ϵ can be measured by studying a beam of K^0 as a function of time. Due to the decay of the K_S^0 content, the beam is expected to perform a damped oscillation from $K^0 = d\bar{s}$ to $\bar{K}^0 = s\bar{d}$, and back. The content of the two components can be studied by looking at the decay rates $K^0 \rightarrow \pi^\mp e^\pm \nu_e$ and $\bar{K}^0 \rightarrow \pi^\mp e^\pm \nu_e$ arising from the decay of the quarks $\bar{s}$ and s , respectively, in accordance with the $\Delta Q = \Delta S$ rule. This permits measuring ϵ directly from the asymmetry

$$\frac{N_{K^0} - N_{\bar{K}^0}}{N_{K^0} + N_{\bar{K}^0}} = \frac{N_{\pi^-} - N_{\pi^+}}{N_{\pi^-} + N_{\pi^+}} = \frac{N_{e^+} - N_{e^-}}{N_{e^+} + N_{e^-}} = \frac{2\text{Re}\epsilon}{1+|\epsilon|^2} \equiv (3.320 \pm 0.074) \times 10^{-3}. \quad (27.116)$$

Thanks to CP -violation, not only K_S^0 but also K_L^0 decays into two pions, and this makes it possible to observe oscillations in the decay of a K^0 -beam into $\pi^+ \pi^-$. The ratio of the decay rates changes as a function of the proper time τ as follows:

$$I_{\pi^+\pi^-}(\tau) = \frac{|\langle \pi^+\pi^- | K^0(\tau) \rangle|}{|\langle \pi^+\pi^- | K_S^0(\tau) \rangle|} = e^{-\Gamma_S \tau} + 2|\eta_{+-}| e^{-(\Gamma_S + \Gamma_L)\tau/2} \cos(\Delta m \tau - \phi_{+-}) + |\eta_{+-}|^2 e^{-\Gamma_L \tau}, \quad (27.117)$$

where

$$\eta_{+-} \equiv |\eta_{+-}| e^{i\phi_{+-}} = \frac{|\langle \pi^+\pi^- | K_L^0(\tau) \rangle|}{|\langle \pi^+\pi^- | K_S^0(\tau) \rangle|}, \quad \Delta m \equiv m_L - m_S. \quad (27.118)$$

This damped oscillation was indeed observed experimentally [18], as shown in Fig. 27.3.

A best fit to the data yields the parameters

$$\tau_S = 1/\Gamma_S = (0.8926 \pm 0.0012) \times 10^{-8} \text{ sec}, \quad (27.119)$$

$$\tau_L = 1/\Gamma_L = (5.17 \pm 0.04) \times 10^{-8} \text{ sec}, \quad (27.120)$$

$$\Delta m = (0.5333 \pm 0.0027) \times 10^{10} \hbar/\text{sec}, \quad (27.121)$$

$$|\eta_{+-}| = (2.269 \pm 0.023) \times 10^{-3} \approx |\epsilon| \quad (27.122)$$

$$\phi_{+-} = (44.3 \pm 0.8)^\circ. \quad (27.123)$$

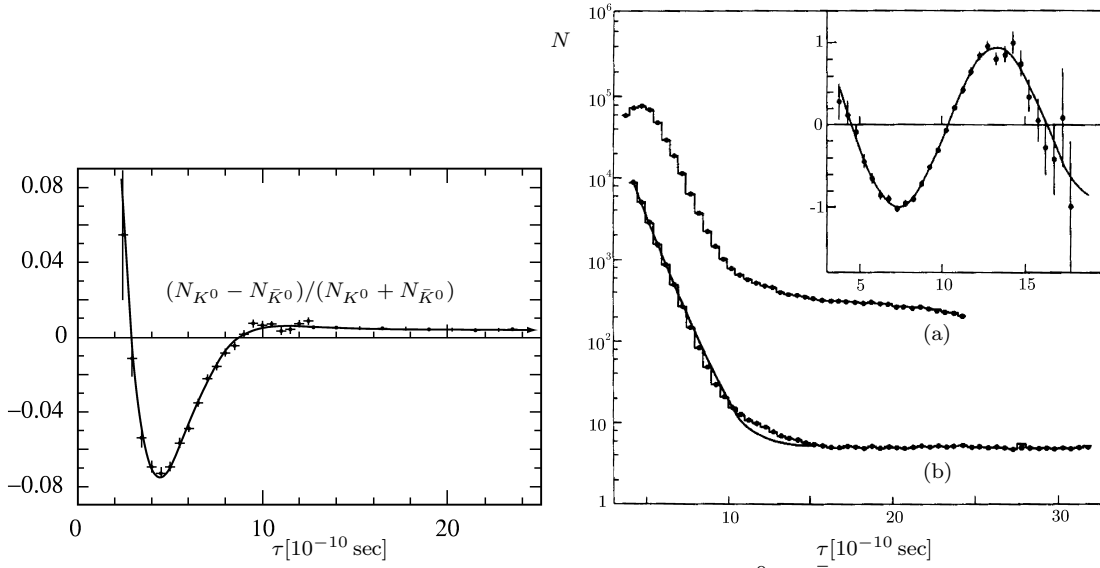


FIGURE 27.3 Left-hand: Asymmetry of the number of $K^0 = \bar{d}s$ mesons with respect to the $\bar{K}^0 = s\bar{d}$ mesons as a function of time [19]. The asymmetry is measured by the ratio of the decays $K^0 \rightarrow \pi^\mp e^\pm \nu_e$ $\bar{K}^0 \rightarrow \pi^\mp e^\pm \nu_e$. After a long time, only K_L^0 survives which does not have an equal content of K^0 and $\bar{K}^0$ as a signal of CP -violation. Right-hand: Oscillation in the decay rate into $\pi^+ \pi^-$ of the K^0 -beam. Curve (a) shows the histogram of the raw data. Curve (b) shows the theoretical decay curve without oscillations, and the insert shows the best fit to the oscillations if the nonoscillating background is subtracted (figure from [18]).

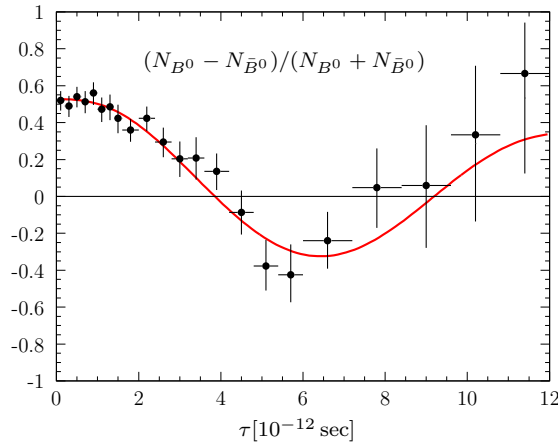


FIGURE 27.4 Asymmetry of the number of $B_d^0 = \bar{d}\bar{b}$ mesons with respect to the $\bar{B}_d^0 = b\bar{d}$ mesons as a function of time [19]. Here the long- and short-lived combinations have almost the same lifetime.

27.11.2 Mesons containing the Bottom Quark

By analogy with the strange mesons K^0 and $\bar{K}^0$ there exist neutral mesons $B_d^0 = d\bar{b}$ and $\bar{B}_d^0 = b\bar{d}$. The masses of their short-lived combination is $m_s = 5721$ MeV which oscillated with the long-lived combination of mass $m_s = 5747$ MeV. For these mesons, the asymmetry measurement yields (see Fig. 27.4) [20]:

$$\frac{N_{B_d^0} - N_{\bar{B}_d^0}}{N_{B_d^0} + N_{\bar{B}_d^0}} = \frac{N_{\pi^-} - N_{\pi^+}}{N_{\pi^-} + N_{\pi^+}} = \frac{N_{e^+} - N_{e^-}}{N_{e^+} + N_{e^-}} = \frac{2\text{Re } \epsilon_{B_d}}{1 + |\epsilon_{B_d}|^2} \equiv (0.0035 \pm 0.0103 \pm 0.0015). \quad (27.124)$$

Similar asymmetries can be observed for $B_s^0 = s\bar{b}$ and $\bar{B}_s^0 = b\bar{s}$.

All such neutral particle mixings can simply be understood by assuming that the Lagrangian density for these particles contains a nondiagonal mass matrix

$$\mathcal{M} = \begin{pmatrix} M_{11} - \frac{i}{2}\Gamma_{11} & M_{12} - \frac{i}{2}\Gamma_{12} \\ M_{21} - \frac{i}{2}\Gamma_{21} & M_{22} - \frac{i}{2}\Gamma_{22} \end{pmatrix}. \quad (27.125)$$

This matrix must be Hermitian, implying that

$$M_{21} = M_{12}^*, \quad \Gamma_{21} = \Gamma_{12}^*. \quad (27.126)$$

Moreover, as a consequence of CPT -invariance, the diagonal elements must satisfy

$$M_{11} = M_{22} = M, \quad \Gamma_{11} = \Gamma_{22} = \Gamma. \quad (27.127)$$

The most general mass matrix is therefore

$$\mathcal{M} = \begin{pmatrix} M - \frac{i}{2}\Gamma & M_{12} - \frac{i}{2}\Gamma_{12} \\ M_{12}^* - \frac{i}{2}\Gamma_{12}^* & M - \frac{i}{2}\Gamma \end{pmatrix}. \quad (27.128)$$

27.11.3 General Flavor Mixing

The Cabibbo theory was set up at a time when only the three quarks u, d, s were known. After the discovery of the heavier three quarks it turned out that all quarks can be grouped into three families of charge $2/3$ and $-1/3$, respectively, and that the weak current (27.43) has the generalization

$$(u, c, t) \gamma^\lambda (1 - \gamma_5) \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}. \quad (27.129)$$

The 3×3 -matrix V is called CKM-matrix, after the initials of the authors Cabibbo, Kobayashi, and Maskawa [7, 13]. It is often expressed in terms of four angles $\theta_{12}, \theta_{13}, \theta_{23}$, and δ_{13} as

$$V = \begin{pmatrix} c_{12} c_{13} & s_{12} c_{13} & s_{13} e^{-i\delta_{13}} \\ -s_{12} c_{23} - c_{12} s_{23} s_{13} e^{i\delta_{13}} & c_{12} c_{23} - s_{12} s_{23} s_{13} e^{i\delta_{13}} & s_{23} c_{13} \\ s_{12} s_{23} - c_{12} c_{23} s_{13} e^{i\delta_{13}} & -c_{12} s_{23} - s_{12} c_{23} s_{13} e^{i\delta_{13}} & c_{23} c_{13} \end{pmatrix}, \quad (27.130)$$

where $s_{12} \equiv \sin\theta_{12}$, $c_{12} \equiv \cos\theta_{12}$. The angle δ_{13} serves to explain the small CP -violation observed in the decay of K_L^0 discussed in the previous subsection. The mixing matrix is permanently updated whenever new experimental data are available. The presently used numbers are [21]:

$$V = \begin{pmatrix} 0.974 \text{ to } 0.9756 & 0.219 \text{ to } 0.226 & 0.0025 \text{ to } 0.0048 \\ 0.219 \text{ to } 0.226 & 0.9732 \text{ to } 0.9748 & 0.038 \text{ to } 0.044 \\ 0.004 \text{ to } 0.014 & 0.037 \text{ to } 0.044 & 0.9990 \text{ to } 0.9993 \end{pmatrix}. \quad (27.131)$$

The most precise constraints on the size of the elements of the CKM-matrix are extracted from the low-energy $s \rightarrow u$ and $d \rightarrow u$ semileptonic transitions. The determination is a specialized part of phenomenological particle physics, on which excellent reviews are available from the Particle Data Group [13].

27.12 Neutrino Mixing

By analogy with the flavor mixing matrix V for quarks in Eq. (27.129), there exists a mixing matrix for the three neutrinos ν_e, ν_μ, ν_τ . It is known as the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix which transforms three bare neutrinos ν_1, ν_2, ν_3 into the physical particles:

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = U \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix} = \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu1} & U_{\mu2} & U_{\mu3} \\ U_{\tau1} & U_{\tau2} & U_{\tau3} \end{pmatrix} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}. \quad (27.132)$$

The matrix U is parametrized in terms of angles in the same way as the matrix V in (27.130), and the best determination at present yields [24]

$$U = \begin{pmatrix} 0.82 \pm 0.01 & 0.54 \pm 0.02 & 0.15 \pm 0.03 \\ 0.35 \pm 0.06 & 0.70 \pm 0.06 & 0.62 \pm 0.06 \\ 0.44 \pm 0.06 & 0.45 \pm 0.06 & 0.77 \pm 0.06 \end{pmatrix}. \quad (27.133)$$

Neutrino flavor mixing is a cause for the notorious detection problem of solar neutrinos [25]. It is also the source of the so-called atmospheric neutrino anomaly [26].

The neutrino masses are too small to be experimentally measurable. What is measurable is the mass difference between the neutrinos associated with the electron and the muon. This is done by counting the number of times by which electron neutrinos are transformed into muon neutrinos and back on their way from the sun to us.

An alternative possibility to measure small mass differences comes from recent observations of the time modulation of two-body weak decays of heavy ions. This reveals the mass content of the electron neutrinos via interference patterns in the recoiling ion wave function. From the modulation period one derives the difference of the square masses $\Delta m^2 \approx 22.5 \times 10^{-5} \text{ eV}^2$, which is about 2.8 times larger than

that derived from a combined analysis of KamLAND and solar neutrino oscillation experiments. It is, however, compatible with a data regime to which the KamLAND analysis attributes a smaller probability.

At the GSI in Darmstadt, Germany, the experimental storage ring ESR permits observing completely ionized heavy atoms I or hydrogen-like heavy ions I_H over a long time [27, 28] and thus to measure the time dependence of their weak two-body decays $I_H \rightarrow I + \nu_e$ or $I \rightarrow I_H + \bar{\nu}_e$. The first decay is due to the well-known electron-capture (EC) process. In the second an electron comes out of the nucleus together with an antineutrino, and the electron remains in an orbit. The virtue of such experiments is that the properties of the neutrino or antineutrino can be deduced from the time dependence of the transition, by observing only the initial and final ions. The special efficiency of these experiments becomes clear in the Dirac sea interpretation of the second process, where the initial ion simply absorbs a negative-energy antineutrino in the vacuum. Since the vacuum has *all* negative-energy states filled, the vacuum is a source of negative-energy neutrinos of *maximally possible* current density, i.e., the best possible neutrino source in the universe. This is why the ESR experiments yield information on neutrino properties with great precision even if the targets and exposure times are quite small, in particular much smaller than the 2.44×10^{32} proton-yrs (2881 ton-yrs) in the famous KamLAND experiments [29], which are only sensitive to the much less abundant positive-energy neutrinos produced by nuclear reactors.

27.13 Simple Theory of Two-Neutrino Mixing

To illustrate this we consider here the small mass difference of the two lightest neutrinos. According to Pontecorvo [30, 31], the Dirac fields of the physical electron and muon-neutrinos $\nu_f = (\nu_e, \nu_\mu)$, the so-called *flavor fields*, are superpositions of neutrino fields $\nu_i(x) = (\nu_1(x), \nu_2(x))$ of masses m_1 and m_2 :

$$\nu_e(x) = \nu_1(x) \cos \theta + \nu_2(x) \sin \theta, \quad \nu_\mu(x) = -\nu_1(x) \sin \theta + \nu_2(x) \cos \theta. \quad (27.134)$$

Here θ is a mixing angle. The free Dirac action has the form

$$\mathcal{A} = \sum_f \int d^4x \bar{\nu}_f(x) (i\gamma^\mu \partial_\mu - \mathcal{M}) \nu_f(x), \quad (27.135)$$

where γ^μ are the Dirac matrices, and $\mathcal{M}$ is a mass matrix, whose diagonal and off-diagonal elements are $m_f = (m_e, m_\mu)$ and $m_{e\mu} = m_{\mu e}$, respectively. The eigenvalues $m_i = (m_1, m_2)$ are related to m_f by [30, 31, 32, 33],

$$\begin{aligned} m_e &= m_1 \cos^2 \theta + m_2 \sin^2 \theta, & m_\mu &= m_1 \sin^2 \theta + m_2 \cos^2 \theta, \\ m_{e\mu} &= m_{\mu e} = (m_2 - m_1) \sin \theta \cos \theta. \end{aligned} \quad (27.136)$$

The weak transition between the electron e and its neutrino ν_e is governed by the interaction

$$\mathcal{A}_{\text{int}} = \frac{g}{\sqrt{2}} \int d^4x W_\mu^-(x) J^{+\mu}(x) + \text{h.c.} \equiv \frac{g}{\sqrt{2}} \int d^4x W_\mu^-(x) \bar{e}(x) \gamma^\mu (1 - \gamma_5) \nu_e(x) + \text{h.c.}, \quad (27.137)$$

where γ_5 is the product of Dirac matrices $i\gamma^0\gamma^1\gamma^2\gamma^3$.

Since the interaction (27.137) involves only two flavor fields in (27.134), the states of masses m_i will always be produced as coherent superpositions. The weakness of the interaction allows us to calculate the shape of the mixed wave packet from perturbation theory. Consider the decay $I \rightarrow I_H + \bar{\nu}_e$ which is a superposition of the states of masses m_1 and m_2 . Let us write down formulas which are applicable for electron capture and, after the interchange of M_H with the mass M of the bare ion, treats the case of outgoing neutrinos. In the center-of-mass (CM) frame of the initial bare ion of mass M , the final H -like ion has the same momentum as the antineutrino $\bar{\nu}_i$ ($i = 1, 2$), whose energy is $\omega_i \equiv \omega_{\mathbf{k},i} = \sqrt{\mathbf{k}_i^2 + m_i^2}$ determined by

$$M \equiv M_H + Q = \omega_i + \sqrt{M_H^2 + \mathbf{k}_i^2} = \omega_i + \sqrt{M_H^2 + \omega_i^2 - m_i^2}, \quad i = 1, 2, \quad (27.138)$$

so that $\omega_i = [(2M_H + Q)Q + m_i^2]/2(M_H + Q)$. Subtracting ω_2 and ω_1 from each other we find the energy difference

$$\Delta\omega \equiv \omega_2 - \omega_1 = \frac{m_2^2 - m_1^2}{2M} \equiv \frac{\Delta m^2}{2M}. \quad (27.139)$$

The denominator M is of the order of 100 GeV and much larger than Δm^2 , so that $\Delta\omega$ is extremely small. It is the difference of the recoil energies transferred to the outgoing ion by the antineutrinos of masses m_1 and m_2 . Without recoil, we would have found an energy difference at the *same* momentum which is four orders of magnitude larger than that, namely

$$\Delta\omega_{\mathbf{k}} = \omega_{\mathbf{k},2} - \omega_{\mathbf{k},1} = (\Delta m^2 + \omega_{\mathbf{k},1}^2)^{1/2} - \omega_{\mathbf{k},1} \approx \Delta m^2/2\omega_{\mathbf{k},1} \approx \Delta m^2/2Q. \quad (27.140)$$

This is the frequency with which the incoming negative-energy neutrino current of momentum $\mathbf{k}$ oscillates in the vacuum. Note that although $\Delta\omega$ is small, the momentum difference $\Delta k \equiv k_2 - k_1$ associated with the energies $\omega_{1,2}$ is as large as $\Delta\omega_{\mathbf{k}}$, but has the opposite sign.

27.14 Experiments

The best experimental results are available for the EC-processes reported in Ref. [27], where an electron is captured from the K-shell and converted into an electron-neutrino which runs off to infinity. On the average, the decay is exponential with a rate expected from a standard-model calculation. In addition, however, the rate shows oscillations with a frequency $\Delta\omega$. The experimental results are [34]

$$^{140}_{59}\text{Pr}^{58+} \rightarrow ^{140}_{58}\text{Ce}^{58+} : \quad \Delta\omega \approx 0.890(11) \text{ sec}^{-1} \quad (Q = 3\,386 \text{ keV}), \quad (27.141)$$

$$^{142}_{61}\text{Pm}^{60+} \rightarrow ^{142}_{60}\text{Nd}^{60+} : \quad \Delta\omega \approx 0.885(31) \text{ sec}^{-1} \quad (Q = 4\,470 \text{ keV}). \quad (27.142)$$

In both cases the period of oscillations is roughly 7 sec, and it scales with M (see Fig. 27.5).

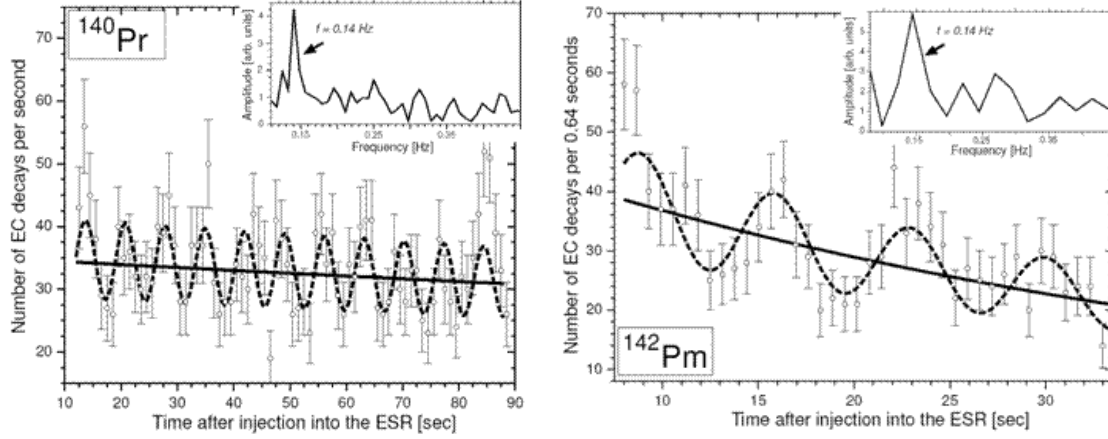


FIGURE 27.5 Oscillations of decay rate for the processes (27.141) and (27.142). The period is in both cases roughly 7 sec. The inserts show the frequency analyses. Plots are from Ref. [27].

We expect these oscillations to be associated with the frequency $\Delta\omega$ determined by Eq. (27.139), and thus to give information on Δm^2 . Inserting the experimental numbers for $\Delta\omega$ into Eq. (27.139) and taking into account that the particles in the storage ring run around with 71% of the light velocity with a Lorentz factor $\gamma \approx 1.43$, we find from the two processes [35]

$$\Delta m^2 \approx 22.5 \times 10^{-5} \text{ eV}^2. \quad (27.143)$$

This is by a factor ≈ 2.8 larger than the result $\Delta m^2 \approx 7.58_{-0.3}^{+0.3} \times 10^{-5} \text{ eV}^2$ favored by the KamLAND experiment [29, 37, 38], but it lies close to their less favored result [36], which the authors excluded by 2.2σ in 2005, now by 6σ [29] (see Fig. 27.6).

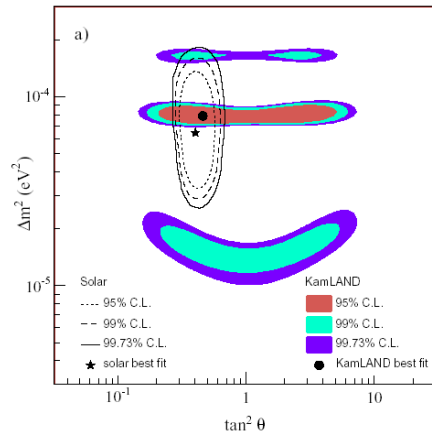


FIGURE 27.6 The upper KamLAND regime of 2006 [36] is compatible with the result $\Delta m^2 \approx 22.5 \times 10^{-5} \text{ eV}^2$.

So far, the origin of this discrepancy is unclear. One explanation has been attempted in Ref. [39] where the authors investigate the influence of the strong Coulomb field around the ion upon the process. We refer the reader to recent discussions of this question [41].

27.15 Entangled Wavefunction

It is easy to describe theoretically the oscillations in Fig. 27.5. Consider the decay of the initial ion I into the ion I_H plus an electron-antineutrino $\bar{\nu}_e$. Ignoring all spins and the finite size of the ions, the effective interaction for this process is

$$\mathcal{A}_{\text{int}} = \int d^4x I_H^\dagger(x) \bar{\nu}_e^\dagger(x) I(x) = \int d^4x \left[\cos \theta I_H^\dagger(x) \bar{\nu}_1^\dagger(x) I(x) + \sin \theta I_H^\dagger(x) \bar{\nu}_2^\dagger(x) I(x) \right], \quad (27.144)$$

where $I(x)$, $\bar{\nu}_e(x)$, and $I_H(x)$ are the field operators of the involved particles. In the CM frame, the initial ion is at rest, while the final moves nonrelativistically. The outgoing wave is spherical. The role of the antineutrinos $\bar{\nu}_1$ and $\bar{\nu}_2$ is simply to create a coherent superposition of two such waves with the two different radial momenta k and associated frequencies ω whose difference was calculated in (27.143):

$$\langle \mathbf{x} | \psi^{(+)}; t \rangle \equiv -\frac{g}{r} \left[\cos \theta e^{i(k_1 r - \omega_1 t)} + \sin \theta e^{i(k_2 r - \omega_2 t)} \right]. \quad (27.145)$$

The resulting wave carries a radial current density of ions I_H :

$$j_r = \frac{g^2}{M_H r^2} \left[\cos^2 \theta k_1 + \sin^2 \theta k_2 + \sin \theta \cos \theta (k_1 + k_2) \cos(\Delta k r - \Delta \omega t) \right]. \quad (27.146)$$

In order to find the decay rate we integrate this over a sphere of radius R surrounding the initial ion. We can choose R any size $\ll 1/\Delta k \approx 10^4$ m. From this surface we find the outgoing probability current density

$$\dot{P} = 4\pi g^2 \frac{\bar{k}}{M} [1 + \sin(2\theta) \cos(\Delta \omega t)], \quad (27.147)$$

where we have approximated k_1 and k_2 by their average $\bar{k}$. This $\dot{P}$ explains directly the observed oscillating decay rate of the initial ions.

A comment is in place on several recent publications [42, 43, 44, 45, 46, 47]. These deny a relation between neutrino oscillations and the nonexponential decay seen in the GSI experiment for various reasons. In Ref. [42], the basic argument is that the antineutrino oscillations set in *after* their emission, so that they cannot be observed in the GSI experiment. The present discussion shows that this argument is true, although it fails to give the correct explanation of the data [48]. Indeed, the GSI data do *not* care about the neutrino oscillations while they propagate away from the decay center. The neutrinos merely serve to give the ion a coherent kick of two different momenta and energies. What is measured are the resulting oscillations of the ion wave function caused by this kick.

It is noteworthy that this analysis, in which we extract the properties of the unobserved antineutrino from the behavior of the ion, corresponds precisely to the usual entanglement analysis of decay processes, such as $\pi^0 \rightarrow \gamma + \gamma$. There the measurement of the polarization of *one* photon tells us immediately the polarization properties of the other, unobserved photon.

Let us finally remind the reader of the similarities of these neutrino oscillations with similar oscillation phenomena in associate production processes of particles, where they appear together with an oscillating partner. These have been proposed and controversially discussed before by many authors. See Subsection 27.11.1, where Λ -hyperons are produced together with neutral Kaons [49]. Or the mixing arising in the production of neutral mesons containing a bottom quark discussed in Subsection 27.11.2. Or the production of μ^- -particles together with antineutrinos in the decay $\pi^- \rightarrow \mu^- + \bar{\nu}_e$ [50]. The presently-discussed data provide us with the most definite experimental confirmation of such a phenomenon.

We refer the reader to the many interesting ideas presented in other publications [44, 45, 46, 47].

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*A little more moderation would be good.
Of course, my life hasn't exactly been one of moderation.*
DONALD TRUMP (1946)

28

Nonabelian Gauge Theory of Strong Interactions

Elementary particles which interact strongly with each other are called *hadrons* (recall the classification in Section 24.1). According to their statistics, one distinguishes baryons and mesons. The most prominent among these are the spin-1/2 particles in nuclear matter, protons and neutrons. The forces between them arise, to lowest approximation, from the exchange of a spin-0 meson called pion, and further mesons (middle-heavy particles).

Hadrons exhibit rich mass spectra, as we have seen in Chapters 24 and 25. These spectra were explained to a good approximation by *quark models* [1]. Just as nuclei are composed of protons and neutrons, baryons are composed of three quarks, mesons of quarks-antiquarks pairs [2].

28.1 Local Color Symmetry

In spite of its success, the initial quark model exhibited several fundamental inconsistencies. Most importantly, it was not compatible with the spin-statistics theorem derived in Section 7.10. For any reasonable potential between quarks, the ground state orbital wave function should always be without zeros implying vanishing relative angular momenta for each pair of quarks. Any higher angular momentum would have at least one zero in the wave function which would increase the gradient and thus the kinetic energy of the Schrödinger field via the centrifugal barrier. The orbital wave function of the ground state of three quarks, the proton, must therefore be symmetric under the exchange of two quarks. On the other hand, the SU(6) wave function involving internal SU(3) and spin has the Yang tableau $\square\square\square$. But this implies that the nucleon wave function is completely symmetric under exchange of all positions, all SU(3), and all spin variables. This seems to contradict the fact that quarks have spin 1/2 so that, by the spin-statistics theorem, they should be fermions and therefore have a completely antisymmetric wave function.

To remedy this contradiction, Han and Nambu suggested that quarks should be a triplet under a further SU(3) group of transformations now called color SU(3) [3]. Color appears as a further label to the quark fields:

$$q(x) = \begin{pmatrix} u(x) \\ d(x) \\ s(x) \\ c(x) \\ t(x) \\ b(x) \end{pmatrix}, \quad (28.1)$$

which may thus be written as

$$q_\alpha(x) = \begin{pmatrix} u_\alpha(x) \\ d_\alpha(x) \\ s_\alpha(x) \\ c_\alpha(x) \\ t_\alpha(x) \\ b_\alpha(x) \end{pmatrix}, \quad (28.2)$$

with a label $\alpha = 1, 2, 3$ specifying the three colors. By postulating that all hadron states are completely antisymmetric in the color indices, so that they are color singlet states, the contradiction disappears and the spin-statistic relation is again valid.

After this somewhat artificial postulate the question arose how nature manages to enforce the color antisymmetry, i.e., how it prevents color non-singlet states to be excited. The answer suggested by Fritzsch and Gell-Mann was that color SU(3) was a local gauge symmetry of hadronic physics. The action had to be invariant under arbitrary nonabelian SU(3)-transformations of the quark fields

$$q(x) \rightarrow e^{-i\alpha^a(x)\lambda^a/2} q(x), \quad (28.3)$$

where the matrices λ^a now act on the three color labels of the quark field $q(x)$ in SU(3). The tripling of the quarks saved not only the validity of the spin-statistics relation for quarks. It also led to the correct rate of the particle decay

$$\pi^0 \rightarrow \gamma\gamma$$

which is observed experimentally at a rate $\Gamma = 8.4 \times 10^{-17}\text{s}$. In addition, it gave the correct total interaction cross section observed in $e^+ e^-$ collisions, which require that each quark occurs in three color versions.

Once it was postulated that the quark action is invariant under local symmetry transformations, it became necessary to introduce a gauge field to maintain the invariance of the gradient term in the action. This led to the quark Lagrangian

$$\mathcal{L}(x) = \bar{q}(x)i\not{D} q(x) - M\bar{q}(x)q(x) \quad (28.4)$$

where $q(x)$ carries flavor indices distinguishing the quarks $u, d, c, s, \dots$ and three color indices. The gradient term contains the covariant derivative

$$\not{D} = \gamma^\mu D_\mu = \gamma^\mu (\partial_\mu + igA_\mu), \quad (28.5)$$

where A_μ is a 3×3 matrix in color space to guarantee that D_μ transforms under local color SU(3) transformations in the same way as the field $\psi(x)$ itself:

$$D_\mu q(x) \rightarrow U(x) D_\mu q(x) = e^{-i\alpha_a(x)\lambda^a/2} D_\mu q(x). \quad (28.6)$$

The covariance property is a bit harder to show than in electromagnetism. The derivative of the field goes over into:

$$\begin{aligned} \partial_\mu q(x) &\rightarrow \partial_\mu U(x) q(x) = U(x) [U^{-1}(x) \partial_\mu U(x) q(x)] \\ &= U(x) \partial_\mu q(x) + U(x) [U^{-1}(x) \partial_\mu U(x)] q(x). \end{aligned} \quad (28.7)$$

In order to remove the second term, the gauge field A_μ has to transform like

$$\begin{aligned} A_\mu(x) &\rightarrow U(x) A_\mu(x) U^{-1}(x) - \frac{1}{ig} [\partial_\mu U(x)] U^{-1}(x) \\ &= U(x) A_\mu(x) U^{-1}(x) + \frac{1}{ig} U(x) \partial_\mu U^{-1}(x). \end{aligned} \quad (28.8)$$

Then

$$\begin{aligned} [\partial_\mu + igA_\mu(x)] q(x) &\rightarrow U(x) [\partial_\mu + igA_\mu(x) + U^{-1}(x) \partial_\mu U(x)] q(x) \\ &= U(x) [\partial_\mu + igA_\mu(x)] q(x), \end{aligned} \quad (28.9)$$

which is the desired covariant transformation law.

28.2 Gluon Action

After the introduction of such a gauge field, an interaction has to be found describing the dynamics of this gauge field itself. If color is never observed, the action of the gauge field should be locally SU(3)-invariant as well. The only Lagrangian which has this property and contains, at most, first derivatives in A_μ is given by

$$\mathcal{L}_{\text{gluon}} = -\frac{1}{2} \text{tr} (F_{\mu\nu} F^{\mu\nu}) \quad (28.10)$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu] \quad (28.11)$$

is the field tensor, which is the nonabelian version of the covariant curl (4.807) of the vector potential A_μ . Just as A_μ , the field tensor is a 3×3 matrix in color space. It is easy to verify that the matrix $F_{\mu\nu}$ transforms under SU(3) covariantly as follows

$$F_{\mu\nu}(x) \rightarrow U(x) F_{\mu\nu}(x) U(x). \quad (28.12)$$

The theory is described by the Lagrangian

$$\mathcal{L}(x) = \bar{q}(x)i[\partial_\mu + igA_\mu(x)]q(x) - \frac{1}{2}\text{tr}[F_{\mu\nu}(x)F^{\mu\nu}(x)]. \quad (28.13)$$

This is a complete nonabelian analog of the gauge field Lagrangian (12.1)–(12.3) in quantum electrodynamics. For this reason it has been given the similar name *quantum chromodynamics* (QCD).

Instead of 3×3 matrices A_μ , $F_{\mu\nu}$, one can also use an octet of vector and tensor fields defined by

$$A_\mu = \frac{\lambda^a}{2}A_\mu^a, \quad F_{\mu\nu} = \frac{\lambda^a}{2}F_{\mu\nu}^a. \quad (28.14)$$

Thus we can write the Lagrangian of QCD as

$$\mathcal{L} = \bar{q}(x)i\gamma^\mu \left[\partial_\mu + ig\frac{\lambda^a}{2}A_\mu^a(x) \right] q(x) - \frac{1}{4}F_{\mu\nu}^a(x)F_{\mu\nu}^a(x), \quad (28.15)$$

where

$$F_{\mu\nu}^a(x) = \partial_\mu A_\nu^a(x) - \partial_\nu A_\mu^a(x) - gf^{abc}A_\mu^b(x)A_\nu^c(x). \quad (28.16)$$

In terms of the eight components $A_\mu^a(x)$, the Lagrangian (28.10) reads

$$\mathcal{L}_{\text{gluon}}^F = -\frac{1}{4}F_{\mu\nu}^a F^{a\mu\nu}. \quad (28.17)$$

There exists an equivalent way of expressing it in terms of two independent fields $A_\mu^a(x)$ and $F_{\mu\nu}^a$, often used by Schwinger:

$$\mathcal{L}_{\text{gluon}} = \frac{1}{4}F_{\mu\nu}^a F^{a\mu\nu} - \frac{1}{2}F_{\mu\nu}^a (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a). \quad (28.18)$$

The spacetime integral over this is the canonical action corresponding to the mechanical action of a free particle [recall (1.14)]:

$$\mathcal{A} = \int dt \left(-\frac{p^2}{2} + p\dot{q} \right). \quad (28.19)$$

In the past, evidence has accumulated that the gauge field A_μ^a is indeed capable of describing the forces which bind together the quarks inside hadrons. The field quanta carried by A_μ^a are called gluons.

28.3 Quantization in the Coulomb Gauge

Let us quantize the theory for the simplest nonabelian symmetry $\text{SU}(2)$, where the gluons A_μ^a ($a = 1, 2, 3$) are vectors in color space. We shall follow the description of

the theory in Ref. [4, 5]. In SU(2)-symmetry, the structure constants f^{abc} reduce to ϵ^{abc} and the covariant curl (28.16) can be written in vector notation as

$$\mathbf{F}_{\mu\nu}(x) = \partial_\mu \mathbf{A}_\nu(x) - \partial_\nu \mathbf{A}_\mu(x) - g \mathbf{A}_\mu(x) \times \mathbf{A}_\nu(x), \quad (28.20)$$

and the Lagrangian (28.18) becomes

$$\mathcal{L}_{\text{gluon}}^F = \frac{1}{4} \mathbf{F}_{\mu\nu} \cdot \mathbf{F}^{\mu\nu} - \frac{1}{2} \mathbf{F}_{\mu\nu} \cdot (\partial^\mu \mathbf{A}^\nu - \partial^\nu \mathbf{A}^\mu - g \mathbf{A}^\mu \times \mathbf{A}^\nu). \quad (28.21)$$

This is invariant under the nonabelian gauge transformations (28.8) whose infinitesimal form is a rotation in isospace by a small angle ϵ around the direction $\hat{\mathbf{n}}$. If $\mathbf{u} \equiv \epsilon \hat{\mathbf{n}}$ denotes the associated infinitesimal rotation vector, the gauge transformations take the form

$$\begin{aligned} \mathbf{A}_\mu(x) &\rightarrow \mathbf{A}_\mu^{\mathbf{u}}(x) = \mathbf{A}_\mu(x) + \mathbf{u}(x) \times \mathbf{A}_\mu(x) + \frac{1}{g} \partial_\mu \mathbf{u}(x) \\ \mathbf{F}_{\mu\nu} &\rightarrow \mathbf{F}_{\mu\nu}^{\mathbf{u}} = \mathbf{F}_{\mu\nu} + \mathbf{u} \times \mathbf{F}_{\mu\nu}. \end{aligned} \quad (28.22)$$

The first Euler-Lagrange equation

$$\frac{\partial \mathcal{L}_{\text{gluon}}^F}{\partial F_{\mu\nu}^a} = 0 \quad (28.23)$$

reproduces the relation (28.20) between the curl and the auxiliary tensor field $F_{\mu\nu}^a$. The second Euler-Lagrange equation

$$\partial_\mu \frac{\partial \mathcal{L}_{\text{gluon}}^F}{\partial (\partial_\mu A_\nu^a)} = \frac{\partial \mathcal{L}}{\partial A_\nu^a} \quad (28.24)$$

yields the field equation

$$D^\mu \mathbf{F}_{\mu\nu} \equiv \partial^\mu \mathbf{F}_{\mu\nu} - g \mathbf{A}^\mu \times \mathbf{F}_{\mu\nu} = 0. \quad (28.25)$$

The combination of Eqs. (28.20) and (28.25) coincides with the field equation that would be obtained from the second-order formulation with the Lagrangian $\mathcal{L}_{\text{gluon}}$ of Eq. (28.17) expressed directly in terms of $\partial^\mu A^\nu$ and A^μ via Eq. (28.11).

In the present first-order formulation, one is given an initial configuration of fields $\mathbf{A}_i$ and $\mathbf{F}_{0i}$ at some time t . From these one determines the fields at any later time by solving the first-order equations of motion

$$\partial_0 \mathbf{A}_i = \mathbf{F}_{0i} + (\nabla_i - g \mathbf{A}_i \times) \mathbf{A}_0, \quad (28.26)$$

$$\partial_0 \mathbf{F}_{0i} = (\partial_j - g \mathbf{A}_j \times) \mathbf{F}_{ji} + g \mathbf{A}_0 \times \mathbf{F}_{0i}. \quad (28.27)$$

As in the abelian case of Maxwell electromagnetism [recall Eq. (7.337)], the field $\mathbf{A}_0$ is not a dynamical variable since the canonical momenta

$$\partial \mathcal{L} / \partial (\partial_0 \mathbf{A}_\mu) = -\mathbf{F}^{0\mu} = \mathbf{F}^{\mu 0} \quad (28.28)$$

vanish for $\mu = 0$. There are only three independent field momenta. The Euler equation for $\mathbf{A}_0$ is not an equation of motion but a constraint equation analogous to the Coulomb law (7.339):

$$(\nabla_k - g\mathbf{A}_k \times) \mathbf{F}_{k0} = 0. \quad (28.29)$$

As in the Abelian case, it tells us that not all of the conjugate momenta $\mathbf{F}_{0k}$ are independent.

Note that in the first-order formulation, the field equation obtained from varying $\mathbf{F}_{ij}$,

$$\mathbf{F}_{ij} = \partial_i \mathbf{A}_j - \partial_j \mathbf{A}_i - g\mathbf{A}_i \times \mathbf{A}_j, \quad (28.30)$$

is also a constraint equation which allows us to calculate $\mathbf{F}_{ij}$ for given $\mathbf{A}_i$ at the same time. In addition we see from Eq. (28.30) that not all field components $\mathbf{A}_k$ can be treated as independent.

In order to remove the redundancy we choose the Coulomb gauge

$$\nabla_k \mathbf{A}_k = 0. \quad (28.31)$$

This is always possible because of the gauge invariance of the second kind of the Lagrangian density [recall (4.255)]. The gauge (28.31) implies that the vector field $\mathbf{A}_i$ must be transverse. Therefore, the longitudinal components $\mathbf{F}_{0i}^L$ of the canonical momentum $\mathbf{F}_{0i}$ are not independent, but they depend on the other degrees of freedom through the constraint (28.29). The splitting of $\mathbf{F}_{0i}$ into longitudinal $\mathbf{F}_{0i}^L$ and transverse parts $\mathbf{F}_{0i}^T$ is defined by the equations

$$\mathbf{F}_{0i} = \mathbf{F}_{0i}^T + \mathbf{F}_{0i}^L, \quad \nabla_i \mathbf{F}_{0i} = \nabla_i \mathbf{F}_{0i}^L, \quad \epsilon^{ijk} \nabla_j \mathbf{F}_{0k}^L = 0. \quad (28.32)$$

Our task is now to express $\mathbf{A}_0$ and $\mathbf{F}_{0i}^L$ in terms of the independent fields and construct the Hamiltonian. As usual we identify the transverse components $\mathbf{F}_{0i}^T$ as the electric field strengths $\mathbf{E}_i$. By rewriting the longitudinal components $\mathbf{F}_{0i}^L$ as a gradient of a scalar isovector $\mathbf{f}$,

$$\mathbf{F}_{0i}^L = -\nabla_i \mathbf{f}, \quad (28.33)$$

we have

$$\nabla_i \mathbf{F}_{0i} = -\nabla^2 \mathbf{f}. \quad (28.34)$$

The independent variables are the transverse vector fields $\mathbf{A}_i$ and its canonically conjugate field momentum $\mathbf{E}_i$.

Inserting (28.33) into the constraint (28.29), we obtain the differential equation for $\mathbf{f}$:

$$(\nabla^2 + g\mathbf{A}_k \times \nabla_k) \mathbf{f} = g\mathbf{A}_i \times \mathbf{E}_i. \quad (28.35)$$

This equation can be solved formally by introducing a Green function $\mathcal{D}^{ab}(\mathbf{x}, \mathbf{x}'; \mathbf{A})$, defined as a solution of the inhomogeneous differential equation

$$\left(\nabla^2 \delta^{ab} + g \epsilon^{acb} A_k^c \nabla_k \right) \mathcal{D}^{bd}(\mathbf{x}, \mathbf{x}'; \mathbf{A}) = \delta^{ad} \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (28.36)$$

With the help of this Green function, Eq. (28.35) can be solved for the components of $\mathbf{f}$ by the integral

$$f^a(\mathbf{x}, t) = g \int d^3 x' \mathcal{D}^{ab}(\mathbf{x}, \mathbf{x}'; \mathbf{A}) \epsilon^{bcd} A_k^c(\mathbf{x}', t) E_k^d(\mathbf{x}', t). \quad (28.37)$$

This may be abbreviated as

$$\mathbf{f} = g \mathbf{D}[\mathbf{A}_k^T, \mathbf{E}_k^T]. \quad (28.38)$$

The solution $\mathcal{D}^{bd}(\mathbf{x}, \mathbf{x}'; \mathbf{A})$ of Eq. (28.36) cannot be found explicitly, but only via a perturbation expansion. The lowest approximation coincides with δ^{ab} times the Green function $-1/\nabla^2$ of electrostatics. A first iteration yields additional terms up to the order g :

$$\mathcal{D}^{ab}(\mathbf{x}, \mathbf{x}'; \mathbf{A}) = \frac{\delta^{ab}}{4\pi|\mathbf{x} - \mathbf{x}'|} + g \int d^3 x'' \frac{1}{4\pi|\mathbf{x} - \mathbf{x}''|} \epsilon^{acb} A_k^c \nabla_k \frac{1}{4\pi|\mathbf{x}' - \mathbf{x}''|} + \dots \quad (28.39)$$

This first-order approximation is easily verified by inserting it into Eq. (28.36).

A similar equation for $\mathbf{A}_0$ is obtained by taking the divergence of Eq. (28.26) and using (28.31) and (28.32) to find

$$\left(\nabla^2 + g \mathbf{A}_i \times \nabla_i \right) \mathbf{A}_0 = \nabla^2 \mathbf{f}. \quad (28.40)$$

This can be solved using once more $\mathcal{D}^{ab}(\mathbf{x}, \mathbf{x}'; \mathbf{A})$, since the operator in brackets is the same as in Eq. (28.35):

$$A_0^a(\mathbf{x}, t) = \int d^3 x' \mathcal{D}^{ab}(\mathbf{x}, \mathbf{x}'; \mathbf{A}) \nabla^2 f^b(\mathbf{x}', t), \quad (28.41)$$

or in short form:

$$\mathbf{A}_0 = \mathcal{D} \nabla^2 \mathbf{f}. \quad (28.42)$$

We can now construct the Hamiltonian density $\mathcal{H}$ by the Legendre transformation of the Lagrangian density (28.18):

$$\mathcal{H} = \mathbf{E}_i \cdot \frac{\partial \mathbf{A}_i}{\partial t} - \mathcal{L}_{\text{gluon}}^F. \quad (28.43)$$

From (28.26), (28.32), (28.33), and (28.42), we find that

$$\partial_t \mathbf{A}_i = \mathbf{E}_i - \left[\nabla_i - (\nabla_i + g \mathbf{A}_i \times) \mathcal{D} \cdot \nabla^2 \right] \mathbf{f}. \quad (28.44)$$

Because of (28.36), the operator in brackets acting on $\mathbf{f}$ is explicitly transverse. Combining further (28.44) and (28.35) or (28.37), we obtain that

$$\begin{aligned} \int d^3x \mathbf{E}_i \cdot \partial_t \mathbf{A}_i &= \int d^3x \left[\mathbf{E}_i^2 + g(\mathbf{E}_i \times \mathbf{A}_i) \cdot \mathcal{D} \cdot \nabla^2 \mathbf{f} \right] \\ &= \int d^3x \left[\mathbf{E}_i^2 - \mathbf{f} \cdot \nabla^2 \mathbf{f} \right] = \int d^3x \left[\mathbf{E}_i^2 + (\nabla_i \mathbf{f})^2 \right]. \end{aligned} \quad (28.45)$$

If we now rewrite the Lagrangian density as

$$\begin{aligned} \mathcal{L}_{\text{gluon}}^F &= \frac{1}{4} \mathbf{F}_{\mu\nu} \cdot \mathbf{F}^{\mu\nu} - \frac{1}{2} \mathbf{F}_{\mu\nu} \cdot (\partial^\mu \mathbf{A}^\nu + g \mathbf{A}^\mu \times \mathbf{A}^\nu) \\ &= \frac{1}{2} (\mathbf{F}_{0k}^2 - \mathbf{B}_i^2) = \frac{1}{2} (\mathbf{E}_k - \nabla_k \mathbf{f})^2 - \frac{1}{2} \mathbf{B}_k^2, \end{aligned} \quad (28.46)$$

and identify the magnetic field strength as

$$\mathbf{B}_i = \frac{1}{2} \epsilon^{ijk} \mathbf{F}_{jk}, \quad (28.47)$$

we find the Hamiltonian

$$H = \frac{1}{2} \int d^3x \left[\mathbf{E}_i^2 + \mathbf{B}_i^2 + (\nabla_i \mathbf{f})^2 \right]. \quad (28.48)$$

The last term is like the familiar instantaneous Coulomb interaction discussed in QED in Section 12.3 [see the last term in Eq. (12.81)].

We now express the generating functional $W_C[\mathbf{j}]$ in the Coulomb gauge in terms of the independent coordinates and momenta, $\mathbf{A}_i$ and $\mathbf{E}_i$, as the functional integral

$$W_C[\mathbf{j}] = \int \mathcal{D}\mathbf{E}_i^T \mathcal{D}\mathbf{A}_i^T \exp \left\{ i \int d^4x \left[\mathbf{E}_k \cdot \dot{\mathbf{A}}_k - \frac{1}{2} \mathbf{E}_k^2 - \frac{1}{2} \mathbf{B}_k^2 - \mathbf{A}_k \cdot \mathbf{j}_k \right] \right\} \quad (28.49)$$

where the superscript T indicates the transverse spatial components of the field, and $\mathbf{f}$ is the functional (28.38) depending on $\mathbf{E}_i^T$ and $\mathbf{A}_i^T$ as specified in Eq. (28.37). Note that the spatial source term at the end has a negative sign, so that the covariant functional to be derived below in Eq. (28.63) will contain the four-dimensional scalar coupling of the vector field to the source with a positive sign: $\mathbf{A}^\mu \cdot \mathbf{j}_\mu$.

The transverse field $\mathbf{E}_i^T$ is somewhat awkward to handle. Therefore we introduce an initially dummy variable $\mathbf{E}^L$ by

$$\int \mathcal{D}\mathbf{E}_i^T = \int \mathcal{D}\mathbf{E}_i^T \mathcal{D}\mathbf{E}^L \delta^{(3)}[\mathbf{E}^L], \quad (28.50)$$

where $\delta^{(3)}[\mathbf{E}^L] \equiv \prod_x \delta^{(3)}(\mathbf{E}^L(x))$ is the δ -functional in four-dimensional spacetime. Then we define three independent transverse and longitudinal components $\mathbf{E}_i$ by

$$\mathbf{E}_i^T = \left(\delta_{ij} - \nabla_i \frac{1}{\nabla^2} \nabla_j \right) \mathbf{E}_j, \quad \mathbf{E}^L \equiv \nabla_i \frac{1}{\nabla^2} \nabla_i \mathbf{E}_i, \quad (28.51)$$

in terms of which we can rewrite the measure (28.50) as

$$\int \mathcal{D}\mathbf{E}_i^T = \int \mathcal{D}\mathbf{E}_i J \delta[\nabla_j \mathbf{E}_j], \quad (28.52)$$

where J is a field-independent, and thus irrelevant, Jacobian of the transformation from the three $\mathbf{E}_i$ to $\mathbf{E}_i^T, \mathbf{E}^L$, and

$$\mathcal{D}\mathbf{E}_i \equiv \prod_x \prod_{i=1}^3 \prod_{a=1}^3 dE_i^a(x).$$

The same decomposition is applied to the gauge fields $\mathbf{A}_i^T$, so that the generating functional has the functional integral representation

$$\begin{aligned} W_C[\mathbf{j}] &= \text{const} \times \int \mathcal{D}\mathbf{E}_i \mathcal{D}\mathbf{A}_i \delta[\nabla_k \mathbf{E}_k] \delta[\nabla_k \mathbf{A}_k] \\ &\times \exp \left\{ i \int d^4x \left[\mathbf{E}_k \cdot \dot{\mathbf{A}}_k - \frac{1}{2} \mathbf{E}_k^2 - \frac{1}{2} \mathbf{B}_k^2 - \frac{1}{2} (\nabla_k \mathbf{f})^2 - \mathbf{A}_k \cdot \mathbf{j}_k \right] \right\}. \end{aligned} \quad (28.53)$$

From this expression we can derive the Feynman diagram rules in the Coulomb gauge. As in the abelian case, these are not covariant, and the Lorentz covariance of the emerging S -matrix is not obvious. The Coulomb gauge is only useful to derive the generating functional from the canonical formalism.

In order to find the Feynman rules for the covariant and gauge invariant S -matrix, one should start out with a covariant-looking form of the generating functional instead of (28.53). There, $\mathbf{f}$ is a function of $\mathbf{E}$ and $\mathbf{A}$ given by Eq. (28.37). It is possible to introduce $\mathbf{f}$ as a variable of integration and fix its value to satisfy (28.37) by a δ -functional

$$\int \mathcal{D}\mathbf{f} \delta[\mathbf{f} - g\mathcal{D} \cdot \mathbf{A}_k \times \mathbf{E}_k] = 1. \quad (28.54)$$

If the generating functional (28.53) is multiplied by this expression, it obviously remains unchanged. Let $\text{Det } M$ be the Jacobian of the transformation from $\mathbf{f}$ to $(\nabla^2 + g\mathbf{A}_i \times \nabla_i)\mathbf{f}$. The factor in front of $\mathbf{f}$ is a functional matrix in isospin space:

$$\begin{aligned} M^{ab}(x, x') &= \left(\nabla^2 \delta^{ab} + g\epsilon^{abc} A_i^c(y) \nabla_i \right) \delta^{(4)}(x - x') \\ &= \nabla^2 \left[\delta^{ab} \delta^{(3)}(\mathbf{x} - \mathbf{x}') + g\epsilon^{abc} G(x, x') A_i^c(x') \nabla_i \right] \delta(x_0 - x'_0), \end{aligned} \quad (28.55)$$

where $G(x, y)$ is the Green function satisfying $\nabla^2 G(x, y) = \delta^{(3)}(\mathbf{x} - \mathbf{x}')$. With the help of Eq. (28.35), we can now rewrite (28.54) as

$$\int \mathcal{D}\mathbf{f} \delta[\mathbf{f} - g\mathcal{D} \cdot \mathbf{A}_k \times \mathbf{E}_k] = \text{Det } M \int \mathcal{D}\mathbf{f} \delta[(\nabla^2 + g\mathbf{A}_i \times \nabla_i)\mathbf{f} - g\mathbf{A}_i \times \mathbf{E}_i], \quad (28.56)$$

and the generating functional (28.53) becomes

$$\begin{aligned} W_C[\mathbf{j}] &= \text{Det } M \int \mathcal{D}\mathbf{A}_i \mathcal{D}\mathbf{E}_i \mathcal{D}\mathbf{f} \delta[\nabla_i \mathbf{A}_i] \delta[\nabla_i \mathbf{E}_i] \delta[(\nabla^2 + g\mathbf{A}_i \times \nabla_i)\mathbf{f} - g\mathbf{A}_i \times \mathbf{E}_i] \\ &\times \exp \left[i \int \left\{ \mathbf{E}_k \cdot \mathbf{A}_k - \frac{1}{2} [\mathbf{f}_k^2 + \mathbf{B}_k^2 + (\nabla_k \mathbf{f})^2] - \mathbf{j}_i \cdot \mathbf{A}_i \right\} d^4x \right]. \end{aligned} \quad (28.57)$$

Next we change variables from $\mathbf{E}_i$ to

$$\mathbf{F}_{0i} = \mathbf{E}_i - \nabla_i \mathbf{f}, \quad (28.58)$$

using (28.32) and (28.33). Then we rewrite the measure of integration in (28.57) as

$$\begin{aligned} \mathcal{D}\mathbf{E}_i \mathcal{D}\mathbf{f} \delta[\nabla_i \mathbf{E}_i] \delta[(\nabla^2 + g\mathbf{A}_i \times \nabla_i)\mathbf{f} - g\mathbf{A}_i \times \mathbf{E}_i] \\ = \mathcal{D}\mathbf{F}_{0i} \mathcal{D}\mathbf{f} \delta[\nabla_i \mathbf{F}_{0i} + \nabla^2 \mathbf{f}] \delta[\nabla^2 \mathbf{f} - g\mathbf{A}_i \times \mathbf{F}_{0i}] \\ = \mathcal{D}\mathbf{F}_{0i} \mathcal{D}\mathbf{f} \delta[\nabla_i \mathbf{F}_{0i} + g\mathbf{A}_i \times \mathbf{F}_{0i}] \delta[\nabla^2 \mathbf{f} - g\mathbf{A}_i \times \mathbf{F}_{0i}]. \end{aligned} \quad (28.59)$$

Now we perform the integration over $\mathcal{D}\mathbf{f}$ using the last δ -function in (28.59). The Jacobian is just $\text{Det } \nabla^2$, i.e., an irrelevant infinite constant which shall be absorbed into the definition of M . Thus we obtain

$$\begin{aligned} W_C[\mathbf{j}] = \text{Det } M \int \mathcal{D}\mathbf{A}_i \mathcal{D}\mathbf{F}_{0i} \delta[\nabla_i \mathbf{A}_i] \delta[\nabla_i \mathbf{F}_{0i} + g\mathbf{A}_i \times \mathbf{F}_{0i}] \\ \times \exp \left\{ i \int d^4x \left[\mathbf{F}_{0i} \cdot \partial_0 \mathbf{A}_i - \frac{1}{2} \mathbf{F}_{0i}^2 - \frac{1}{4} (\nabla_i \mathbf{A}_j - \nabla_j \mathbf{A}_i + g\mathbf{A}_i \times \mathbf{A}_j)^2 - \mathbf{j}_i \cdot \mathbf{A}_i \right] \right\}. \end{aligned} \quad (28.60)$$

The exponent has been found by setting in the exponent of (28.57)

$$\mathbf{E}_k^2 + (\nabla_k \mathbf{f})^2 = (\mathbf{E}_k - \nabla_k \mathbf{f})^2 = \mathbf{F}_{0k}^2,$$

and omitting the mixed term since it vanishes upon integration over x , due to the transversality of $\mathbf{E}_k$.

Next we express the last factor in the measure of (28.60) as a functional integral over a dummy field variable $\mathbf{A}_0$:

$$\begin{aligned} \delta[\nabla_i \mathbf{F}_{0i} + g\mathbf{A}_i \times \mathbf{F}_{0i}] = \prod_x \int \frac{d\mathbf{A}_0}{2\pi} \exp \{ i \mathbf{A}_0 \cdot (\nabla_0 \mathbf{F}_{0i} - g\mathbf{A}_i \times \mathbf{F}_{0i}) \} \\ = \text{const.} \times \int \mathcal{D}\mathbf{A}_0 \exp \left\{ i \int d^4x \mathbf{F}_{0i} (g\mathbf{A}_0 \times \mathbf{A}_i - \nabla_i \mathbf{A}_0) \right\}. \end{aligned} \quad (28.61)$$

Finally, we write the term $\frac{1}{4}(\nabla_i \mathbf{A}_j - \nabla_j \mathbf{A}_i + g\mathbf{A}_i \times \mathbf{A}_j)^2$ in the exponent of (28.60) as

$$\int \mathcal{D}\mathbf{F}_{ij} \exp \left\{ i \left[\frac{1}{4} \mathbf{F}_{ij} \cdot \mathbf{F}_{ij} - \frac{1}{2} \mathbf{F}_{ij} \cdot (\nabla_i \mathbf{A}_j - \nabla_j \mathbf{A}_i + g\mathbf{A}_i \times \mathbf{A}_j) \right] \right\}, \quad (28.62)$$

which is a standard Gaussian integral. Inserting (28.62) and (28.61) into (28.60), we obtain

$$\begin{aligned} W_C[\mathbf{j}] &= \text{Det } M \int \mathcal{D}\mathbf{A}_\mu \mathcal{D}\mathbf{F}_{\mu\nu} \delta[\nabla_i \mathbf{A}_i] \\ &\times \exp \left[i \int d^4x \left\{ -\frac{1}{2} \mathbf{F}_{0i} \cdot \mathbf{F}_{0i} + \frac{1}{4} \mathbf{F}_{ij} \cdot \mathbf{F}_{ij} \right. \right. \\ &\quad \left. \left. - \frac{1}{2} \mathbf{F}_{ij} \cdot (\nabla_i \mathbf{A}_j - \nabla_j \mathbf{A}_i + g\mathbf{A}_i \times \mathbf{A}_j) + \mathbf{F}_{0i} (\partial_0 \mathbf{A}_i - \nabla_i \mathbf{A}_0 + g\mathbf{A}_0 \times \mathbf{A}_i) \right\} \right] \\ &= \text{Det } M \int \mathcal{D}\mathbf{A}_\mu \mathcal{D}\mathbf{F}_{\mu\nu} \delta[\nabla_i \mathbf{A}_i] \exp \left\{ i \int d^4x [\mathcal{L}_{\text{gluon}}^F + \mathbf{j}^\mu \cdot \mathbf{A}_\mu] \right\}. \end{aligned} \quad (28.63)$$

Were it not for the factor $\text{Det } M$, this would directly define covariant Feynman rules. In order to calculate the effect of the factor, it is useful to reexpress it in terms of an effective Lagrangian density. Recalling the explicit form of the functional matrix (28.55), we factorize it as

$$\text{Det } M = \text{Det } \nabla^2 \cdot \text{Det } [\hat{1} + \hat{M}], \quad (28.64)$$

where

$$\hat{M} = g\epsilon^{abc}G(x, y)A_i^c(y) \cdot \nabla_i \delta(x_0 - y_0), \quad \hat{1} = \delta^{ab}\delta^4(x - y). \quad (28.65)$$

The determinant $\text{Det } \nabla^2$ is again an irrelevant infinite constant. The second factor is expanded as

$$\begin{aligned} \text{Det } (\hat{1} + \hat{M}) &= \exp \text{Tr} \log(\hat{1} + \hat{M}) \\ &= \exp \sum_{n=0}^{\infty} \frac{(-1)^{n-1}}{n} \int d^4x_1 \dots d^4x_n \text{tr} [\hat{M}(x_1, x_2) \hat{M}(x_2, x_3) \dots \hat{M}(x_n, x_1)]. \end{aligned} \quad (28.66)$$

The trace symbol tr runs only over isospin indices. Inserting (28.65), this becomes

$$\begin{aligned} \text{Det } (\hat{1} + \hat{M}) &= \exp \left[\delta(0) \left\{ - \sum_{n=0}^{\infty} \frac{g^n}{n} \int d^3x_1 \dots d^3x_n \int dt \text{tr} [\mathbf{T} \cdot \mathbf{A}_{i_1}(\mathbf{x}_1, t) \nabla_{i_1} G(\mathbf{x}_1, \mathbf{x}_2) \right. \right. \\ &\quad \left. \left. \times \mathbf{T} \cdot \mathbf{A}_{i_2}(\mathbf{x}_2, t) \nabla_{i_2} G(\mathbf{x}_2, \mathbf{x}_3) \dots \mathbf{T} \cdot \mathbf{A}_{i_n}(\mathbf{x}_n, t) \nabla_{i_n} G(\mathbf{x}_n, \mathbf{x}_1) \right\} \right], \end{aligned} \quad (28.67)$$

where $(T^a)_{bc} = \epsilon^{abc}$ and Tr includes the trace over isospin indices.

Since (28.67) is a power series in the exponent, it is an effective correction in each order to the Feynman rules obtained from $\mathcal{L}_{\text{gluon}}^F$ alone.

28.4 General Functional Quantization of Gauge Fields

Equation (28.63) can be further simplified. We can perform the functional integration over $F_{\mu\nu}^a$ and obtain

$$W[\mathbf{j}] = \text{Det } M \int \mathcal{D}\mathbf{A}_\mu \delta[\nabla_i \mathbf{A}_i(x)] \exp \left\{ i \int d^4x [\mathcal{L}_{\text{gluon}}(x) + \mathbf{j}_\mu(x) \cdot \mathbf{A}^\mu(x)] \right\}, \quad (28.68)$$

where $\mathcal{L}(x)$ is the second-order Lagrangian density (28.17). Except for the factor $\text{Det } M \delta[\nabla_i \mathbf{A}_i(x)]$, this expression looks the same as for a standard scalar field theory:

$$W[\mathbf{j}] \sim \int \mathcal{D}\phi \exp \left\{ i \int d^4x [\mathcal{L}(x) + j(x)\phi(x)] \right\}. \quad (28.69)$$

For the abelian gauge theory QED we have shown in Section 14.16 how to derive such a factor following an intuitive argument due to Faddeev and Popov. Here we may do the same for the nonabelian case. Recall how the argument went in the

abelian case. There we expressed the quadratic part of the action in the bilocal form

$$\mathcal{A}_0 = - \int d^4x \frac{1}{4} (\partial_\mu \mathbf{A}_\nu - \partial_\nu \mathbf{A}_\mu)^2 = \int d^4x d^4x' \frac{1}{2} \mathbf{A}_\mu(x) D^{\mu\nu}(x, x') \mathbf{A}_\nu(y), \quad (28.70)$$

with a functional matrix

$$D^{\mu\nu}(x, x') = - \left(\partial^2 g^{\mu\nu} - \partial^\mu \partial^\nu \right) \delta^4(x - x').$$

This cannot be inverted, since it involves only the transverse components of $\mathbf{A}_\mu$, while ignoring the longitudinal components. Hence the Euclidean version of the functional integral of Eq. (28.68) contains no Gaussian exponential involving the longitudinal components of $\mathbf{A}_\mu$, and therefore the functional integral over these diverges. In the abelian case this was a consequence of the invariance of the exponent in (14.347) under the gauge transformation (14.345). Here it is a consequence of the invariance of the exponent of (28.68) under the gauge transformation

$$\mathbf{A}_\mu \rightarrow \mathbf{A}_\mu^g. \quad (28.71)$$

The right-hand side emerges as a result of applying the element g of the gauge group G to the field $\mathbf{A}_\mu$:

$$\mathbf{A}_\mu^g \cdot \mathbf{L} = U(g) \left[\mathbf{A}_\mu \cdot \mathbf{L} + \frac{1}{ig} U^{-1}(g) \partial_\mu U(g) \right] U^{-1}(g). \quad (28.72)$$

The exponent in the functional integral (28.72) is constant on the orbits of the gauge group, which are formed by all $\mathbf{A}_\mu^g$ for fixed $\mathbf{A}_\mu$, while dg runs over the entire group G . This causes a divergence of the functional integral for the generating functional $W[\mathbf{j}]$. The amplitude $W[\mathbf{j} = 0]$ is therefore proportional to the “volume” of orbits $\prod_x dg(x)$, and this factor should be extracted before defining $W[\mathbf{j} = 0]$. Thus the functional integral should not be performed over all fluctuations of the gauge fields, but only over the different orbits of $\mathbf{A}_\mu$ defined by the symmetry transformations of the gauge group.

To implement this idea, we choose a “hypersurface” in the manifold of all fields which intersects each orbit only once. Let

$$f_a(\mathbf{A}_\mu) = 0, \quad a = 1, 2, \dots, N \quad (28.73)$$

describe such hypersurface, where N is the dimension of the group. We shall assume that the equation

$$f_a(\mathbf{A}_\mu^g) = 0$$

has a unique solution g for any given field $\mathbf{A}_\mu$. We are going to integrate over all different hypersurfaces of this kind, instead of integrating over the manifold of all fields. The conditions $f_a(\mathbf{A}_\mu) = 0$ define a particular gauge, the Coulomb gauge $f_a(\mathbf{A}_\mu) = \nabla_i A_i^a$ being just a particular example.

Before proceeding further, let us recall briefly some simple facts about group representations. For any two group elements $g, g' \in G$, the product gg' is also $\in G$, and their representations satisfy the same multiplication law

$$U(g)U(g') = U(gg').$$

The invariant Hurwitz measure over the group G is invariant under this operation, so that

$$dg' = d(gg'). \quad (28.74)$$

If we parametrize $U(g)$ in the neighborhood of the identity as

$$U(g) = 1 + i\mathbf{u} \cdot \mathbf{L} + \mathcal{O}(u^2),$$

then in the neighborhood of the identity we may choose

$$dg = \prod_a du_a, \quad g \sim 1. \quad (28.75)$$

Let us define the functional $\Delta_f[\mathbf{A}_\mu]$ by

$$\Delta_f[\mathbf{A}_\mu] \int \mathcal{D}g \prod_a \delta[f_a(\mathbf{A}_\mu^g(x))] = 1, \quad (28.76)$$

where

$$\int \mathcal{D}g \equiv \prod_x \left[\int dg(x) \right]. \quad (28.77)$$

Without the gauge invariance, the vacuum-to-vacuum amplitude would be given by

$$\int \mathcal{D}\mathbf{A}_\mu \exp \left\{ i \int d^4x \mathcal{L}_{\text{gluon}}(x) \right\}. \quad (28.78)$$

We now insert the left-hand side of Eq. (28.76) into the functional integral (28.78) without changing the result:

$$\int \mathcal{D}g \mathcal{D}\mathbf{A}_\mu \Delta_f[\mathbf{A}_\mu] \prod_a \delta[f_a(\mathbf{A}_\mu^g(x))] \exp \left\{ i \int d^4x \mathcal{L}_{\text{gluon}}(x) \right\}. \quad (28.79)$$

Now we perform a gauge transformation $\mathbf{A}_\mu(x) \rightarrow \mathbf{A}_\mu^g(x)$ defined by (28.72) on $\mathbf{A}_\mu(x)$. Under this, the action in (28.78) is invariant. We may also convince ourselves that the functional $\Delta_f[\mathbf{A}_\mu]$ defined by (28.76) is gauge invariant:

$$\begin{aligned} \Delta_f^{-1}[\mathbf{A}_\mu^g] &= \int \prod_{\mathbf{x}} dg'(x) \prod_{x,a} \delta[f_a(\mathbf{A}_\mu^{gg'}(x))] \\ &= \int \prod_{\mathbf{x}} d(g(x)g'(x)) \prod_{x,a} \delta[f_a(\mathbf{A}_\mu^{gg'}(x))] \\ &= \int \prod_{\mathbf{x}} dg''(x) \prod_{x,a} \delta[f_a(\mathbf{A}_\mu^{g''}(x))], \end{aligned}$$

so that indeed

$$\Delta_f[\mathbf{A}_\mu^g] = \Delta_f[\mathbf{A}_\mu]. \quad (28.80)$$

Hence we may write Eq. (28.79) also as

$$\int \mathcal{D}g \int \mathcal{D}\mathbf{A}_\mu \Delta_f[\mathbf{A}_\mu] \prod_{x,a} \delta[f_a(\mathbf{A}_\mu)] \exp \left\{ i \int d^4x \mathcal{L}_{\text{gluon}}(x) \right\},$$

and we find that the integrand of the group integration is independent of $g(x)$. This was the observation of Faddeev and Popov, who saw that the functional integral $\int \mathcal{D}g$ is simply an infinite factor independent of the fields. It can therefore be dropped from the amplitude, so that the generating functional $W[\mathbf{j}]$ may be defined as

$$W_f[\mathbf{j}] = \int \mathcal{D}\mathbf{A}_\mu \Delta_f[\mathbf{A}_\mu] \prod_a \delta[f^a(\mathbf{A})] \exp \left\{ i \int d^4x [\mathcal{L}(x) + \mathbf{j}^\mu(x) \cdot \mathbf{A}_\mu(x)] \right\}. \quad (28.81)$$

Faddeev and Popov also gave the canonical derivation of Eq. (28.63) as discussed in the preceding section.

Before demonstrating the equivalence of Eqs. (28.68) and (28.81), we shall compute $\Delta_f[\mathbf{A}_\mu]$. Since the factor $\Delta_f[\mathbf{A}_\mu]$ is multiplied by $\prod_a \delta[f^a(\mathbf{A}_\mu(x))]$ in Eq. (28.81), it suffices to compute $\Delta_f[\mathbf{A}_\mu]$ only for vector fields $\mathbf{A}_\mu$ which satisfy Eq. (28.73). Let us define the functional matrix M_f by

$$f^a(\mathbf{A}_\mu^g(x)) = f^a(\mathbf{A}_\mu(x)) + \int d^4y \sum_b [M_f(x, y)]^{ab} u_b(y) + \mathcal{O}(u^2). \quad (28.82)$$

Then we find from Eq. (28.76) that

$$\Delta_f^{-1}[\mathbf{A}_f] = \int \prod_{x,a} \left\{ du_a(x) \delta[f^a(\mathbf{A}_\mu^g(x))] \right\} = \int \prod_{x,a} \left\{ du_a(x) \delta[M_f \mathbf{u}] \right\}.$$

The integral receives a contribution only from $\mathbf{A}$ -fields satisfying $f_a(\mathbf{A}_\mu) = 0$, so that

$$\Delta_f[\mathbf{A}_\mu] = \text{Det } M_f = \exp \{ \text{Tr } \log M_f \}. \quad (28.83)$$

The hypersurface equation $f_a = 0$ is just the gauge condition, and for the Coulomb gauge adopted in the preceding section, we had

$$f^a(\mathbf{A}_\mu) = \nabla_i A_i^a = 0,$$

which becomes, after an infinitesimal gauge transformation,

$$f^a(\mathbf{A}_\mu^g) = \nabla_i A_i^a + \frac{1}{g} \left(\nabla^2 \delta^{ab} - g \epsilon^{abc} A_i^c \nabla_i \right) u_b(x) + \mathcal{O}(u^2). \quad (28.84)$$

From this we identify

$$[M_f(x, x')]_{ab} \sim \frac{1}{g} \nabla^2 \left(\delta^{ab} - g \epsilon^{abc} \frac{1}{\nabla^2} A_i^c \nabla_i \right) \delta^4(x - x') \sim [M(x, x')]_{ab}, \quad (28.85)$$

which shows that Eq. (28.68) is indeed a special case of Eq. (28.81) for $f^a = \nabla_i A_i^a$.

Being in possession of Eq. (28.81), we are free to use many different gauges other than the Coulomb gauge. If we choose, for example, the manifestly covariant Landau gauge condition $\partial^\mu \mathbf{A}_\mu = 0$, then Eq. (28.82) takes the form

$$\partial^\mu \mathbf{A}_\mu^g(x) = \partial^\mu \mathbf{A}_\mu(x) + \frac{1}{g}[\partial^2 \mathbf{u} + g\partial^\mu(\mathbf{A}_\mu \times \mathbf{u})] + \mathcal{O}(u^2), \quad (28.86)$$

so that M_f is given by

$$[M_L(x, x')]_{ab} = \frac{1}{g}(\partial^2 \delta_{ab} - g\epsilon_{abc} A_\mu^c \partial^\mu) \delta^4(x - x') \quad (28.87)$$

when $\mathbf{A}_\mu$ is restricted to $\partial^\mu \mathbf{A}_\mu = 0$. Removing the trivial factor $(1/g)\partial^2$ from $M_L(x, x')$, we have

$$\Delta_L \equiv \text{Det } M_L \sim \exp \left\{ \text{Tr } \ln(\hat{1} + \hat{M}_L) \right\}, \quad (28.88)$$

where

$$\hat{M}_L^{ab}(x, x') = g\epsilon_{abc} \int D_F(x - z) A_\mu^c(z) \frac{\partial}{\partial z_\mu} \delta^4(z - y) d^4 z, \quad (28.89)$$

and $D_F(x - z)$ is the usual Feynman propagator satisfying $-\partial^2 D_F(x - y) = \delta^4(x - y)$. More explicitly we can write

$$\begin{aligned} \Delta_L = \exp \left\{ - \sum_{n=0}^{\infty} \frac{(-g)^n}{n} \int d^4 x_1 \dots d^4 x_n \text{tr} \left[\partial^\lambda D_F(x_1 - x_2) \mathbf{T} \cdot \mathbf{A}_\mu(x_2) \partial^\mu D_F(x_2 - x_3) \right. \right. \\ \left. \left. \times \dots D_F(x_n - x_1) \mathbf{T} \cdot \mathbf{A}_\lambda(x_1) \right] \right\}. \end{aligned} \quad (28.90)$$

The need to have the extra factor $\Delta_f[A_\mu] \prod_a \delta[f^a(\mathbf{A}_\mu(x))]$ was first noted by Feynman.

We can write Eq. (28.81) as

$$W_f[\mathbf{j}] = \int \mathcal{D}\mathbf{A}_\mu \prod_a \delta[f^a(\mathbf{A}_\mu(x))] \exp \left\{ i \left[S_{\text{eff}} + \int d^4 x \mathbf{j}^\mu(x) \cdot \mathbf{A}_\mu(x) \right] \right\}, \quad (28.91)$$

where

$$\mathcal{A}_{\text{eff}} = \int d^4 x \mathcal{L}_{\text{gluon}}(x) - i \text{Tr } \ln M_L. \quad (28.92)$$

At this point it is useful to observe that the additional term $-i \text{Tr } \ln M_L$ in the effective action may be thought of as arising from loops generated by a fictitious isotriplet of complex scalar fields $\mathbf{c}$ obeying Fermi statistics, whose presence and interactions can be described by the following action

$$\begin{aligned} \mathcal{A}_{\mathbf{c}} = - \int d^4 x \left[\partial^\mu \mathbf{c}^\dagger(x) \cdot \mathbf{A}_\mu(x) \times \mathbf{c}(x) \right] \sim \int d^4 x d^4 x' \sum_{a,b} \mathbf{c}_a^\dagger(x) [M_L(x, x')]_{ab} \mathbf{c}_b(x'). \end{aligned} \quad (28.93)$$

With this, Eq. (28.91) may be written as

$$W_L[\mathbf{j}] = \int \mathcal{D}\mathbf{A}_\mu \prod_a \delta[f^a(\mathbf{A}_\mu(x))] \int \mathcal{D}\mathbf{c}^\dagger \mathcal{D}\mathbf{c} \exp \left\{ i \left[\mathcal{A} + \mathcal{A}_c + \int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu(x) \right] \right\}. \quad (28.94)$$

Since $\mathbf{c}$ and $\mathbf{c}^\dagger$ appear quadratically in the action (28.93), the path integral $\int \mathcal{D}\mathbf{c}^\dagger \mathcal{D}\mathbf{c}$ can trivially be done with the result

$$\int \mathcal{D}\mathbf{c}^\dagger \mathcal{D}\mathbf{c} \exp(i\mathcal{A}_c) \sim \text{Det } M_L = \exp \{ \text{Tr } \ln M_L \}, \quad (28.95)$$

and we can expand

$$\begin{aligned} \exp \{ \text{Tr } \ln M_L \} &\sim \exp \left[\text{Tr } \ln(1 + \hat{M}_L) \right] \\ &= \exp \left\{ \text{Tr } \hat{M}_L - \frac{1}{2} \text{Tr } \hat{M}_L^2 + \dots - (-)^n \frac{1}{n} \text{Tr } \hat{M}_L^n + \dots \right\}. \end{aligned} \quad (28.96)$$

The terms in the exponent may arise from loop diagrams of the Fermi fields $\mathbf{c}$.

Let us now specify the Feynman rules resulting from $W_L[\mathbf{j}]$ of Eq. (28.94), following from the general rules described in Chapter 14. The gauge boson propagator is determined from the free-field functional

$$W_L^0[\mathbf{j}] = \int \mathcal{D}\mathbf{A}_\mu \delta[\partial^\mu \mathbf{A}_\mu] e^{i \int d^4x \left\{ -\frac{1}{4} (\partial_\mu \mathbf{A}_\nu - \partial_\nu \mathbf{A}_\mu)^2 + \mathbf{j}^\mu(x) \cdot \mathbf{A}_\mu(x) \right\}}. \quad (28.97)$$

A convenient way of evaluating Eq. (28.97) is to express the δ -functional as

$$\delta[\partial^\mu \mathbf{A}_\mu(x)] \sim \lim_{\alpha \rightarrow 0} \exp \left\{ \frac{i}{2\alpha} \int d^4x [\partial^\mu \mathbf{A}_\mu(x)]^2 \right\}, \quad (28.98)$$

where we have discarded an irrelevant infinite constant $\prod_x \sqrt{2\pi\alpha}$. Then we arrive at the generating functional of free vector boson Green functions:

$$\begin{aligned} W_L^0[\mathbf{j}] &= \lim_{\alpha \rightarrow 0} \int \mathcal{D}\mathbf{A}_\mu \exp \left\{ -\frac{i}{2} \int d^4x \mathbf{A}_\mu(x) \cdot \left[-\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu \left(1 - \frac{1}{\alpha} \right) \right] \mathbf{A}_\nu(x) \right. \\ &\quad \left. + i \int d^4x \mathbf{j}^\mu(x) \cdot \mathbf{A}_\mu(x) \right\} \\ &= \lim_{\alpha \rightarrow 0} \exp \left[-\frac{i}{2} \int d^4x d^4x' \mathbf{j}_\mu(x) D_F^{\mu\nu}(x - x'; \alpha) \mathbf{j}_\nu(x') \right], \end{aligned} \quad (28.99)$$

where $D_F^{\mu\nu}(x - x'; \alpha)$ is the free vector boson propagator

$$D_F^{\mu\nu}(x - x'; \alpha) = \int \frac{d^4k}{(2\pi)^4} \exp \{ ik \cdot (x - x') \} \frac{1}{k^2 + i\epsilon} \left[-g_{\mu\nu} + \frac{k_\mu k_\nu}{k^2} (1 - \alpha) \right]. \quad (28.100)$$

In the limit $\alpha \rightarrow 0$, this becomes

$$D_F^{\mu\nu}(x - x') = \int \frac{d^4k}{(2\pi)^4} \exp \{ ik \cdot (x - x') \} \frac{1}{k^2 + i\epsilon} \left(-g_{\mu\nu} + \frac{k_\mu k_\nu}{k^2} \right), \quad (28.101)$$

which is transverse in spacetime. The rest of the Feynman rules can be derived as usual. They are recorded in Figs. 28.1 and 28.2. In addition, the following rule must be kept in mind: the ghost-ghost-vector vertex may carry a “dot” which indicates that a ghost line is differentiated. Note that a ghost line cannot be dotted at both ends and that a ghost loop carries an extra minus sign.

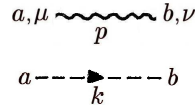


FIGURE 28.1 Propagators in the Yang-Mills theory. Wavy lines are vector mesons. Dashed lines are scalar ghosts.

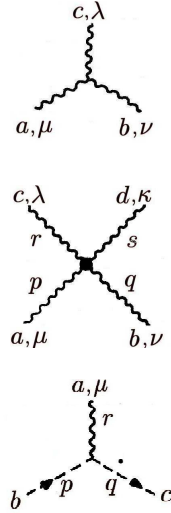


FIGURE 28.2 Vertices in the Yang-Mills theory. Note that the ghost with index c in the last diagram is pictured by a *dotted* line.

28.5 Equivalence of Landau and Coulomb Gauges

Formally, the S -matrix computed in the Landau gauge is the same as that computed in the Coulomb gauge [5]. An element of the unrenormalized S -matrix is obtained from the corresponding Green functions by removing single particle propagators corresponding to external lines, taking the Fourier transform of the resulting “amputated” Green function, and placing external momenta on the mass shell. The demonstration to be presented is basically correct, except that the S -matrix of a gauge theory is plagued by infrared divergences and may not even be defined. In fact, this may be the reason why massless Yang-Mills particles are not seen in nature. The point of presenting this demonstration is at this point purely pedagogical. The technique will be useful in the discussion of spontaneously broken versions of gauge theories.

Let us first establish a relation between $W_C[\mathbf{j}]$ and $W_L[\mathbf{j}]$. From Eq. (28.68) we obtain for the first:

$$W_C[\mathbf{j}] = \int \mathcal{D}\mathbf{A}_\mu \Delta_C[\mathbf{A}_\mu] \delta[\nabla_i \mathbf{A}_i] \exp \left\{ i\mathcal{A}[\mathbf{A}_\mu] + i \int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu \right\}, \quad (28.102)$$

where $\Delta_C = \text{Det } M$ satisfies

$$\Delta_C[\mathbf{A}_\mu] \int \mathcal{D}g \delta[\partial^\mu \mathbf{A}_\mu^g(x)] = 1. \quad (28.103)$$

Inserting the left-hand side of Eq. (28.103) into the integrand of the functional integration in Eq. (28.102), we write

$$\begin{aligned} W_C[\mathbf{j}] &= \int \mathcal{D}g \int \mathcal{D}\mathbf{A}_\mu \Delta_C[\mathbf{A}_\mu] \Delta_C[\mathbf{A}_\mu] \delta[\nabla_i \mathbf{A}_i] \\ &\times \delta[\partial^\mu \mathbf{A}_\mu^g] \exp \left\{ i\mathcal{A}[\mathbf{A}_\mu] + i \int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu \right\}. \end{aligned}$$

Now we perform a gauge transformation of the integration variables $\mathbf{A}_\mu(x)$:

$$\mathbf{A}_\mu(x) \rightarrow \mathbf{A}_\mu^g(x).$$

Recalling the gauge invariance of the action $\mathcal{A}$, the functional Δ_f , and the metric $\mathcal{D}\mathbf{A}_\mu(x)$, we find that

$$\begin{aligned} W_C[\mathbf{j}] &= \int \mathcal{D}\mathbf{A}_\mu \Delta_C[\mathbf{A}_\mu] \delta[\partial^\mu \mathbf{A}_\mu] \exp(i\mathcal{A}[\mathbf{A}_\mu]) \\ &\times \Delta_C[\mathbf{A}_\mu] \int \prod_{\mathbf{x}} dg(x) \prod_{\mathbf{x}} \delta(\nabla_i \mathbf{A}_i^{g^{-1}}) \exp \left\{ i \int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu^{g^{-1}} \right\} \\ &= \int \mathcal{D}\mathbf{A}_\mu \Delta_L[\mathbf{A}_\mu] \prod_{\mathbf{x}} \delta(\partial^\mu \mathbf{A}_\mu(x)) \exp \left\{ i\mathcal{A}[\mathbf{A}_\mu] + i \int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu^{g_0} \right\}. \end{aligned} \quad (28.104)$$

As before, $\mathbf{A}_\mu^{g_0}$ is the gauge transform of $\mathbf{A}_\mu$, which satisfies $\partial^\mu \mathbf{A}_\mu = 0$, such that

$$\mathbf{L} \cdot \nabla_i \mathbf{A}_i^{g_0} = \nabla_i \left\{ U(g_0) \left[\mathbf{L} \cdot \mathbf{A}_i + \frac{1}{ig} U^{-1}(g_0) \nabla_i U(g_0) \right] U^{-1}(g_0) \right\} = 0. \quad (28.105)$$

When deriving Eq. (28.104), we have used the fact that

$$\begin{aligned} \Delta_C[\mathbf{A}_\mu] \int \prod_{\mathbf{x}} dg(x) \prod_{\mathbf{x}} \delta(\nabla_i \mathbf{A}_i^{g^{-1}}) &= \Delta_C[\mathbf{A}_\mu] \int \left\{ \prod_{\mathbf{x}} \prod_a du_a(x) \right\} \\ &\times \prod_{\mathbf{x}} \delta \left(\nabla_i \mathbf{A}_i^{g_0} - \frac{1}{g} M[\mathbf{A}_\mu^{g_0}] u \right) \sim \Delta_C[\mathbf{A}_\mu] \Delta_C^{-1}[\mathbf{A}_\mu^{g_0}] = 1. \end{aligned}$$

It is possible to solve Eq. (28.105) for $\mathbf{A}_\mu^{g_0}$ as a power series in $\mathbf{A}_\mu$. This can be done beginning with

$$\mathbf{A}_i^{g_0} = \left(\delta_{ij} - \nabla_i \frac{1}{\nabla^2} \nabla_j \right) \mathbf{A}_j + \mathcal{O}(\mathbf{A}_\mu^2).$$

The source $\mathbf{j}_\mu$ in the Coulomb gauge will be restricted to

$$\mathbf{j}_0 = 0, \quad \nabla_i \mathbf{j}_i = 0, \quad (28.106)$$

so that we may write

$$\int d^4x \mathbf{j}^\mu \cdot \mathbf{A}_\mu^{g_0} = \int d^4x \mathbf{j}^\mu \cdot \mathbf{F}_\mu(x; \mathbf{A}_\lambda),$$

where

$$\mathbf{F}_\mu(x; \mathbf{A}_\lambda) = \mathbf{A}_\mu(x) + \mathcal{O}(\mathbf{A}_\lambda^2). \quad (28.107)$$

Carrying this construction to high orders we can finally express W_C in terms of W_L as follows:

$$W_C[\mathbf{j}] = \left[\exp \left\{ i \int d^4x \mathbf{j}^\mu(x) \cdot \mathbf{F}_\mu \left(x; \frac{1}{i} \frac{\delta}{\delta \mathbf{j}_\lambda} \right) \right\} \right] W_L[\mathbf{j}]|_{\mathbf{j}=0}. \quad (28.108)$$

It is helpful to visualize the generating functionals (28.104) or (28.108) with the help of Feynman diagrams. The two expressions imply that the Green functions in the Coulomb gauge are the same as those in the Landau gauge, if the source is suitably restricted by equations like those in (28.106). We only must take into account extra vertices between source and field, represented by the term

$$\int d^4x \mathbf{j}^\mu \cdot (\mathbf{F}_\mu - \mathbf{A}_\mu). \quad (28.109)$$

Then one may construct Green functions in the Coulomb gauge from the Feynman rules of the Landau gauge. This relationship becomes much simpler if we go to the mass shell. In this case, we ought to compare only the terms having a pole in each of the external momentum square p_i^2 . Of all the diagrams generated by the extra couplings of (28.109), only those survive in this limit in which the whole effect of the extra vertices can be reduced to a type of self-energy insertion into the corresponding external line. The other corrections introduced by (28.109) do not contribute to poles of the Green functions at $p_i^2 = 0$, and therefore do not contribute to the S -matrix. Hence in the limit $p_i^2 \rightarrow 0$, the unrenormalized S -matrix elements in Coulomb gauge C and Landau gauge L with propagators differ by coming from the different propagators

$$\lim_{p^2 \rightarrow 0} D'_{\mu\nu}(p; L) = \frac{Z_L}{p^2 + i\epsilon} (g_{\mu\nu} + \dots), \quad \lim_{p^2 \rightarrow 0} D'_{\mu\nu}(p; C) = \frac{Z_C}{p^2 + i\epsilon} (g_{\mu\nu} + \dots).$$

In particular, the ratio

$$\sigma^2 = Z_C/Z_L \quad (28.110)$$

is different from unity. In general, the unrenormalized S -matrix elements in the two gauges C and L are related to each order by

$$S_C = \sigma^n S_L = (Z_C/Z_L)^{n/2} S_L,$$

so that the renormalized S -matrix element

$$S_{\text{ren}} \equiv Z_C^{-n/2} S_C = Z_L^{-n/2} S_L$$

is independent of the gauge in which the calculation was done.

As a consequence, $W_C[\mathbf{j}]$ is equal to the expression (28.104), and thus it is equal to $W_L[\mathbf{j}]$ except that the coefficient of $\mathbf{j}^\mu$ is the gauge-transformed vector field

$\mathbf{A}_\mu^{g_0}$, instead of $\mathbf{A}_\mu$ itself. For the S -matrix, the only consequence of this difference is that the renormalization constants attached to each external line depend on the gauge. Thus we have shown that ultimately the S -matrix can be calculated from $W_L[\mathbf{j}]$.

As pointed out earlier, the only flaw in the above argument is that the singularity at $p_i^2 = 0$ is not in general a simple pole.

28.6 Perturbative QCD

For scattering processes at high energy, the strong interaction becomes effectively so weak that quarks behave approximately like free pointlike particles. This phenomenon of strong interactions is called *asymptotic freedom*. It was discovered experimentally in deep-inelastic scattering at the Stanford Linear Accelerator and led Feynman to his famous *parton hypothesis* [11, 12, 13]. By combining this hypothesis with Gell-Mann's field theory of quarks held together by a color octet of non-abelian gauge fields, the present-day quantum field theory of strong interactions was born. It was called *Quantum Chromo Dynamics* (QCD) [3]. Theoretically the asymptotic freedom was first observed for charged vector bosons by V.S. Vanyashin and M.V. Terantjev as early as 1965 [8], and for the nonabelian gauge theory with local $SU(2)$ -symmetry by I.B. Khriplovich [9]. But it was not until 1972 that it was noted in the western physics community, first by 't Hooft who failed to publish it and told it only to colleagues, and later by Politzer, Gross, and Wilczek [14, 15] who earned the Nobel prize of 1973 for it.

For a sufficiently small number of quark flavors $N_f < 33/2$, the behavior of the beta function in QCD is opposite to that in Eq. (20.31) of ϕ^4 -theory and in Eq. (27.30) for QED. It starts out with negative slope and remains negative at least for a certain range. This is what causes the asymptotic freedom when the energy-momenta of the particles in all Feynman diagrams grow large. To study this behavior analytically, we introduce a small number ϵ and imagine living in $4 + \epsilon$ dimensions with less than $N_f = 17$ quark flavors. Then we define an analogue of the fine-structure constant $\alpha = e^2/4\pi$ for strong interactions, namely the constant “alpha-strong” $\alpha_s \equiv g^2/(4\pi)^2$. By a perturbative calculation of the scale dependence of the coupling constant, one finds the β -function of the theory as $\beta(g) \equiv \mu \partial_\mu \alpha_s$ [recall (20.59)]. To lowest order, this is

$$\beta(\alpha_s) = \epsilon \alpha_s - b \alpha_s^2, \quad \text{with} \quad b = 11 - 2N_f/3. \quad (28.111)$$

Then the solution of the differential equation for the scale-dependent coupling constant becomes, by analogy with (20.126):

$$\log \mu = \int_{\alpha_s}^{\alpha_s(\mu)} \frac{d\alpha_s}{\epsilon \alpha_s - b \alpha_s^2}. \quad (28.112)$$

Because of the sign change with respect to (20.126), the movement of α_s for increasing mass scale μ is opposite to that in the ϕ^4 -theory and in QED. The coupling constant $\alpha_s = g^2/(4\pi)^2$ goes towards a fixed point $g^* = \epsilon/b$ in the ultraviolet limit.

By comparison with (20.289), we find the solution after changing the signs of ϵ and b to satisfy

$$\frac{\mu^{-\epsilon}}{\alpha_s(\mu_0)} = \frac{1}{\alpha_s(\mu)} - \frac{b}{\epsilon}. \quad (28.113)$$

This shows that α_s tends to the fixed point $\alpha_s^* = \epsilon/b$ in the limit of large μ , i.e., in the UV-limit. In four spacetime dimensions, we let the auxiliary parameter ϵ go to zero and see that the solution (28.113) tends to

$$\frac{1}{\alpha_s(\mu_0)} = \frac{1}{\alpha_s(\mu)} - \frac{b}{\epsilon} \ln \frac{\mu}{\mu_0}. \quad (28.114)$$

This is solved for $\alpha_s(\mu)$ by

$$\alpha_s(\mu) = \frac{1}{\alpha_s^{-1}(\mu_0) + b \log \frac{\mu}{\mu_0}}. \quad (28.115)$$

The first term in the denominator can be absorbed in the logarithm, and we can rewrite $\alpha_s(\mu)$ as

$$\alpha_s(\mu) = \frac{1}{\frac{1}{2}b \log \frac{\mu^2}{\Lambda_{\text{QCD}}^2}} = \frac{4\pi}{\left(11 - \frac{2}{3}N_f\right) \log \frac{\mu^2}{\Lambda_{\text{QCD}}^2}}. \quad (28.116)$$

The mass Λ_{QCD} is the *dimensionally transmuted coupling constant* of QCD. For $\mu \rightarrow \infty$, the coupling constant $\alpha_s(\mu)$ goes to zero. This is why the nonabelian gauge theory with less than $N_f < 33/2$ flavors is *ultraviolet-free*.

If higher loops are included in the calculations of QCD, the β -function has the expansion [18]

$$\beta(g) = \epsilon \alpha_s - 2(\beta_0 \alpha_s^2 + \beta_1 \alpha_s^3 + \beta_2 \alpha_s^4 + \beta_3 \alpha_s^5) + \dots, \quad (28.117)$$

where

$$\begin{aligned} \beta_0 &= 11 - \frac{2}{3}N_f = \frac{b}{2}, \\ \beta_1 &= 102 - \frac{38N_f}{3}, \\ \beta_2 &= \frac{325N_f^2}{54} - \frac{5033N_f}{18} + \frac{2857}{2}, \\ \beta_3 &= \frac{1093N_f^3}{729} + N_f^2 \left(\frac{6472\zeta(3)}{81} + \frac{50065}{162} \right) - N_f \left(\frac{6508\zeta(3)}{27} + \frac{1078361}{162} \right) \\ &\quad + 3564\zeta(3) + \frac{149753}{6}. \end{aligned} \quad (28.118)$$

The various partial sums are plotted in Fig. 28.3.

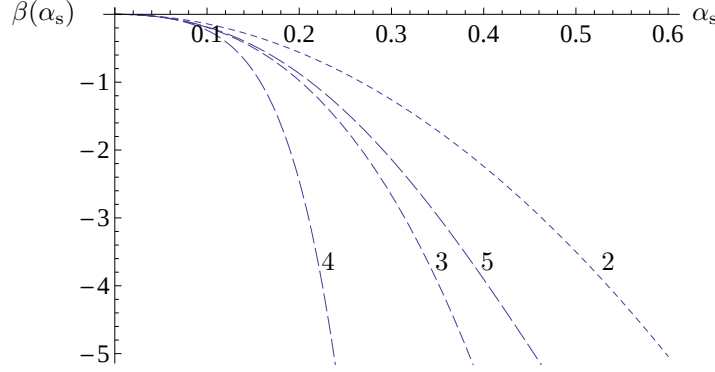


FIGURE 28.3 Flow of the coupling constant α_s towards the origin as the scale parameter μ approaches infinity (ultraviolet limit). For the opposite flow direction (infrared limit), the arrows are reversed and the coupling strength becomes large leading to the formation of a fat attractive flux bundle between quarks.

If only the term α_s^3 is included in the differential equation for the scale-dependence of the coupling constant, the result changes from (28.116) to

$$\frac{\alpha_s(\mu)}{4\pi} = \frac{1}{b_0 \ln \frac{\mu^2}{\Lambda_{\text{QCD}}^2}} - \frac{b_1}{b_0^3} \frac{\ln \ln \frac{\mu^2}{\Lambda_{\text{QCD}}^2}}{\ln^2 \frac{\mu^2}{\Lambda_{\text{QCD}}^2}}. \quad (28.119)$$

The presently best fit to the experimental coupling constants yields the value

$$\Lambda_{\text{QCD}} \approx 217 \pm 25 \text{ MeV}. \quad (28.120)$$

Since the theory is asymptotically free, many properties of it can be studied in perturbation theory. The results can be compared quite well with the experimental data observed in high-energy collisions. Details are amply available in the literature [16, 17].

28.7 Approximate Chiral Symmetry

At first, the masses of the quarks are approximated to be equal to zero. Then the Lagrangian density has an additional invariance. If we restrict our attention only to the three quarks u, d, s , the flavor group is $\text{SU}(3)$. For massless quarks, the symmetry is extended to $\text{SU}(3) \times \text{SU}(3)$, where the extension involves $\text{SU}(3)$ flavor. Its Noether current densities are

$$\begin{aligned} j_a^\mu(x) &= \bar{q}(x) \gamma^\mu \frac{\lambda_a}{2} q(x), \\ j_{5a}^\mu(x) &= \bar{q}(x) \gamma^\mu \gamma_5 \frac{\lambda_a}{2} q(x), \end{aligned} \quad (28.121)$$

where the λ_a matrices act on the flavor-SU(3) indices. The current densities are color singlets. The corresponding color octet currents are not observable, due to local SU(3) color invariance.

After field quantization the field components satisfy the local SU(3) $\times$ SU(3) commutation rules derived in (8.281) and discussed in Section 25.3. The charges Q_a and axial charges Q_{5a} , defined by

$$\begin{aligned} Q_a &= \int d^3x j^0, \\ Q_{5a} &= \int d^3x j_{5a}^0, \end{aligned} \quad (28.122)$$

form the Lie algebra

$$[Q_a, Q_b] = if_{abc} Q_c, \quad (28.123)$$

$$[Q_a, Q_{5b}] = if_{abc} Q_{5c}, \quad (28.124)$$

$$[Q_{5a}, Q_{5b}] = if_{abc} Q_c. \quad (28.125)$$

From these we may form the chiral charges

$$Q_a^L = (Q_a - Q_{5a})/2, \quad Q_a^R = (Q_a + Q_{5a})/2, \quad (28.126)$$

which generate the two commuting groups SU(3)_L and SU(3)_R, respectively. Due to the chiral invariance of the massless quark gluon Lagrangian density (28.15), the currents are conserved:

$$\begin{aligned} \partial_\mu j^\mu(x) &= 0, \\ \partial_\mu j_5^\mu(x) &= 0. \end{aligned} \quad (28.127)$$

The ground state of the theory breaks the axial part of this symmetry spontaneously. This gives rise to non-zero quark masses. The spontaneous breakdown is accompanied by massless pseudoscalar Nambu-Goldstone bosons, which are identified with the pion and its flavor octet partners.

In nature, quarks are not massless and the axial charges are not conserved. The masses of non-strange quarks are, however, very small so that the axial charges with the SU(2)-indices $a = 1, 2$ are approximately conserved. This is the basis of the PCAC hypothesis (Partial Conservation of Axial vector Current). The nonzero masses of $m_u, m_d, m_s \dots$ raise the mass of the pion and the other pseudoscalar mesons to the experimental nonzero values. The quark masses which give a consistent picture of experimental data are [7]

$$\begin{pmatrix} m_u \\ m_d \\ m_s \\ m_c \\ m_t \\ m_b \end{pmatrix} = \begin{pmatrix} 4.5 \pm 1.4 \\ 7.9 \pm 2.4 \\ 155 \pm 50 \\ 1270 \pm 50 \\ 40000 \pm 10000 \\ 4250 \pm 100 \end{pmatrix} \text{ MeV}. \quad (28.128)$$

In recent years, much insight into the theory has been gained from computer simulations of lattice models of the theory. They have confirmed that the theory has the desired properties to explain the many strongly interacting particles observed in the laboratory.

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*Do not worry about your difficulties in Mathematics.
I can assure you mine are still greater.*
ALBERT EINSTEIN (1879-1955)

29

Cosmology with General Curvature-Dependent Lagrangian

According to a sixty-year-old idea of Andrei Sakharov [1], the gravitational properties of spacetime should not be considered a consequence of a fundamental action associated with the metric of spacetime. Instead they may be viewed as an emerging property caused by the bending stiffness of all quantum fields. This idea of induced gravity has inspired many subsequent generalization attempts of Einstein's theory. More than four decades ago, Buchdahl set up a nonlinear Lagrangian for the metric tensor which was supposed to govern the evolution of the cosmos [2]. This led Starobinsky to work with a simple specific version of it that was restricted to linear and quadratic terms in curvature and Ricci tensors [3]. Later Adler [4] proposed to consider Einstein gravity as a scale-breaking effect in a quantum field theory. Other recent versions of induced gravity were inspired by string theories [5].

Another early generalization [6] of Einstein gravity was inspired by theories of the elasticity and plasticity [7] of solid materials. When a steel tape is bent, it initially resists linearly to the deformations, following Hooke's law of elasticity. If the deformation becomes strong, however, defects are created which lead to tiny cracks in the material and make a further bending increasingly easier. If gravity arises in a similar way from the bending stiffness of all matter fields, it may be assumed to lose stiffness in a similar way. For small curvature R , the Lagrange density starts out following a Hooke-like law which is linear in R , so that gravity is described by the Einstein-Hilbert action. When the curvature becomes larger, however, the Lagrangian density $\mathcal{L}(R)$ grows at a smaller pace and may even saturate at a finite value that is observable as a cosmological constant Λ .

Many present-day discussions generalize our proposal for $\mathcal{L}(R)$ and discuss it under the name of $f(R)$ -gravity (see the review article [8]). Whatever specific function is used, all such Lagrangians start out linearly for small R , and continue in various ways for larger R .

29.1 Simple Curvature-Saturated Model

As a warm-up, let us investigate the physical consequences of the simple Lagrangian density proposed in [6]. It interpolates smoothly between the Einstein-Hilbert Lagrangian in (4.352) for small R and a pure cosmological constant for large R . It will be referred to as *curvature-saturated model* [6] and its Lagrangian density has the form

$$\mathcal{L}_{\text{cs}}(R) = -\frac{1}{2\kappa} \frac{R}{\sqrt{1 + l^4 R^2}}. \quad (29.1)$$

Here κ is related to Newton's gravitational constant by Eq. (4.354). It contains a length parameter l that may be much larger than the Planck length l_{P} in Eq. (4.355). According to present cosmological data, l^2 is larger than l_{P}^2 by roughly a factor $10^{122}/2$. This is seen, for example, in Eq. (19.157) of the textbook [9], or in the data of Ref. [11], according to which $\mathcal{L}_{\text{cs}}(R)$ seems to saturate at the cosmological constant Λ :

$$\mathcal{L}_{\text{cs}}(R) \underset{R \rightarrow \infty}{=} -\Lambda \approx -10^{-122} \frac{1}{l_{\text{P}}^4}. \quad (29.2)$$

Let us derive the cosmological consequences of such an $\mathcal{L}_{\text{cs}}(R)$, and compare the ansatz (29.1) with other possible model functions of R . The mathematical techniques for this were developed in Refs. [12, 13, 14, 15, 16].

One of the motivations for a renewed interest in a more detailed consideration of cosmology with non-linear curvature terms comes from the so-called M-theory (see Ref. [17] “Brane New World”). In that theory, a conformal anomaly becomes relevant, and this turns out to have similar consequences as the R^2 -term in Starobinsky's model. The latest results concerning the effective Λ -term in such models are contained in Ref. [18].

A general argument why we should expect the full gravitational action to interpolate between the linear behavior in R and a saturation at large curvature can be seen in the treatment of the vacuum energy in Ref. [19]. A study of finite-size effects on the quantum field states in a closed Friedmann universe [10] shows that instead of a continuous distribution of the energy levels one has a discrete spectrum. If the radius a of the spatial part of spacetime shrinks to small values, the scalar curvature R becomes large. The spacings between the energy levels increase, and after a certain threshold, all fields wind up in the ground state. It is this general behavior that is summarized in an effective Lagrangian density $\mathcal{L}_{\text{cs}}(R)$. The concrete form of $\mathcal{L}(R)$ cannot yet be fully determined, but the discussion suggests that the R -dependence at large curvature should approach a cosmological constant $-\Lambda$. The model (29.1) represents the simplest analytic function connecting this large- R behavior with the correct weak-field shape à la Einstein-Hilbert.

This chapter is organized as follows. First we calculate the consequences of the Lagrangian density (29.1). In particular we want to see how the cosmological

evolution is influenced by the R -dependence of the effective gravitational constant $\kappa_{\text{eff}}(R)$. This is defined by the derivative

$$\frac{1}{2\kappa_{\text{eff}}(R)} \equiv -\frac{d\mathcal{L}(R)}{dR}. \quad (29.3)$$

For the Lagrangian density (29.1), it reads explicitly:

$$\kappa_{\text{eff}}(R) = \kappa \sqrt{1 + l^4 R^2}^3. \quad (29.4)$$

It corresponds to an effective Newton constant

$$G_{\text{eff}}(R) = G_N \sqrt{1 + l^4 R^2}^3, \quad (29.5)$$

that tends to infinity for large R .

Then we apply two different conformal transformations to $\mathcal{L}_{\text{cs}}(R)$. One of them will make $\mathcal{L}_{\text{cs}}(R)$ asymptotically equivalent to the Gurovich-ansatz [20, 21]:

$$\mathcal{L}_G(R) = -\frac{R}{2\kappa} - c_1 |R|^{4/3}. \quad (29.6)$$

The other makes use of Bicknell's theorem that will be discussed in Section 29.4. That theorem establishes a conformal relation of the $\mathcal{L}_{\text{cs}}(R)$ -theory to Einstein's theory by coupling it minimally to a scalar field ϕ with a suitably chosen potential $\tilde{V}(\phi)$. Up to now, only the second of these conformal transformations has been employed in the literature.¹ The physical consequences of different conformal transformations are quite different since the resulting metrics are *not* related to each other by any coordinate transformation.

Our approach differs fundamentally from that derived from the *limiting curvature hypothesis* (LCH) in Refs. [23], where the gravitational Lagrangian reads

$$\mathcal{L}_{\text{LHC}}(R) = -R - \frac{\Lambda}{2} \left(\sqrt{1 - R^2/\Lambda^2} - 1 \right). \quad (29.7)$$

Its derivative with respect to R diverges for $R \rightarrow \Lambda$. This divergence was supposed to prevent a curvature singularity to appear in cosmological evolution. This goal not completely reached by the model (29.7), since other curvature invariants may still diverge. Some of them are discussed in Ref. [24]. All these considerations have remained restricted to isotropic models. In more general spacetimes one faces the problem that sometimes a curvature singularity exists, even though all polynomial curvature invariants stay finite. In contrast to Eq. (29.7), which limits large curvatures, our model (29.1) *favors* increasing curvature values.

¹See, for instance, Ref. [22] or references cited therein.

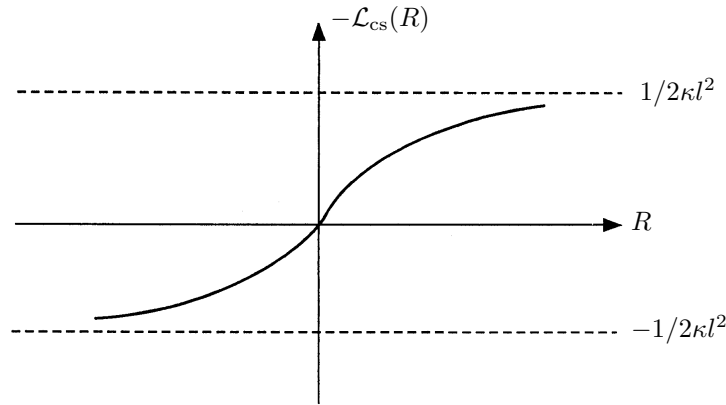


FIGURE 29.1 Curvature-saturated Lagrangian as a function of the curvature scalar R .

29.2 Field Equations of Curvature-Saturated Gravity

The curvature-saturated Lagrangian (29.1) interpolates between the Einstein-Hilbert Lagrangian

$$\mathcal{L}_{\text{EH}} = -\frac{R}{2\kappa}, \quad (29.8)$$

which is experimentally well confirmed at weak fields, and a pure cosmological constant Λ at strong fields:

$$\mathcal{L}_{\text{cs}}(R) \underset{R \rightarrow \infty}{=} -\Lambda = -\frac{1}{2\kappa l^2}. \quad (29.9)$$

The R -dependence is plotted in Fig. 29.1.

From our curvature-saturated Lagrangian (29.1) we obtain, via the derivative with respect to R , an effective gravitational constant (29.5). If one considers the Newtonian limit for a general Lagrangian $\mathcal{L}(R)$ which may tend asymptotically to a nonvanishing cosmological constant, the potential between two point masses contains a Newtonian $1/r$ -part plus a Yukawa-like part $\exp(-r/r_Y)$ stemming from the nonlinearities of the Lagrangian. Details will be given in the Appendix. At distances much larger than r_Y , but much smaller than $1/\sqrt{|R|}$, only the $1/r$ -term survives, and the coupling strength of the $1/r$ -term is given by the effective gravitational constant $G_{\text{eff}}(R)$.

For a general Lagrangian $\mathcal{L}(R)$ such as ours in (29.1), the calculation of the field equation is somewhat tedious, since the Palatini formalism, which simplifies calculations in Einstein's theory, is no longer applicable. Recall that in this formalism, metric and affine connections are varied independently, and the latter are identified with the Christoffel symbols only at the end. Fortunately, the following indirect procedure leads rather efficiently to the correct field equations. We define

$$\mathcal{L}' \equiv \frac{d\mathcal{L}}{dR}, \quad \mathcal{L}'' \equiv \frac{d^2\mathcal{L}}{dR^2}, \quad (29.10)$$

and calculate the covariant energy-momentum tensor of the gravitational field. It is given by the variational derivative of $\mathcal{L}(R)$ with respect to the metric $g_{\mu\nu}(x)$:

$$\overset{\text{f}}{T}_{\mu\nu} \equiv -\frac{2}{\sqrt{-g}} \frac{\delta \mathcal{L}(R) \sqrt{-g}}{\delta g^{\mu\nu}}, \quad (29.11)$$

where g denotes the determinant of $g_{\mu\nu}(x)$. For dimensional reasons, $\overset{\text{f}}{T}_{\mu\nu}$ has the following structure:

$$\overset{\text{f}}{T}_{\mu\nu} = \alpha \mathcal{L}' R_{\mu\nu} + \beta \mathcal{L}' R g_{\mu\nu} + \gamma \mathcal{L} g_{\mu\nu} + \delta \square \mathcal{L}' g_{\mu\nu} + \epsilon \mathcal{L}'_{;\mu\nu}, \quad (29.12)$$

with the 5 real constants $\alpha, \beta, \dots, \epsilon$. The index separated by a semicolon abbreviates the covariant derivative, i.e., $v_{\nu;\mu}(x) \equiv D_\mu v_\nu(x)$, and the symbol $\square$ denotes the Laplace-Beltrami operator (1.390) in four spacetime dimensions. The 5 constants can be uniquely determined, up to a common overall constant, by the covariant conservation law

$$\overset{\text{f}}{T}^{\mu\nu}_{;\nu} = 0. \quad (29.13)$$

Recalling the coupling of matter to gravity in Eq. (5.66), we obtain the generalization of the Einstein-Hilbert equation (5.71):

$$\overset{\text{m}}{T}_{\mu\nu} = -\frac{1}{2\kappa} (2\mathcal{L}' R_{\mu\nu} - \mathcal{L} g_{\mu\nu} + 2\square \mathcal{L}' g_{\mu\nu} - 2\mathcal{L}'_{;\mu\nu}). \quad (29.14)$$

The calculation is straightforward if one carefully distinguishes between $(\square \mathcal{L}')_{;\mu}$ and $\square(\mathcal{L}'_{;\mu})$, which differ from one another by a multiple of the scalar curvature R . Inserting the curvature-saturated Lagrangian (29.1) into (29.10), we have

$$\mathcal{L}' = \frac{d\mathcal{L}}{dR} = -\frac{1}{2} (1 + l^4 R^2)^{-3/2}, \quad (29.15)$$

and we find from (29.14):

$$\overset{\text{m}}{T}_{\mu\nu} = \frac{1}{\kappa} \left\{ \frac{R_{\mu\nu}}{(1 + l^4 R^2)^{3/2}} - \frac{R g_{\mu\nu}}{2(1 + l^4 R^2)^{1/2}} + g_{\mu\nu} \square \left[\frac{1}{(1 + l^4 R^2)^{3/2}} \right] - \left[\frac{1}{(1 + l^4 R^2)^{3/2}} \right]_{;\mu\nu} \right\}. \quad (29.16)$$

Setting $l = 0$, the right-hand side reduces to $1/\kappa$ times the Einstein tensor.

For the trace of the energy-momentum tensor, the equation (29.16) yields

$$\overset{\text{m}}{T}_{\mu}{}^{\mu} = \frac{1}{\kappa} \left\{ \frac{R + 2l^4 R^3}{(1 + l^4 R^2)^{3/2}} - 3\square \left[\frac{1}{(1 + l^4 R^2)^{3/2}} \right] \right\}. \quad (29.17)$$

This implies that in vacuum, the only constant curvature scalar is $R = 0$. Therefore, this model does not possess a de Sitter solution. Furthermore, we can see from Eq. (29.16) that a curvature singularity does not necessarily imply a divergence in the energy-momentum tensor.

29.3 Effective Gravitational Constant and Weak-Field Behavior

Let us compare the effective gravitational constant G_{eff} of our curvature-saturated model with those of other models discussed in the literature. From (29.5), we see that $G_{\text{eff}}(R)$ has the weak-field expansion

$$G_{\text{eff}}(R) = G_{\text{N}} \left(1 + \frac{3}{2} l^4 R^2 + \dots \right), \quad (29.18)$$

and the strong-field expansion

$$G_{\text{eff}} = G_{\text{N}} l^6 |R|^3 \left(1 + \frac{3}{2 l^4 R^2} + \dots \right). \quad (29.19)$$

The full R -behavior is plotted in Fig. 31.1.

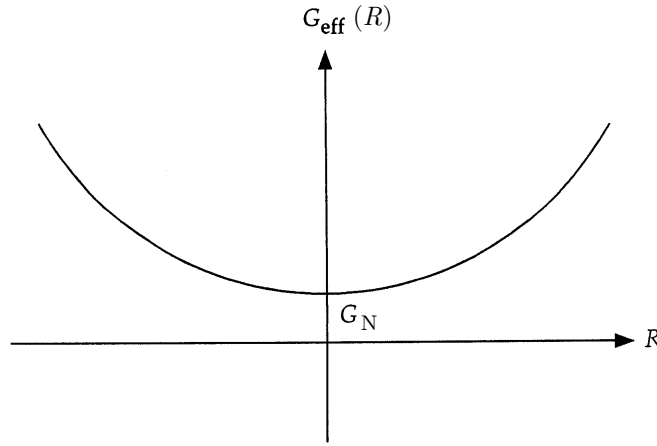


FIGURE 29.2 Effective gravitational constant as a function of the scalar curvature R .

The weak-field expansion of $\mathcal{L}_{\text{cs}}(R)$ is given by

$$\mathcal{L}_{\text{cs}}(R) = -\frac{R}{2\kappa\sqrt{1+l^4R^2}} = -\frac{R}{2\kappa} - \sum_{k=1}^{\infty} b_k R^{2k+1} \quad (29.20)$$

with real coefficients b_k , where $b_1 = -l^4/32\pi G$.

29.4 Bicknell's Theorem

This theorem was published four decades ago [25]. It relates general R -dependent Lagrangians of the type (29.15) to ordinary Einstein's theory coupled minimally to a scalar field ϕ with a suitably chosen interaction potential $\tilde{V}(\phi)$. More details are given in Ref. [12]. The full Lagrangian density is given by

$$\mathcal{L}_{\text{EH}} + \frac{1}{2} \phi_{,\mu} \phi^{,\mu} - \tilde{V}(\phi). \quad (29.21)$$

The relation of $\tilde{V}(\phi)$ with $\mathcal{L}_{\text{cs}}(R)$ is expressed most simply by introducing a field with a different normalization $\psi \equiv \sqrt{2/3}\phi$, in terms of which the potential reads

$$\tilde{V}(\phi) \equiv V(\psi) = \mathcal{L}_{\text{cs}}(R)e^{-2\psi} - \frac{R}{2}e^{-\psi}, \quad (29.22)$$

with R being the inverse function of

$$\psi(R) = \ln[2\mathcal{L}'_{\text{cs}}(R)]. \quad (29.23)$$

The metric in the transformed Lagrangian (29.21) is a conformally transformed version of $g_{\mu\nu}$:

$$\tilde{g}_{\mu\nu} = e^{\psi}g_{\mu\nu}. \quad (29.24)$$

For our particular Lagrangian (29.15) we have from (29.23):

$$\psi(R) = -\frac{3}{2}\ln(1 + l^4 R^2). \quad (29.25)$$

Now we restrict our attention to the range $R > 0$ and $\psi < 0$; the other sign can be treated analogously. Then (29.25) is inverted to

$$R = \frac{1}{l^2}\sqrt{e^{-2\psi/3} - 1}, \quad (29.26)$$

and (29.22) becomes

$$V(\psi) = \frac{1}{2l^2}(e^{-5\psi/3} - e^{-\psi})\sqrt{e^{-2\psi/3} - 1}. \quad (29.27)$$

In the range under consideration, this is a positive and monotonously increasing function of $-\psi$ shown in Fig. 29.3, with the large- ψ behavior

$$V(\psi) = \frac{1}{2l^2}e^{-2\psi}. \quad (29.28)$$

This is the typical exponential potential used in cosmological theories with power-law inflation. As mentioned before, there exists no exact de Sitter inflation. For $\psi \rightarrow 0$, also $V(\psi)$ tends to zero like a power $4\sqrt{2/3}\psi^{3/2}$.

If $V(\psi)$ has a quadratic minimum at some ψ_0 with a positive value $V_0 = V(\psi_0)$, then there exists a stable de Sitter inflationary phase. As a pleasant feature, the potential $V(\psi)$ has no maximum which would have given rise to undesired tachyons. From Eq. (29.25) one can see that for weak fields, the function ψ starts out like R^2 . A theory whose Lagrangian density behaves like $R + R^2$ would have $\psi \sim R$.

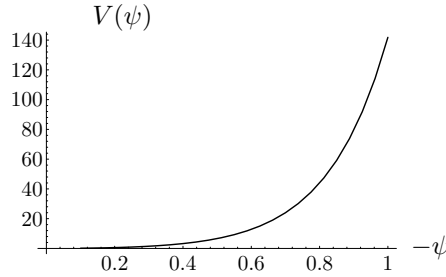


FIGURE 29.3 Potential $V(\psi)$ associated with the curvature-saturated action (29.1) via Bicknell's theorem.

Appendix 29A Newtonian Limit in a Nonflat Background

The Newtonian limit of a theory of gravity in a nonflat background is defined as being the weak-field slow-motion limit of fields whose energy-momentum tensor $\overset{\text{m}}{T}_{\mu\nu}(x)$ is dominated by the component $\overset{\text{m}}{T}_{00}(x)$ in comoving time. In textbooks, the limit is formed in a flat background, and sometimes it is believed that the flatness is a necessary assumption. This is, however, not true, and we show here briefly how the limit can be calculated in a nonflat background. Note that the result is different from what is usually called a *Newtonian cosmology* [26].

To have a concrete example, we take as a background the de Sitter spacetime. The slow-motion assumption allows us to work with static spacetime and matter, assuming the energy-momentum tensor to be

$$\overset{\text{m}}{T}_{ij} = \rho \delta^0_i \delta^0_j, \quad (29A.1)$$

where ρ is the energy density, and time is assumed to be synchronized. The length element in de Sitter spacetime in its static form can be written as

$$ds^2 = -(1 - kr^2)dt^2 + \frac{dr^2}{1 - kr^2} + r^2 d\Omega^2, \quad (29A.2)$$

where $x^0 = t$, $x^1 = r$, $x^2 = \chi$, $x^3 = \theta$ and $d\Omega^2 = d\chi^2 + \sin^2 \chi d\theta^2$ is the metric of the 2-sphere. In this Appendix, we have changed the signature of the metric from $(+---)$, which is usual in cosmology, to $(-+++)$, which leads to the standard definition of the Laplacian. The parameter k characterizes the following physical situations: For $k = 0$, we have the usual flat background. By setting $k = 0$ we can therefore compare the equations with well-known results. The case $k > 0$ corresponds to a positive cosmological constant Λ . In the calculations, we must observe that the time coordinate t fails to be synchronized for $k \neq 0$, but it is obvious from the context how to obtain the synchronized time from it. In the coordinates (29A.2), there is a horizon at $r = r_0 \equiv 1/\sqrt{k}$. So, our approach makes sense in the interval $0 < r < r_0$. However, r_0 will be quite large in comparison with the system under consideration, so that we do not encounter any problem here. Then the following ansatz is appropriate:

$$ds^2 = -(1 - kr^2)(1 - 2\varphi)dt^2 + \left(\frac{dr^2}{1 - kr^2} + r^2 d\Omega^2 \right) (1 + 2\psi), \quad (29A.3)$$

where φ and ψ depend on the spatial coordinates only. The weak-field assumption allows us to linearize the metric with respect to φ and ψ . An extended matter configuration can be obtained by superposition of point particles, so we only need to solve the problem for a δ -source at $r = 0$.

Assuming this to be spherically symmetric, we may take $\varphi = \varphi(r)$ and $\psi = \psi(r)$ in Eq. (29A.3). For the metric components we get:

$$g_{00} = -(1 - kr^2)(1 - 2\varphi), \quad g_{11} = \frac{1 + 2\psi}{1 - kr^2}, \quad g_{22} = r^2(1 + 2\psi), \quad g_{33} = g_{22} \cdot \sin^2 \chi. \quad (29A.4)$$

The inverted components are, up to linear order in φ and ψ ,

$$g^{00} = -\frac{1 + 2\varphi}{1 - kr^2}, \quad g^{11} = (1 - kr^2)(1 - 2\psi), \quad g^{22} = \frac{1 - 2\psi}{r^2}, \quad g^{33} = g^{22} \sin^2 \chi, \quad (29A.5)$$

which gives the Christoffel symbols

$$\Gamma_{01}^0 = -\varphi' - \frac{kr}{1 - kr^2}, \quad (29A.6)$$

$$\Gamma_{00}^1 = (1 - kr^2) [-kr + 2kr(\varphi + \psi) - \varphi'(1 - kr^2)], \quad (29A.7)$$

$$\Gamma_{11}^1 = \psi' + \frac{kr}{1 - kr^2}, \quad (29A.8)$$

$$\Gamma_{12}^2 = \Gamma_{13}^3 = \psi' + \frac{1}{r}, \quad (29A.9)$$

$$\Gamma_{22}^1 = -r(1 - kr^2) - \psi' r^2(1 - kr^2), \quad (29A.10)$$

$$\Gamma_{33}^1 = \sin^2 \chi \Gamma_{22}^1, \quad (29A.11)$$

$$\Gamma_{32}^3 = \cot \chi, \quad (29A.12)$$

$$\Gamma_{33}^2 = -\sin \chi \cos \chi, \quad (29A.13)$$

and the Ricci tensor reads

$$R_{00} = -3k(1 - kr^2) - \varphi''(1 - kr^2)^2 - \frac{2\varphi'}{r}(1 - kr^2) + 6k(\varphi + \psi)(1 - kr^2) + kr(1 - kr^2)(5\varphi' - \psi'), \quad (29A.14)$$

$$R_{11} = -2\psi'' + \varphi'' - \frac{2}{r}\psi' + \frac{3k}{1 - kr^2} + \frac{kr}{1 - kr^2}(\psi' - 3\varphi'), \quad (29A.15)$$

$$R_{22} = 3kr^2 - \psi'' r^2(1 - kr^2) - \psi'(2r - 4kr^3) + (\varphi' - \psi')(r - kr^3), \quad (29A.16)$$

$$R_{33} = R_{22} \sin^2 \chi. \quad (29A.17)$$

Before we discuss these equations, we consider two obvious limits:

For $k = 0$, we see that

$$R_{00} = -\varphi'' - 2\varphi'/r = -\Delta\varphi, \quad (29A.18)$$

which leads to the usual Newtonian field equation $\Delta\varphi = -4\pi G\rho$.

For $\varphi = \psi = 0$, we get for the Ricci tensor:

$$R_0^0 = R_1^1 = R_2^2 = R_3^3 = 3k, \quad (29A.19)$$

and thus the de Sitter spacetime with $R = 12k$ for $k > 0$.

Returning to the general case we have

$$\frac{R}{2} = 6k - 12k\psi + (\varphi'' - 2\psi'')(1 - kr^2) + \frac{2}{r}\varphi' - 5kr\varphi' - \frac{4}{r}\psi' + 7kr\psi', \quad (29A.20)$$

and thus

$$R_0^0 - \frac{R}{2} = -3k + 6k\psi + 2\psi''(1 - kr^2) - 6kr\psi' + \frac{4}{r}\psi'. \quad (29A.21)$$

The other components have a similar structure and can be calculated easily from the above equations. The first term $-3k$ on the right-hand side will be compensated by the Λ -term. The usual gauging to $\psi \rightarrow 0$ and $\varphi \rightarrow 0$ for $r \rightarrow \infty$ is impossible since the above approximation is no more applicable for $r > r_0$. As an alternative gauge we add to ψ and φ suitable constant values so that they are approximately zero in the region under consideration. So we may disregard the term $6k\psi$. All remaining terms with k can be obtained from those without k by multiplying with factors of the type $1 + \epsilon$ where $\epsilon \approx kr^2$, $k = 1/r_0^2$, with r_0 being of the order of magnitude of the world radius. In a first approximation, this gives only a small correction to the gravitational constant. In a second approximation, there are deviations from the $1/r$ -behavior. An analogous discussion for the Lagrangian $R + l^2 R^2$ tells us that, in a range where $l \ll r \ll r_0$, the potential behaves like $(1 - c_1 e^{-r/l})/r$, as in flat space.

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*By three methods we may learn wisdom:
 First, by reflection, which is noblest;
 Second, by imitation, which is easiest;
 And third by experience, which is the bitterest.*
 CONFUCIUS (551 BC- 471 BC)

30

Einstein Gravity from Fluctuating Conformal Gravity

Among the many possible gravitational theories, set up in the previous section to generalize the Einstein-Hilbert action

$$\mathcal{A}_{\text{EH}} = -\frac{1}{2\kappa} \int d^4x (-g)^{1/2} R, \quad (30.1)$$

there exists a special one that has a chance of leading to a renormalizable quantum field theory. Its action is based on the conformally invariant expression¹

$$\mathcal{A}_{\text{conf}} = -\frac{1}{8e_c^2} \int d^4x (-g)^{1/2} C_{\lambda\mu\nu\kappa} C^{\lambda\mu\nu\kappa}, \quad (30.2)$$

where $C_{\lambda\mu\nu\kappa}$ is the conformal *Weyl tensor* composed of the Riemann curvature tensor $R_{\lambda\mu\nu\kappa}$ and the Ricci tensor $R_{\mu\kappa} \equiv g^{\nu\lambda} R_{\mu\nu\lambda\kappa}$ as [1]

$$C_{\lambda\mu\nu\kappa} = R_{\lambda\mu\nu\kappa} + \frac{1}{2}(g_{\lambda\nu} R_{\mu\kappa} - g_{\lambda\kappa} R_{\mu\nu} - g_{\mu\nu} R_{\lambda\kappa} + g_{\mu\kappa} R_{\lambda\nu}) - \frac{1}{6}R(g_{\lambda\nu} g_{\mu\kappa} - g_{\lambda\kappa} g_{\mu\nu}). \quad (30.3)$$

Inserting this decomposition into (30.2), we obtain

$$\mathcal{A}_{\text{conf}} = -\frac{1}{8e_c^2} \int d^4x (-g)^{1/2} (R_{\lambda\mu\nu\kappa} R^{\lambda\mu\nu\kappa} - 2R_{\mu\nu} R^{\mu\nu} + \frac{1}{3}R^2). \quad (30.4)$$

Using the fact that the Lanczos integral [2]

$$\int d^4x (-g)^{1/2} (R_{\lambda\mu\nu\kappa} R^{\lambda\mu\nu\kappa} - 4R_{\mu\nu} R^{\mu\nu} + R^2) \quad (30.5)$$

is a topological invariant that does not contribute to the equations of motion, the conformal action (30.4) can be rewritten as

$$\mathcal{A}_{\text{conf}} = -\frac{1}{4e_c^2} \int d^4x (-g)^{1/2} (R_{\mu\nu} R^{\mu\nu} - \frac{1}{3}R^2). \quad (30.6)$$

¹Note that $1/e_c^2$ has the dimension $\hbar$.

We have neglected surface terms which do not contribute to the equation of motion.

The action (30.2), and thus also (30.6), does not contain any mass scale and is invariant under local *conformal transformations* of the metric introduced by Hermann Weyl [1] as:

$$g_{\mu\nu}(x) \rightarrow \Omega^2(x)g_{\mu\nu}(x) \equiv e^{2\alpha(x)}g_{\mu\nu}(x). \quad (30.7)$$

Based on this action it will eventually be possible to construct a theory of all matter with its weak, electromagnetic, and strong interactions. For this we shall have to extend it with the actions of various extra fields. Before we come to this, we shall study the behavior of spacetime itself as it would follow from the action (30.6) alone.

Up to this point, it is not yet clear that we should choose a negative overall sign of the action (30.2). Since the fluctuations are quantum-mechanical and the path integral in the linear approximation is of the Fresnel type, there is no convergence criterion to settle the sign. Recall that in the Einstein-Hilbert action (4.352), the sign was fixed by the fact that the linearized action (4.372) corresponded in the Euclidean formulation to a strictly positive energy. In the quantum mechanical formulation, this led to the attractive Newton law (5.99) between masses. For the conformally-invariant action, the determination of the sign is nontrivial. Only later, after the calculation of the gravitational potential in Eqs. (30.53) and (30.54), it will turn out that no matter whether we quantize the gravitational field without tachyons (i.e., correctly) or with them (i.e., wrongly), we must choose the negative overall sign. In either quantization, the long-range forces are Newton-like.

For simplicity, we shall first focus attention upon the vicinity of the Minkowski metric $\eta_{\mu\nu}$. For this we set $g_{\mu\nu}(x) = \eta_{\mu\nu} + h_{\mu\nu}(x)$, as in (4.350), and expand the action (30.6) in powers of the field $h_{\mu\nu}(x)$, assuming all ten components of $h_{\mu\nu}(x)$ to be much smaller than 1. A functional integral over $e^{i\mathcal{A}_{\text{conf}}}$ takes into account all quantum fluctuations of $h_{\mu\nu}(x)$. The important observation made in this chapter is that these fluctuations are so violent that they are capable of spontaneously generating an Einstein-Hilbert term in the effective action. This will become clear after Eq. (30.44). The Einstein-Hilbert term introduces a nonzero mass scale into the conformal action (30.2). This mass plays the role of a *dimensionally transmuted coupling constant*. It appears in the same way as in scalar QED in Section 17.12. The formal reason for this is that the conformal action has, in the weak-field limit, a term that is quadratic in the fields $h_{\mu\nu}(x)$ and contains four field derivatives. These lead to propagators of $h_{\mu\nu}(x)$ which behave like $\int d^4k e^{ikx}/k^4$. This makes them logarithmically divergent at small k . Such divergencies are quite familiar from two-dimensional many-body field theories. There they prevent the existence of long-range ordered states [3, 4, 5]. In quantum field theories of elementary particles, they lead to a *no-go theorem* for fields of spinless particles of zero mass [6]. A similar phenomenon has been observed long ago in the context of bio-membranes [7], pion condensation [8], ferromagnetism [9], later in string theories with extrinsic curvature [10, 11], and after that in a gravity-like theory [12]. The fourth power of derivatives in the free graviton action makes the long-wavelength fluctuations so violent that the theory spontaneously creates a new mass term. In the case of

biomembranes and stiff strings, this is responsible for the appearance of a surface tension. In conformal gravity, the violent long-wavelength fluctuations produce an effective action à la Einstein-Hilbert that is responsible for the correct long-range behavior of gravitational forces.

30.1 Classical Conformal Gravity

Conformal Gravity has become a fashionable object of study. The initial motivation was to investigate it as an interesting extension of Einstein gravity [25]. It is a purely metric theory that exhibits general coordinate invariance and satisfies the equivalence principle of standard gravity. In addition, it is invariant under the local Weyl transformation (30.7) of the metric. Let us take $R_{\mu\nu\lambda}{}^\kappa$ from Eq. (4.360), and write it as a covariant curl

$$R_{\mu\nu\lambda}{}^\kappa = \{\partial_\mu \Gamma_\nu - \partial_\nu \Gamma_\mu - [\Gamma_\mu, \Gamma_\nu]\}_\lambda{}^\kappa \quad (30.8)$$

of four 4×4 -matrices built from the Christoffel symbols $\{\Gamma_\nu\}_\lambda{}^\kappa \equiv \Gamma_{\nu\lambda}{}^\kappa$. Then the curvature tensor may be viewed as a set of 4×4 -matrices $(R_{\mu\nu})_\lambda{}^\kappa$. These have a form completely analogous to the field strength tensor (28.11) of the SU(3)-invariant nonabelian gauge theory of strong interactions (QCD). This similarity is part of the esthetical appeal of the conformal action (30.2).

As in the QCD action (28.10), the coupling constant e_c^2 is dimensionless, and this ensures that all Feynman diagrams in a perturbation expansion of the theory can be made finite by counter terms that have the same form as those in the initial action. This is what makes the conformal action an attractive candidate for a quantum theory of gravitation.

Adding to (30.2) a source term for the coupling of the gravitational field with matter, which reads [compare with (5.1) and (5.66)]

$$\overset{\text{m}}{\mathcal{A}} = -\frac{1}{2} \int d^4x (-g)^{1/2} g_{\mu\nu} \overset{\text{m}}{T}{}^{\mu\nu}, \quad (30.9)$$

we obtain, from a variation of the total action $\mathcal{A}_{\text{conf}} + \overset{\text{m}}{\mathcal{A}}$ with respect to the metric $g_{\mu\nu}$, the field equation [25]:

$$\frac{1}{2e_c^2} B^{\mu\nu} = \overset{\text{m}}{T}{}^{\mu\nu}, \quad (30.10)$$

where $B^{\mu\nu}$ on the left-hand side is the symmetric and conserved *Bach tensor* defined by

$$\frac{1}{2e_c^2} B^{\mu\nu} \equiv 2(-g)^{-1/2} \frac{\delta \mathcal{A}_{\text{conf}}}{\delta g_{\mu\nu}}. \quad (30.11)$$

Functional differentiation of (30.2) yields the expression

$$B^{\mu\nu} \equiv 2C^{\mu\lambda\nu\kappa}{}_{;\lambda;\kappa} + C^{\mu\lambda\nu\kappa} R_{\lambda\kappa}, \quad (30.12)$$

whose explicit form is

$$B^{\mu\nu} = \frac{1}{2}g^{\mu\nu}R^{;\kappa}_{;\kappa} + R^{\mu\nu;\kappa}_{;\kappa} - R^{\mu\kappa;\nu}_{;\kappa} - R^{\nu\kappa;\mu}_{;\kappa} - 2R^{\mu\kappa}R^{\nu}_{\kappa} + \frac{1}{2}g^{\mu\nu}R_{\lambda\kappa}R^{\lambda\kappa} \\ + \frac{2}{3}g^{\mu\nu}R^{;\kappa}_{;\kappa} - \frac{2}{3}R^{;\mu;\nu} + \frac{2}{3}RR^{\mu\nu} - \frac{1}{6}g^{\mu\nu}R^2. \quad (30.13)$$

Note that the Bach tensor is traceless so that Eq. (30.10) can be satisfied only if the energy-momentum tensor is also traceless.

30.2 Quantization

Let us now study the quantum field theory associated with the action (30.2). It is formally defined by the functional integral ($\hbar = c = 1$) [13]:

$$Z = \sum_i \int_{\Sigma_i} \mathcal{D}g_{\mu\nu} e^{i\mathcal{A}_{\text{conf}}}. \quad (30.14)$$

Here $\mathcal{D}g_{\mu\nu}$ denotes the measure of the functional integral. Its proper treatment requires fixing of both gauge symmetries, the first with respect to coordinate transformations, the second with respect to conformal transformations (30.7). Alternatively, we can use the decomposition (4.435) of the field tensor $h_{\mu\nu}$ into its different irreducible parts under Lorentz transformations, and extend them to the metric tensor to factorize

$$\mathcal{D}g_{\mu\nu} \equiv \mathcal{D}g_{\mu\nu}^{(2)} \mathcal{D}g_{\mu\nu}^l \mathcal{D}g_{\mu\nu}^s. \quad (30.15)$$

The sum in (30.14) comprises a sum over topologically distinct manifolds Σ_i , although it is not clear how to do that, even in principle, since so far four-dimensional manifolds cannot even be classified [13, 14, 15].

Due to the invariance of the theory under general coordinate transformations, only the spin-2 content of the field is physical. This fact may be taken care of by inserting into this measure a δ -functional for the unphysical field components $g_{\mu\nu}^l$. In order to do this in a covariant way we adapt the Faddeev-Popov method of quantum electrodynamics to the present field theory. We go to the weak-field limit and fix the gauge of $h_{\mu\nu}(x)$ by requiring the divergence to satisfy the Hilbert condition (4.399). This can be achieved by inserting into the functional integral (30.14) a gauge-fixing functional analogous to one of the various possible choices (14.353). For example we may use the functional

$$F_4[h] = \exp \left\{ -\frac{i}{2\zeta} \int d^4x [\partial^\mu h_{\mu\nu}(x) - \frac{1}{2}\partial_\nu h(x)]^2 \right\}, \quad (30.16)$$

where ζ is an arbitrary parameter. To find the effect of this choice upon the measure of functional integration, we proceed as in Section 14.16 and insert into $F_4[h]$ the gauge-transformed $h_{\mu\nu}$ -field à la (4.380),

$$h_{\mu\nu}^\Lambda = h_{\mu\nu} + \partial_\mu \Lambda_\nu + \partial_\nu \Lambda_\mu. \quad (30.17)$$

This yields

$$F_4[h^\Lambda] = \exp \left\{ -\frac{i}{2\zeta} \int d^4x [\partial^\mu h_{\mu\nu}(x) - \tfrac{1}{2} \partial_\nu h(x) + \partial^2 \Lambda_\nu] \right\}. \quad (30.18)$$

Integrating this over all $\Lambda_\mu(x)$ determines the normalization functional for the measure [compare (14.365)]:

$$\Phi_4[h] = \int \mathcal{D}^4 \Lambda_\mu F_4[h^\Lambda] \propto \text{Det} (\partial^4)^{-2}. \quad (30.19)$$

With the gauge fixing functional $F_4[h]/\Phi_4[h]$, the measure (30.15) is free of the components $g_{\mu\nu}^l$.

Finally, we account for the conformal invariance of the theory. For this we insert a δ -functional ensuring the vanishing of the scalar part $g_{\mu\nu}^s$ of the metric. In the linear approximation, this is done by inserting a gauge-fixing functional for the scalar part of the field $h^s \equiv h_\mu{}^\mu - \partial_\mu \partial^{-2} \partial_\nu h^{\mu\nu}$ [recall (4.367)]. As an example we insert

$$F_{4'}[h] = \exp \left\{ -\frac{i}{2\xi} \int d^4x (\partial^2 h^s)^2 \right\} = \exp \left\{ -\frac{i}{2\xi} \int d^4x [\partial^2 h_\mu{}^\mu - \partial^\mu \partial^\nu h_{\mu\nu}]^2 \right\}. \quad (30.20)$$

Here ξ is another arbitrary parameter. Subjecting $F_{4'}[h]$ to an infinitesimal Weyl transformation (30.7), which reads

$$h_{\mu\nu} \rightarrow h_{\mu\nu} + 2\alpha(x)\eta_{\mu\nu}, \quad (30.21)$$

we obtain the transformed functional

$$F_{4'}[h^\alpha] = \exp \left\{ -\frac{i}{2\xi} \int d^4x [\partial^2 h_\mu{}^\mu(x) - \partial^\mu \partial^\nu h_{\mu\nu}(x) - 6\partial^2 \alpha]^2 \right\}. \quad (30.22)$$

This can be integrated functionally over all $\alpha(x)$ to yield the normalization functional

$$\Phi_{4'}[h] \propto \text{Det}^{-1/2}(\partial^4). \quad (30.23)$$

Thus, by analogy with the quantum electrodynamic gauge-fixing factor $F_4[A]/\Phi_4$ in (14.366), we obtain in the weak-field approximation the proper measure of quantum gravity in the functional integral (30.14) as

$$\mathcal{D}h_{\mu\nu}^{(2)} \mathcal{D}h_{\mu\nu}^l \mathcal{D}h_{\mu\nu}^s \equiv \mathcal{D}h_{\mu\nu} \frac{F_4[h]}{\Phi_4} \frac{F_{4'}[h]}{\Phi_{4'}} = \text{Det}^{5/2}(\partial^4) \mathcal{D}h_{\mu\nu} F_4[h] F_{4'}[h]. \quad (30.24)$$

A great advantage of the conformal action (30.2) is that the coupling constant α_c is dimensionless so that, by pure power counting, the Feynman diagrams of its perturbation expansions can be renormalized order by order. In addition, the β -function governing the flow of the coupling constant is asymptotically free [16].

It has been explained in the beginning of this chapter that the fluctuations of the field around the Minkowski metric are controlled by a term with four derivatives. As a negative consequence, the propagator in four dimensions $\int d^4k e^{ikx}/k^4$, when

treated à la Feynman, contains modes that move faster than light (tachyons) [17]. They are a signal of the fact that the weak-field expansion of the metric around the Minkowski metric $\eta_{\mu\nu}$ is not an expansion around a state of minimal energy. There exist field configurations of lower energy, and a consistent perturbative expansions must be based on oscillations around that. These are necessarily free of tachyons, as discussed in Section 18.7.

Similar stability arguments have been used in QCD to find an optimal field configuration around which one can perform a perturbation expansion of the theory. In QCD, a first search for a lower minimum was successfully performed by Savvidy [18]. Improvements of his result were found by various authors [19]. If QCD is formulated on a lattice and studied numerically, the formation of a nontrivial vacuum can be followed most explicitly [20].

The instability of Minkowski spacetime against small fluctuations and the associated tachyon problem in quantized gravity have prevented many authors from accepting the conformal action as a viable extension of Einstein's theory. The problem has been discussed in detail by Stelle [21], who showed that tachyonic states are a serious obstacle for making a unitary quantum field theory. One possible way out of the dilemma is by reducing the requirement of renormalizability of the quantum field theory to the more modest requirement of *asymptotic safety* [22, 23]. Another proposal is based on the choice of suitable boundary conditions at large infinity [24]. A third proposal has been made by Bender and Mannheim to use a different quantization procedure [25] of the gravitational fields. They point out that, by studying fluctuation in complex phase space rather than in the real phase space we live in, the tachyonic states disappear [26]. This is a simple generalization of the obvious fact that the unstable potential $V(x) = -x^2/2$ is stable if x is permitted to fluctuate only along the imaginary axis ix . Of course, this consideration does not produce a truly stable minimum of the energy, over which the metric fluctuations would necessarily represent only physical particles which move slower than light. However, if we focus attention upon some important effects of quantum fluctuations, a true stability is not really needed. The reason is that quantum mechanical integrals are of the Fresnel type and can be calculated not only for a stable minimum but also for the inverted potential. In any quantum theory whose action involves four derivatives, an analogous situation exists in the extended phase space consisting of coordinates and their derivatives. In the complex version of it, a quantum theory can be constructed after slight modification of Feynman's rule for calculating propagators of the theory. These will be discussed in detail in Appendix 30B.

In this chapter we want to emphasize the positive consequences of the four derivatives in (30.2). At small k , they make the quantum fluctuations of the gravitational field so violent, that they spontaneously generate Newton forces which will govern the long-distance attraction between celestial bodies. In particular, we shall demonstrate that this type of mechanism spontaneously creates an effective gravitational action that has been proposed long time ago by Starobinsky [27]:

$$\mathcal{A}_{\text{St}} = -\frac{1}{2\kappa} \int d^4x (-g)^{1/2} (R - \xi^2 R^2). \quad (30.25)$$

Here ξ is Starobinsky's parameter that is determined by the inflational scale of the Planck satellite data to be $\xi/\sqrt{\kappa} \sim 10^5$ (see Ref. [28]).

To derive this we begin by expanding the conformal action around a flat background up to quadratic order in $h_{\mu\nu}(x) = g_{\mu\nu}(x) - \eta_{\mu\nu}$, using the weak-field expansions (4.362), (4.363), (4.364), (4.366), and (4.367):

$$\mathcal{A}_{\text{conf}} = -\frac{1}{8e_c^2} \left[\frac{1}{2} \int d^4x h^{\mu\nu} \partial^4 h_{\mu\nu} - \int d^4x \partial^\lambda h_{\lambda\mu} H^{\mu\nu} \partial^\rho h_{\rho\nu} - \frac{1}{6} \int d^4x h^s \partial^4 h^s \right]. \quad (30.26)$$

Here we have introduced the tensors $H_{\mu\nu} = \frac{1}{2} \partial_\mu \partial_\nu - \partial^2 \eta_{\mu\nu}$ and the scalar field $h^s = h_\mu{}^\mu - \partial_\mu \partial^{-2} \partial_\nu h^{\mu\nu}$, as before in (4.367). We have also omitted constant contributions from total derivatives. After some algebra, relegated to Appendix 30A on page 1535, the action (30.26) may be rewritten as

$$\mathcal{A}_{\text{conf}} = -\frac{1}{16e_c^2} \int d^4x \partial^2 h^{\lambda\mu} P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial) \partial^2 h^{\lambda\kappa}, \quad (30.27)$$

where $P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial)$ is the projection operator into the spacetime-dependent symmetric tensor fields of spin 2. It is composed of products of transverse projection operators $P_{\mu\nu}^t(i\partial) = \eta_{\mu\nu} - \partial_\mu \partial_\nu / \partial^2$ as

$$P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial) \equiv \frac{1}{2} [P_{\mu\lambda}^t(i\partial) P_{\nu\kappa}^t(i\partial) + P_{\mu\kappa}^t(i\partial) P_{\nu\lambda}^t(i\partial)] - \frac{1}{3} P_{\mu\nu}^t(i\partial) P_{\lambda\kappa}^t(i\partial) \quad (30.28)$$

[recall Eq. (4G.4)]. Inserting $P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial)$ into (30.27), performing some integrations by part and discarding pure volume terms, we find indeed agreement with (30.26).

It has been shown in Ref. [29] that a conformally invariant action can be derived, in the spirit of Sakharov [30], from the fluctuations of the conformal factor in the partition function of all matter fields of spin s . In a D -dimensional Riemann spacetime with metric $g_{\mu\nu}$, the conformal action receives contributions from the fields of various spins s . Integrating out the conformal transformations of the various spin fields, one obtains the conformal action (30.2) with the inverse coupling constant

$$\frac{1}{4e_c^2} = \frac{1}{8\pi^2(4-D)} \left(\frac{1+N_0}{120} + \frac{N_{1/2}}{40} + \frac{N_1}{10} - 233 \frac{N_{3/2}}{720} + 53 \frac{N_2}{45} \right), \quad (30.29)$$

where N_s is the number of fields of spin s . In four dimensions, this is divergent and requires a conformal action (30.2) to supply a counter term to end up with a finite coupling constant that can eventually be chosen to fit experiments.

Apart from these divergent terms, there are also finite contributions to the conformal action which come from loop diagrams. If all fields of the total action are massless, the classical energy momentum tensor is traceless, as long as we work with the so-called improved energy-momentum tensor of Callan, Coleman, and Jackiw [31]. Apart from that classical part, there are contributions caused by loop diagrams. These are the famous *conformal anomalies* of gravitational theories. For example, a large part of the matter of the universe comes from spin-1/2 Dirac particles. These are believed to be originally created without a mass, so that their

classical energy-momentum tensor is traceless. But if we calculate loop diagrams, each massless Dirac field contributes an anomaly of the gravitational action of the form [32]:

$$\mathcal{A}^{\text{anom}} = \frac{1}{2880\pi^2} \left[\frac{11}{2} C_{\mu\nu\lambda\kappa} C^{\mu\nu\lambda\kappa} - 6 \square R \right], \quad (30.30)$$

where the symbol $\square$ denotes the Laplace-Beltrami operator (1.390) in four space-time dimensions. A similar effective action comes from the loops of other massless particles. The sum of the anomalies of all fields has to be zero, if we want to make sure that quantum gravity can truly be renormalized. It will be important to know at the end which are precisely the fields in the ultimate theory of field and matter.

As usual, we assume that all particle masses arise from a spontaneous symmetry breakdown in scalar field theories of the Higgs type. The precise set of scalar fields in the theory is not yet fully known and will certainly be subject to change in the future. To simulate their typical effect upon gravity we shall couple, *pars pro toto*, a charged scalar fields φ to the gravitational field in an almost minimal way. For this we add, to the conformal action (30.2), the generic Higgs-type action (27.83) that contains the simplest conformally invariant term proportional to R , namely $R|\varphi|^2$. Formulated in curved spacetime with a metric $g_{\mu\nu}(x)$, this has the form [33, 34, 35, 36]:

$$\mathcal{A}^{\text{m}} = \int d^4x (-g)^{1/2} \left\{ \frac{1}{2} g^{\mu\nu} D_\mu^* \varphi^* D_\nu \varphi + \frac{R}{12} |\varphi|^2 - \frac{m^2}{2} |\varphi|^2 - \frac{g}{4} |\varphi|^4 \right\}. \quad (30.31)$$

Here $D_\mu \equiv \partial_\mu + ieA_\mu$ denotes the covariant derivatives defined as in (27.84), with e denoting the respective coupling constant, for example the electromagnetic one. We have omitted the action $-\frac{1}{4} F_{\mu\nu} F^{\mu\nu}$ of the gauge fields themselves that was written down in Eq. (27.83), where the field tensor $F_{\mu\nu}$ collects the covariant curls of all relevant gauge fields, as explained in (27.88). The masses m^2 break the conformal invariance of the theory.

Since the Higgs actions are supposed to generate the correct mass terms of all matter fields, we have constructed them to be invariant under the Weyl transformations

$$g_{\mu\nu}(x) \rightarrow \Omega^2(x) g_{\mu\nu}(x), \quad \varphi(x) \rightarrow \Omega^{-1}(x) \varphi(x). \quad (30.32)$$

Under these the gradient term of the scalar field transforms as follows [43]:

$$\begin{aligned} g^{\mu\nu} D_\mu^* \varphi^* D_\nu \varphi &\rightarrow \Omega^{-2} g^{\mu\nu} D_\mu^* (\Omega^{-1} \varphi^*) D_\nu (\Omega^{-1} \varphi) \\ &\rightarrow \Omega^{-4} [D_\mu^* \varphi^* D^\mu \varphi - \varphi^* (D_\mu \varphi) \Omega^{-1} \partial^\mu \Omega - (D_\mu^* \varphi^*) \varphi \Omega^{-1} \partial^\mu \Omega + \varphi^* \varphi \Omega^{-2} \partial_\mu \Omega \partial^\mu \Omega] \\ &\rightarrow \Omega^{-4} [D_\mu^* \varphi^* D^\mu \varphi + \varphi^* \varphi \Omega^{-1} \square \Omega - \partial_\mu (\varphi^* \varphi \partial^\mu \ln \Omega)]. \end{aligned} \quad (30.33)$$

In the action, the last term can be neglected since it is a total derivative.

The scalar curvature term in (30.31) changes under Weyl transformations like

$$R \rightarrow \Omega^{-2} (R - 6 \Omega^{-1} \square \Omega). \quad (30.34)$$

Therefore a scalar action is properly Weyl invariant if it contains the invariant combination

$$\int d^4x (-g)^{1/2} \left(g^{\mu\nu} D_\mu^* \varphi^* D_\nu \varphi + \frac{1}{6} R |\varphi|^2 \right). \quad (30.35)$$

After the electroweak phase transition, where some of the Higgs fields acquire a nonzero vacuum expectation value, each of them contributes a term of the type

$$\int d^4x (-g)^{1/2} \left(\frac{1}{6} R |\varphi_i|^2 \right). \quad (30.36)$$

For a smooth expectation value of $|\varphi|^2$ in spacetime, this is a term that produces stiffness in spacetime proportionally to the scalar curvature R . When comparing this with the Einstein-Hilbert action (30.1), we see that it has, unfortunately, the wrong overall sign in front of R . Hence the associated gravitational field is unstable. The weak-field gravitational fluctuations of the metric would contain tachyons, and this cannot be, as discussed in Section 18.7. The universe would collapse.

Fortunately, there is a possibility of rescuing stability. This can be done with the help of a modified Higgs-like action which is not made Weyl-invariant by an $R/12$ -term in (30.31), but with the help of a gauge field $w^\mu(x)$ introduced by Weyl in his original work. This can be used to make any derivative of scalar or fermion fields covariant under Weyl transformation. A minimal way of achieving this is by considering a single scalar field ϕ and forming the action

$$\mathcal{A}_{\text{WT}} = \int d^4x (-g)^{1/2} \left\{ \frac{1}{2} \left(g^{\mu\nu} D_\mu^w \phi D_\nu^w \phi - \frac{g}{2} \phi^4 \right) - \frac{1}{4g_w} \overset{w}{F}_{\mu\nu} \overset{w}{F}^{\mu\nu} \right\}. \quad (30.37)$$

Here w_μ is the Weyl gauge field. It was introduced by him to convert a globally Weyl-invariant field into a locally Weyl-invariant form. The symbol

$$D_\mu^w \equiv D_\mu - \Omega^{-1}(x) \partial_\mu \Omega(x) = D_\mu - w_\mu \quad (30.38)$$

denotes the associated covariant derivative, and $F_{\mu\nu}^w \equiv \partial_\mu w_\nu - \partial_\nu w_\mu$ the four-curl. If the Weyl transformation is written in an exponential form as $\Omega(x) = e^{\alpha(x)}$, the Weyl field changes by

$$w_\mu \rightarrow w_\mu + \partial_\mu \alpha(x). \quad (30.39)$$

The gauge field $w(x)$ has the virtue that it makes the action (30.37) Weyl-invariant without an extra R -term. In the action (30.37), the ϕ -fluctuations are stable.

The important observation is now that by a combination of the actions (30.37) and the Higgs-type actions (30.35) it is possible to generate spontaneously an Einstein-Hilbert action whose spacetime fluctuations around Minkowski spacetime are stable. To achieve this we simply add to (30.37) a small admixture of a Higgs-type action with the opposite sign to that of (30.35):

$$\mathcal{A}_{\text{WT}'} = \frac{1}{2} \int d^4x (-g)^{1/2} \left(-g^{\mu\nu} D_\mu \phi D_\nu \phi - \frac{R}{6} \phi^2 \right). \quad (30.40)$$

While doing this we must make sure that the accompanying gradient term of the scalar field remains smaller than that in (30.37) to maintain the *stability* of the ϕ -fluctuations. The admixture of (30.40) will bring in an R -term with the correct sign to ensure *stable* metric fluctuation. The admixture must be small enough to ensure that the total action still has ϕ -stability. But it must be large enough to ensure that the metric fluctuations follow Einstein's theory.

In order to achieve both goals we choose the mixing to be hyperbolic. We multiply action (30.37) by a factor $\cosh^2 \theta$ that is larger than unity, and the admixture of (30.40) by a factor $\sinh^2 \theta$ that is smaller than unity. Thus we form the combination

$$\mathcal{A}_{\text{mixture}} = \cosh^2 \theta \mathcal{A}_{\text{WT}} - \sinh^2 \theta \mathcal{A}_{\text{WT}'}. \quad (30.41)$$

To this we add the curvature terms (30.36) coming from the Higgs fields. After this, the field ϕ is governed by an action

$$\mathcal{A}_{\text{mix}} = \frac{1}{2} \int d^4x (-g)^{1/2} \left[g^{\mu\nu} D_\mu \phi D_\nu \phi - \frac{R}{6} (\phi^2 \sinh^2 \theta - 2 \sum_i |\varphi_i|^2) - \frac{g \cosh^2 \theta}{2} \phi^4 \right], \quad (30.42)$$

where the sum over i runs over all Higgs fields. In going from (30.41) to (30.42), we have omitted the action $-(1/4g_w) F^w_{\mu\nu} F^{w\mu\nu}$ of the Weyl field in (30.37), as well as the accompanying mixing factor $\cosh^2 \theta$.

We can now choose a small enough coupling constant g so that $\langle \phi^2 \rangle \sinh^2 \theta$ becomes much larger than the sum of the $\langle |\varphi_i|^2 \rangle$'s of all Higgs-fields. Then the effective gravitational action spontaneously generated by the scalar field expectations reads

$$\mathcal{A}_{\text{ind}} = - \frac{(\langle \phi^2 \rangle \sinh^2 \theta - 2 \sum_i |\varphi_i|^2)}{12} \int d^4x (-g)^{1/2} R = - \frac{1}{2\bar{\kappa}} \int d^4x (-g)^{1/2} R. \quad (30.43)$$

This corresponds to an induced gravitational constant

$$\frac{1}{\bar{\kappa}} \equiv \frac{(\langle \phi^2 \rangle \sinh^2 \theta - 2 \sum_i |\varphi_i|^2)}{6}, \quad (30.44)$$

which can be adjusted to be equal to the experimental value $1/\kappa$.

Hyperbolic mixing angles of this type have been introduced before in Refs. [34]–[37]. If the Higgs fields are neglected and only a single scalar field ϕ is assumed to be present, the theory is similar to the modified gravity in the Brans-Dicke formulation [38], for which a quantization has been proposed in Ref. [39].

Let us study the consequences of the generated R -term (30.43) in the conformal gravity. The new terms coming from the expectation values $\langle \phi^2 \rangle$ and $\langle |\varphi_i|^2 \rangle$ carry mass dimensions and therefore break the conformal symmetry of the action. The action governing the fluctuations of the metric comes from the sum of (30.27) and (30.43), in which we have made $\bar{\kappa}$ equal to the experimental gravitational coupling κ :

$$\mathcal{A}_{\text{conf}'} = - \frac{1}{16e_c^2} \int d^4x \partial^2 h^{\lambda\mu} P_{\mu\nu, \lambda\kappa}^{(2)} \partial^2 h^{\lambda\kappa} + \frac{1}{4\kappa} \int d^4x h_{\mu\nu} G^{\mu\nu}. \quad (30.45)$$

The last term in this action can also be composed in terms of the projection operators discussed in Appendix 4G. From these we derive Eq. (5.77), thus obtaining the action

$$\begin{aligned}\mathcal{A}_{\text{conf}'} &= -\frac{1}{16e_c^2} \int d^4x \partial^2 h^{\lambda\mu} P_{\mu\nu,\lambda\kappa}^{(2)} \partial^2 h^{\lambda\kappa} - \frac{1}{8\kappa} \int d^4x h^{\mu\nu} P_{\mu\nu,\lambda\kappa}^{(2)} \partial^2 h^{\lambda\kappa} \\ &+ \frac{1}{4\kappa} \int d^4x h^{\mu\nu} P_{\mu\nu,\lambda\kappa}^s \partial^2 h_{\lambda\mu}.\end{aligned}\quad (30.46)$$

This governs the fluctuations of $h_{\mu\nu}(x)$ for smooth average values of $\langle\phi^2\rangle$ and $\langle|\varphi_i|^2\rangle$.

We can now integrate out the gravitational field fluctuations $h_{\mu\nu}(x)$. For this purpose, we rewrite the action (30.46) as

$$\mathcal{A}_{\text{conf}'} = -\frac{1}{16e_c^2} \int d^4x h^{\lambda\mu} P_{\mu\nu,\lambda\kappa}^{(2)} \left(\partial^4 + \frac{2e_c^2}{\kappa} \partial^2 \right) h^{\lambda\kappa} + \frac{1}{4\kappa} \int d^4x h^{\mu\nu} P_{\mu\nu,\lambda\kappa}^s h^{\lambda\kappa}.\quad (30.47)$$

Integrating out the spin-2 part yields the effective action

$$\Gamma^{(2)} = \int \frac{d^D k}{(2\pi)^D} \log \left(k^4 - \frac{2e_c^2}{\kappa} k^2 \right).\quad (30.48)$$

The divergent momentum integral can be made finite by standard counterterms.

The logarithm contains the denominator of the propagator

$$G^{(2)}(k) = \frac{i}{k^2(k^2 - 2e_c^2/\kappa)}\quad (30.49)$$

of the graviton in this theory. It shows that the nonzero average values of $|\phi|^2$ and $|\varphi_i|^2$ in (30.43) and (30.46) change the initial free-field propagator associated with the conformal action (30.27),

$$\langle h_{\mu\nu}^{(2)}(k) h_{\lambda\kappa}^{(2)*}(k) \rangle = 8e_c^2 \frac{P_{\mu\nu,\lambda\kappa}^{(2)}(k)}{k^4}\quad (30.50)$$

into the propagator (30.49) associated with the action (30.47). In spacetime, the propagator requires calculating a Fourier transform

$$G^{(2)}(x - x') = \int \frac{d^4 k}{(2\pi)^4} \frac{i}{k^2(k^2 - 2e_c^2/\kappa)} e^{-ik(x-x')}.\quad (30.51)$$

For this we have to specify the boundary conditions. This is commonly done by prescribing the path in the complex plane along which the integral over k^0 should encircle the zeros in the denominator of the integral. If this is done in the same way as in Feynman's QED, one would find [compare (30B.15)]

$$G^{(2)}(x - x') = \int \frac{d^4 k}{(2\pi)^4} \frac{i}{(k^2 + i\epsilon)(k^2 - 2e_c^2/\kappa + i\epsilon)} e^{-ik(x-x')}.\quad (30.52)$$

This would imply that the nonzero average values of $|\phi|^2$ and $|\varphi_i|^2$ in (30.43) and (30.46) would change the free-field propagator (30.50) into

$$\langle h_{\mu\nu}^{(2)}(k) h_{\lambda\kappa}^{(2)*}(k) \rangle = 4\kappa P_{\mu\nu,\lambda\kappa}^{(2)}(k) \left(\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - 2e_c^2/\kappa + i\epsilon} \right). \quad (30.53)$$

The negative sign in front of the second term is a signal of the “wrong quantization” in which the states with the nonzero square mass $2e_c^2/\kappa$ have a negative norm. As announced before, this can be corrected by exchanging the Feynman rules for calculating the propagators with new $i\epsilon$ -prescriptions (discussed in detail in Appendix 30B; see in particular the poles in Fig. 30.2). Thus, after a proper quantization the massive contributions to the propagator will appear with an opposite sign with respect to (30.53), and with an opposite $i\epsilon$ -term, so that (30.53) turns into [compare with (30B.38) and (30B.41)]:

$$\langle h_{\mu\nu}^{(2)}(k) h_{\lambda\kappa}^{(2)*}(k) \rangle = 4\kappa P_{\mu\nu,\lambda\kappa}^{(2)}(k) \left(\frac{1}{k^2 + i\epsilon} + \frac{1}{k^2 - 2e_c^2/\kappa - i\epsilon} \right). \quad (30.54)$$

The spin-0 part adds to this the propagator

$$\langle h_{\mu\nu}^s(k) h_{\lambda\kappa}^{s*}(k) \rangle = 2\kappa P_{\mu\nu,\lambda\kappa}^s(k) \frac{1}{k^2 + i\epsilon}. \quad (30.55)$$

As a cross check we verify that the sum of the first term in (30.54) plus the spin-0 term (30.55) is equal to the fluctuations (5.98) in Einstein gravity. At long distances, this guarantees the Newton potential $-G_N M_1 M_2 / r$ between celestial bodies of masses M_1 and M_2 [recall the derivation in (5.100)].

At very short distances of the order of $r_Y = \sqrt{\kappa/2e_c^2}$, the gravitational potential $1/r$ is modified by the addition of a repulsive Yukawa potential. It becomes $1/r + e^{-r/r_Y}/r$.

Experimentally, such quantum corrections to the gravitational forces are extremely hard to measure. If two bodies are brought together to atomic distances, there are immediately other forces which are much stronger than gravity and will dominate any measurement. Even if the bodies are carefully kept neutral, to avoid Coulomb interactions, there are molecular forces of the van-der-Waals type, which will win at the nanometer scale. It is therefore not astonishing that present experimental limits for the Newton forces are quite rough. They do not reach below 5 micrometers [40]. So far, one must be quite inventive to find observations which allow better tests [41]. The data produced by the Planck satellite [28] seem to be attractive candidates for this purpose, albeit only after a generous use of a theory that is still being discussed in the literature [42].

Let us see what phenomenological R^2 -term emerges from the action developed so far as a correction in the Starobinsky action (30.25). It can be found from the weak-field approximation to the scalar curvature in the actions (30.31) and (30.43). In the former, we simply take the effective potentials

$$V(\varphi_i) = \frac{1}{2} \left(m_i^2 + \frac{R}{6} \right) |\varphi_i|^2 + \frac{g_i}{4} |\varphi_i|^4. \quad (30.56)$$

For negative m_i^2 , these give an unstable contribution to the Einstein action (30.43) for each Higgs field φ_i . From the minima, we obtain the condensation energies

$$V_{\min} = - \sum_i \frac{1}{4g_i} (m_i^2 + R/6)^2. \quad (30.57)$$

The sum of these yields the effective action of the R^2 -type

$$\mathcal{A}_{R^2 \varphi}^{\text{eff}} = \sum_i \frac{1}{4g_i} \int d^4x (-g)^{1/2} \frac{R^2}{36}. \quad (30.58)$$

A further term proportional to R^2 is found from the action (30.42):

$$\mathcal{A}_{R^2 \phi}^{\text{eff}} = \frac{1}{4g} \int d^4x (-g)^{1/2} \frac{R^2}{36} \frac{\sinh^4 \theta}{\cosh^2 \theta}. \quad (30.59)$$

Adding this to (30.58), we find a total effective action of the R^2 -type:

$$\mathcal{A}_{R^2}^{\text{eff}} = \frac{1}{2} \int d^4x (-g)^{1/2} \frac{R^2}{36} \left(\frac{1}{2g} \frac{\sinh^4 \theta}{\cosh^2 \theta} + \sum_i \frac{1}{2g_i} \right). \quad (30.60)$$

This can be brought into agreement with the R^2 -correction term in the Starobinsky action (30.25), if we choose the dimensionless parameters g and g_i to satisfy the condition

$$\frac{\xi^2}{\kappa} = \frac{1}{36} \left(\frac{1}{2g} \frac{\sinh^4 \theta}{\cosh^2 \theta} + \sum_i \frac{1}{2g_i} \right). \quad (30.61)$$

Then we obtain the correct prefactor of the R^2 -term in Starobinsky's action (30.25), thus reproducing optimally the data of the Planck satellite.

Let us also calculate loop corrections to these results. For this we assume all coupling constants g_i in the scalar Higgs actions (30.31) to be small, at most of the order of e_c^4 . Then we can ignore higher order perturbations of the order of g_i^2 , and find that the gravitational fluctuations produce an effective potential as a function of φ_i :

$$V(\varphi_i) = \frac{g_i}{4} |\varphi_i|^4 + \frac{3e_c^4}{64\pi^2} |\varphi_i|^4 \left(\log \frac{|\varphi_i|^2}{\mu^2} - \frac{25}{6} \right). \quad (30.62)$$

Here we may introduce a dimensionally transmuted coupling constant M defined by the equation

$$\frac{g_i}{4} = \frac{3e_c^4}{64\pi^2} \left(\log \frac{\mu^2}{M_i^2} + \frac{11}{3} \right). \quad (30.63)$$

Then Eq. (30.62) becomes

$$V(\varphi_i) = \frac{3e_c^4}{64\pi^2} |\varphi_i|^4 \left(\log \frac{|\varphi_i|^2}{M_i^2} - \frac{1}{2} \right). \quad (30.64)$$

This potential has a minimum at $\varphi_i = \varphi_{i,f}$ which satisfies

$$\langle |\varphi_{i,f}|^2 \rangle = M_i^2. \quad (30.65)$$

To see what this minimum implies for the effective potential (30.64), we expand around $|\varphi_i|^2 = M_i^2$ up to the second order in $\Delta_i \equiv |\varphi_i|^2 - M_i^2$ and find

$$V(\varphi_i) = V(0) - RM_i^2 - R\Delta_i + \frac{3e_c^4}{64\pi^2}\Delta_i^2 + \mathcal{O}(\Delta_i^3), \quad (30.66)$$

where $V(0) \equiv -3M^4e_c^4/128\pi^2$. The minimum with respect to Δ_i lies at $\Delta_i = 32\pi^2/3e_c^4$. It has the value

$$V_{\min} = V(0) - RM_i^2 - \frac{32\pi^2}{6e_c^4}R^2. \quad (30.67)$$

The sum of second terms over i changes the spontaneously generated Einstein action.

30.3 Outlook

We have discussed a quantum field theory based on a conformally invariant action for the gravitational field. The standard problem has appeared that small fluctuations around Minkowski spacetime possess tachyonic excitation. It implies that spacetime is unstable with respect to these fluctuations. To solve this problem, one must find a new nontrivial spacetime configuration that is analogous to a confining field configuration of QCD. That started from an approximate configuration found by Savvidy and others. In gravity, a solution of this problem must be left to the future.

In this chapter we have dealt with a more modest problem. We have used the fact that by extending the phase space of the spacetime of our universe into certain complex directions and by allowing fluctuations to take place only along the new axes, we have succeeded in constructing a conformal quantum field theory. Its restricted phase space fluctuations have only physical properties. As shown at the end of Appendix 30B, the perturbative expansions contain no tachyons and are capable of generating spontaneously an Einstein-Hilbert action. The resulting theory reproduces the presently known forces between celestial bodies, and specifies their fluctuation corrections.

We did not enter into a discussion of the very fundamental problem whether it makes sense to consider quantum fluctuations of a field system that is intrinsically classical [13, 45]. Indeed, famous quantum field theorists like Freeman Dyson have expressed severe doubts about this [46].

Appendix 30A Some Algebra

Inserting the projection operator $P_{\mu\nu,\lambda\kappa}^{(2)}(i\partial)$ of Eq. (30.28) into (30.27), we find with $\hat{\partial} \equiv \partial/\sqrt{\partial^2}$:

$$\int d^4x \partial^2 h^{\mu\nu} P_{\mu\nu,\lambda\kappa}^{(2)}(\hat{q}) \partial^2 h^{\lambda\kappa} = \int d^4x \partial^2 h^{\mu\nu} \partial^2 [h_{\mu\nu} - 2\hat{\partial}_\mu(\hat{\partial}^\lambda h_{\lambda\nu}) + \hat{\partial}_\mu\hat{\partial}_\nu(\hat{\partial}^\lambda\hat{\partial}^\kappa h_{\lambda\kappa})]$$

$$\begin{aligned}
& -\frac{1}{3} \int d^4x \partial^2 h^{\mu\nu} (g_{\mu\nu} - \hat{\partial}_\mu \hat{\partial}_\nu) (g_{\lambda\kappa} - \hat{\partial}_\lambda \hat{\partial}_\kappa) \partial^2 h^{\lambda\kappa} \\
& = \int d^4x \partial^2 h^{\mu\nu} \partial^2 [h_{\mu\nu} - 2\hat{\partial}_\mu (\partial^\lambda h_{\lambda\nu}) + \hat{\partial}_\mu \hat{\partial}_\nu (\partial^\lambda \hat{\partial}^\kappa h_{\lambda\kappa})] - \frac{1}{3} \int d^4x \partial^2 h_s \partial^2 h_s \\
& = \int d^4x \partial^2 h^{\mu\nu} \partial^2 h_{\mu\nu} + \int d^4x (\partial_\mu h^{\mu\nu}) \partial^2 [2(\partial^\lambda h_{\lambda\nu}) - \hat{\partial}_\nu \hat{\partial}^\kappa (\partial^\lambda h_{\lambda\kappa})] - \frac{1}{3} \int d^4x \partial^2 h_s \partial^2 h_s \\
& = \int d^4x \partial^2 h^{\mu\nu} \partial^2 h_{\mu\nu} - 2 \int d^4x (\partial_\mu h^{\mu\nu}) \partial^2 H_\nu{}^\kappa (\partial^\lambda h_{\lambda\kappa}) - \frac{1}{3} \int d^4x \partial^2 h_s \partial^2 h_s. \tag{30A.1}
\end{aligned}$$

Using (4.366), we see that

$$\begin{aligned}
& \int d^4x (-g)^{1/2} R_{\mu\nu} R^{\mu\nu} \\
& = \frac{1}{4} \int d^4x (\partial^2 h_{\mu\nu} - \partial_\mu \partial^\lambda h_{\lambda\nu} - \partial_\nu \partial^\lambda h_{\lambda\mu} + \partial_\mu \partial_\nu h) (\partial^2 h_{\mu\nu} - \partial_\mu \partial^\lambda h_{\lambda\nu} - \partial_\nu \partial^\lambda h_{\lambda\mu} + \partial_\mu \partial_\nu h) \\
& = \frac{1}{4} \int d^4x [(\partial^2 h_{\mu\nu})^2 + 2(\partial_\mu \partial^\lambda h_{\lambda\nu})^2 + 2(\partial^\lambda \partial^\nu h_{\lambda\nu})(\partial^\mu \partial^\kappa h_{\mu\kappa}) + (\partial_\mu \partial_\nu h)^2 \\
& \quad + 4\partial^2 (\partial^\mu h_{\mu\nu})(\partial^\lambda h_{\lambda\nu}) + 2\partial^2 (\partial^\mu \partial^\nu h_{\mu\nu})h - 4\partial^2 (\partial^\lambda \partial^\nu h_{\lambda\nu})h] \\
& = \frac{1}{4} \int d^4x [(\partial^2 h_{\mu\nu})^2 - \partial^\nu \partial^\kappa (\partial^\lambda h_{\lambda\nu})(\partial^\mu h_{\mu\kappa}) + \partial^2 (\partial^\mu h_{\mu\nu})(\partial^\lambda h_{\lambda\nu}) + [(\partial_\mu \partial_\nu - \eta_{\mu\nu} \partial^2)h^{\mu\nu}]^2] \\
& = \frac{1}{4} \int d^4x [(\partial^2 h_{\mu\nu})^2 - 2(\partial^\lambda h_{\lambda\nu})H^{\nu\kappa}(\partial^\mu h_{\mu\kappa}) + (\partial^2 h_s)^2]. \tag{30A.2}
\end{aligned}$$

Hence

$$\begin{aligned}
2 \int d^4x (-g)^{1/2} (R_{\mu\nu} R^{\mu\nu} - \frac{1}{3} R^2) & = \frac{1}{2} \int d^4x [(\partial^2 h_{\mu\nu})^2 - 2(\partial^\lambda h_{\lambda\nu})H^{\nu\kappa}(\partial^\mu h_{\mu\kappa}) - \frac{1}{3}(\partial^2 h_s)^2] \\
& = \frac{1}{2} \int d^4x \partial^2 h^{\mu\nu} P_{\mu\nu, \lambda\kappa}^{(2)} \partial^2 h^{\lambda\kappa}. \tag{30A.3}
\end{aligned}$$

Note that the linearized Einstein tensor (4.376) can be expressed in terms of the projection operator $P_{\mu\nu, \lambda\kappa}^{(2)}(i\partial)$ of Eq. (30.28) and the spin-zero projection operator $P_{\mu\nu, \lambda\kappa}^s(i\partial)$ of Eq. (5.76). The result was stated in Eq. (5.77). We may use that formula to find a more convenient expression for the weak-field Einstein-Hilbert action (4.378). Inserting formula (5.77) for the Einstein tensor $G_{\mu\nu}$ into the weak-field action (4.378), we obtain:

$$\mathcal{A} = \frac{1}{4\kappa} \int d^4x (-g)^{1/2} h_{\mu\nu} G^{\mu\nu} = \frac{1}{4\kappa} \int d^4x (-g)^{1/2} \left[h^{\mu\nu} \left(-\frac{1}{2} P_{\mu\nu, \lambda\kappa}^{(2)} \right) \partial^2 h^{\lambda\kappa} + \frac{1}{3} h_s \partial^2 h_s \right]. \tag{30A.4}$$

The last term in the brackets may also be written as $h^{\mu\nu} P_{\mu\nu, \lambda\kappa}^s \partial^2 h^{\lambda\kappa}$.

Appendix 30B Quantization without Tachyons

The simplest prescription for quantizing a scalar field with an action

$$\mathcal{A} = \frac{1}{2} \int dt x (-\partial_t^2 - \omega_0^2) x \tag{30B.1}$$

was found by Feynman. He inverted the differential operator between the fluctuating field variable in Fourier space and defined

$$G(\omega) = \frac{i}{\omega^2 - \omega_0^2} = \frac{1}{2\omega_0} \left(\frac{i}{\omega - \omega_0} - \frac{i}{\omega + \omega_0} \right). \tag{30B.2}$$

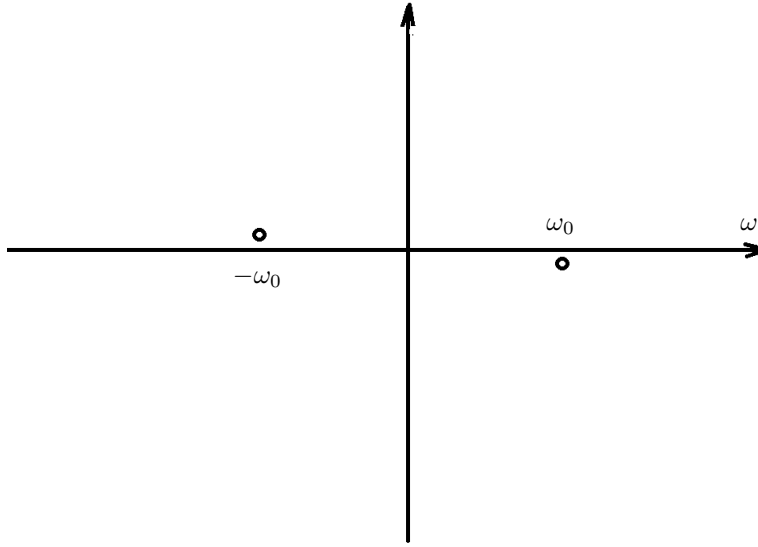


FIGURE 30.1 Calculation of Feynman propagator in Green function (30B.3). Compare with Fig. (7.1) on p. 495.

From this he calculated the Fourier transformation and settled the boundary conditions by circumventing the poles in the complex ω -plane at ω_0 and $-\omega_0$ as shown in Fig. 30.1. The result of the ω -integration is [recall (1.319)]

$$\begin{aligned} G^F(t) &= \frac{1}{2\pi} \int d\omega e^{-i\omega t} G(\omega) \\ &= \theta(t) \frac{e^{-i\omega_0 t}}{2\omega_0} + \theta(-t) \frac{e^{i\omega_0 t}}{2\omega_0}. \end{aligned} \quad (30B.3)$$

Equivalently, we can place the poles at the slightly shifted positions $\omega_0 - i\epsilon$ and $-\omega_0 + i\epsilon$ with an infinitesimal positive ϵ . Then the Feynman propagator is given by the integral

$$G^F(t) = \frac{1}{2\pi} \int d\omega \frac{i}{\omega^2 - \omega_0^2 + i\epsilon} e^{-i\omega t} \quad (30B.4)$$

$$= \frac{1}{2\pi} \int d\omega e^{-i\omega t} \frac{1}{2\omega_0} \left(\frac{i}{\omega - \omega_0 + i\epsilon} - \frac{i}{\omega + \omega_0 - i\epsilon} \right) e^{-i\omega t}. \quad (30B.5)$$

Let us now perform the quantization in the canonical formulation of the model. Then we replace the action (30B.1) by

$$\mathcal{A}_{\text{can}} = \int dt (ip_x \dot{x} - H), \quad (30B.6)$$

where H is the Hamiltonian:

$$H = \frac{p^2}{2} + \frac{\omega_0^2}{2} x^2. \quad (30B.7)$$

The quantization proceeds via the canonical path integral

$$(x' t | x 0) = \int \mathcal{D}p \frac{\mathcal{D}x}{2\pi} e^{i\mathcal{A}_{\text{can}}}. \quad (30B.8)$$

The variables $x(t)$ and $p(t)$ can be expressed in terms of creation and annihilation operators $a^\dagger$ and a as [compare (7.12) and (7.10)]:

$$x = \frac{1}{\sqrt{2\omega_0}} (a e^{-i\omega_0 t} + a^\dagger e^{i\omega_0 t}),$$

$$p = \frac{-i\omega_0}{\sqrt{2}\omega_0} (ae^{-i\omega_0 t} - a^\dagger e^{i\omega_0 t}) = \dot{x}. \quad (30B.9)$$

In terms of these, the Hamiltonian reads [compare 7.30) and 7.31)]

$$H = \frac{1}{2} (\dot{x}^2 + \omega_0^2 x^2) = (a^\dagger a + \frac{1}{2})\omega_0. \quad (30B.10)$$

Let us now quantize a theory whose fluctuating variable has four time derivatives in its action

$$\mathcal{A} = \frac{1}{2} \int dt x (-\partial_t^2 - \omega_1^2)(-\partial_t^2 - \omega_2^2)x. \quad (30B.11)$$

For this we have to calculate the Fourier transform of

$$G(\omega) = \frac{i}{(\omega^2 - \omega_1^2)(\omega^2 - \omega_2^2)}. \quad (30B.12)$$

The integrand can be decomposed as

$$G(\omega) = \frac{1}{\omega_1^2 - \omega_2^2} \left(\frac{i}{\omega^2 - \omega_1^2} - \frac{i}{\omega^2 - \omega_2^2} \right) \quad (30B.13)$$

and further as

$$\begin{aligned} G(\omega) &= \frac{1}{2\omega_1(\omega_1^2 - \omega_2^2)} \left(\frac{i}{\omega - \omega_1} - \frac{i}{\omega + \omega_1} \right) \\ &- \frac{1}{2\omega_2(\omega_1^2 - \omega_2^2)} \left(\frac{i}{\omega - \omega_2} - \frac{i}{\omega + \omega_2} \right). \end{aligned} \quad (30B.14)$$

If one had to calculate a propagator according to the Feynman prescription, one would find

$$\begin{aligned} G^F(t) &= \frac{1}{2\pi} \int d\omega e^{-i\omega t} G(\omega) \\ &= \frac{\theta(t)}{\omega_1^2 - \omega_2^2} \left(\frac{e^{-i\omega_1 t}}{2\omega_1} - \frac{e^{-i\omega_2 t}}{2\omega_2} \right) + \frac{\theta(-t)}{\omega_1^2 - \omega_2^2} \left(\frac{e^{i\omega_1 t}}{2\omega_1} - \frac{e^{i\omega_2 t}}{2\omega_2} \right). \end{aligned} \quad (30B.15)$$

This propagator arises from the following quantization procedure. We rewrite the action (30B.11) as

$$\mathcal{A} = \frac{1}{2} \int dt [\ddot{x}^2 - (\omega_1^2 + \omega_2^2) \dot{x}^2 + \omega_1^2 \omega_2^2 x^2], \quad (30B.16)$$

and identify the velocity $\dot{x}$ as a new variable v . Then we replace the action (30B.16) by

$$\mathcal{A}_{\text{can}} = \int dt (ip_x \dot{x} + ip_v \dot{v} - H), \quad (30B.17)$$

with the Hamiltonian

$$H = \frac{p_v^2}{2} + p_x v + \frac{1}{2} (\omega_1^2 + \omega_2^2) v^2 - \frac{1}{2} \omega_1^2 \omega_2^2 x^2. \quad (30B.18)$$

The quantization of this canonical system was performed a long time ago in Ref. [44]. The amplitude is the result of a path integral

$$(x' v'; t | x v; 0) = \int \mathcal{D}p_v \frac{\mathcal{D}v_v}{2\pi} \mathcal{D}p_x \frac{\mathcal{D}x}{2\pi} e^{i\mathcal{A}_{\text{can}}}. \quad (30B.19)$$

The operator form of this quantization was obtained by the substitution (assuming $\omega_2 > \omega_1$)

$$\begin{aligned} x &= x_1 + x_2, \\ p_x &= -\frac{1}{\omega_2^2 - \omega_1^2} (\omega_2^2 \dot{x}_1 - \omega_1^2 \dot{x}_2), \\ v &= \dot{x}_1 + \dot{x}_2, \\ p_v &= -\frac{1}{\omega_2^2 - \omega_1^2} (\omega_1^2 x_1 + \omega_2^2 x_2). \end{aligned} \quad (30B.20)$$

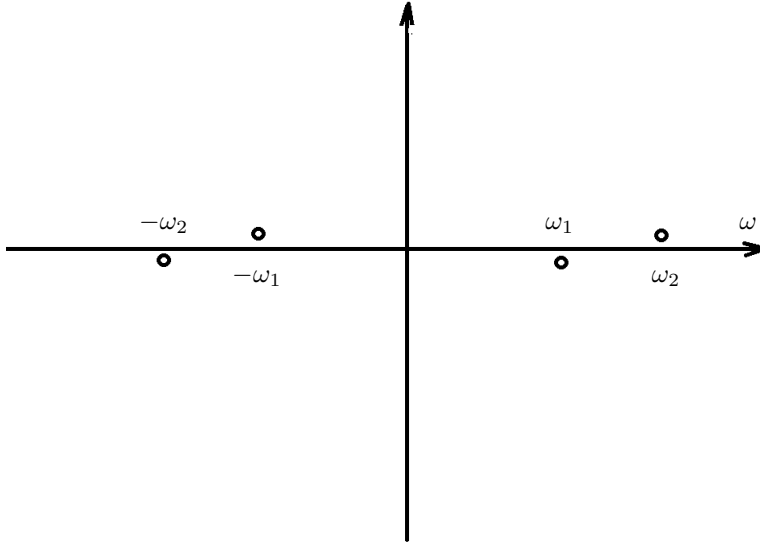


FIGURE 30.2 Calculation of Feynman propagator without tachyons in Green function (30B.12).

If we express the real variables x_1 and x_2 in terms of creation and annihilation operators $a^\dagger$ and a as in (30B.9), but with a slightly more convenient normalization of these, we obtain [compare Section 2.22.2]

$$\begin{aligned}
 x &= a_1 e^{-i\omega_1 t} + a_1^\dagger e^{i\omega_1 t} + a_2 e^{-i\omega_2 t} + a_2^\dagger e^{i\omega_2 t}, \\
 p_x &= \frac{1}{2(\omega_2^2 - \omega_1^2)} [i\omega_1 \omega_2^2 (a_1 e^{-i\omega_1 t} - a_1^\dagger e^{i\omega_1 t}) + i\omega_1^2 \omega_2 (a_2 e^{-i\omega_2 t} - a_2^\dagger e^{i\omega_2 t})], \\
 v &= -i\omega_1 (a_1 e^{-i\omega_1 t} - a_1^\dagger e^{i\omega_1 t}) - i\omega_2 (a_2 e^{-i\omega_2 t} - a_2^\dagger e^{i\omega_2 t}), \\
 p_v &= -\frac{1}{2(\omega_2^2 - \omega_1^2)} [\omega_1^2 (a_1 e^{-i\omega_1 t} + a_1^\dagger e^{i\omega_1 t}) + \omega_2^2 (a_2 e^{-i\omega_2 t} + a_2^\dagger e^{i\omega_2 t})], \quad (30B.21)
 \end{aligned}$$

and the Hamiltonian operator takes the form

$$H = \omega_1 a_1^\dagger a_1 - \omega_2 a_2^\dagger a_2 + \frac{1}{2}(\omega_1 + \omega_2). \quad (30B.22)$$

The states created by powers of $a_2^\dagger$ have an energy that can be lowered arbitrarily which makes the ground state unstable.

Let us now quantize the same theory without such unwanted states [26]. Once this is done for each momentum eigenmode and integrated over all momenta, one obtains a quantum field theory without tachyons. We simply use an ω -integration with a contour as shown in Fig. (30.2). The pole at $\omega = \omega_2$ is circumnavigated for negative t in the anticlockwise sense, and this cancels the negative sign in the last term of (30B.15). A similar sign change happens with the second term in (30B.15) for positive t from the pole at $\omega = -\omega_2$. Thus the integral yields the positive-definite expression (assuming that $\omega_2 > \omega_1$):

$$\begin{aligned}
 G^{\text{pos}}(t) &= \frac{1}{2\pi} \int d\omega e^{-i\omega t} G(\omega) \\
 &= \frac{\theta(t)}{\omega_2^2 - \omega_1^2} \left(\frac{e^{-i\omega_1 t}}{2\omega_1} + \frac{e^{i\omega_2 t}}{2\omega_2} \right) + \frac{\theta(-t)}{\omega_2^2 - \omega_1^2} \left(\frac{e^{i\omega_1 t}}{2\omega_1} + \frac{e^{-i\omega_2 t}}{2\omega_2} \right). \quad (30B.23)
 \end{aligned}$$

The corresponding quantization comes about after a unitary transformation of the canonical pairs of variables z, p_z and v, p_v by an operator

$$\mathcal{Q} = i\alpha p_v p_z - i\beta v z. \quad (30B.24)$$

This yields

$$\begin{aligned} e^{-\mathcal{Q}} v e^{\mathcal{Q}} &= v \cosh(\sqrt{\alpha\beta}) - \sqrt{\frac{\alpha}{\beta}} p_z \sinh(\sqrt{\alpha\beta}), \\ e^{-\mathcal{Q}} p_v e^{\mathcal{Q}} &= p_v \cosh(\sqrt{\alpha\beta}) + \sqrt{\frac{\beta}{\alpha}} z \sinh(\sqrt{\alpha\beta}), \\ e^{-\mathcal{Q}} z e^{\mathcal{Q}} &= z \cosh(\sqrt{\alpha\beta}) - \sqrt{\frac{\alpha}{\beta}} p_v \sinh(\sqrt{\alpha\beta}), \\ e^{-\mathcal{Q}} p_z e^{\mathcal{Q}} &= p_z \cosh(\sqrt{\alpha\beta}) + \sqrt{\frac{\beta}{\alpha}} v \sinh(\sqrt{\alpha\beta}). \end{aligned} \quad (30B.25)$$

We shall choose α and β to have the ratio

$$\frac{\beta}{\alpha} = \omega_1^2 \omega_2^2, \quad (30B.26)$$

and satisfy

$$\sinh(\sqrt{\alpha\beta}) = \frac{2\omega_1\omega_2}{\omega_2^2 - \omega_1^2}, \quad \cosh(\sqrt{\alpha\beta}) = \frac{\omega_1^2 + \omega_2^2}{\omega_2^2 - \omega_1^2}, \quad (30B.27)$$

so that

$$\sqrt{\frac{\alpha}{\beta}} \sinh(\sqrt{\alpha\beta}) = \frac{2}{\omega_2^2 - \omega_1^2}. \quad (30B.28)$$

Then the transformations (30B.25) can also be written as

$$\begin{aligned} e^{-\mathcal{Q}} v e^{\mathcal{Q}} &= v \frac{\omega_1^2 + \omega_2^2}{\omega_2^2 - \omega_1^2} - p_z \frac{2}{\omega_2^2 - \omega_1^2}, \\ e^{-\mathcal{Q}} p_v e^{\mathcal{Q}} &= p_v \frac{\omega_1^2 + \omega_2^2}{\omega_2^2 - \omega_1^2} + z \frac{2\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2}, \\ e^{-\mathcal{Q}} z e^{\mathcal{Q}} &= z \frac{\omega_1^2 + \omega_2^2}{\omega_2^2 - \omega_1^2} - p_v \frac{2}{\omega_2^2 - \omega_1^2}, \\ e^{-\mathcal{Q}} p_z e^{\mathcal{Q}} &= p_z \frac{\omega_1^2 + \omega_2^2}{\omega_2^2 - \omega_1^2} + v \frac{2\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2}, \end{aligned} \quad (30B.29)$$

$$(30B.30)$$

and the canonical form of the action (30B.18) becomes

$$\mathcal{A}_{\text{can}} = \int dt (ip_z \dot{z} + ip_v \dot{v} - H), \quad (30B.31)$$

with the Hamiltonian

$$H = \frac{p_v^2}{2} + \frac{p_z^2}{2\omega_2^2} + \frac{1}{2} (\omega_1^2 + \omega_2^2) v^2 + \frac{1}{2} \omega_1^2 \omega_2^2 z^2. \quad (30B.32)$$

This is a positive-definite operator. The canonical variables in H can be expressed in terms of two variables with frequencies ω_1 and $\omega_2 > \omega_1$ defined by

$$z = x_1 + ix_2,$$

$$\begin{aligned}
p_v &= \frac{1}{2(\omega_2^2 - \omega_1^2)}(-\omega_1^2 x_1 - i\omega_2^2 x_2), \\
v &= \dot{x}_1 - i\dot{x}_2, \\
p_z &= \frac{1}{2(\omega_2^2 - \omega_1^2)}(\omega_2^2 \dot{x}_1 + i\omega_1^2 \dot{x}_2).
\end{aligned} \tag{30B.33}$$

The corresponding creation-annihilation operator forms are

$$\begin{aligned}
z &= a_1 e^{-i\omega_1 t} + a_1^\dagger e^{i\omega_1 t} + i(a_2 e^{-i\omega_2 t} + a_2^\dagger e^{i\omega_2 t}), \\
p_v &= \frac{1}{2(\omega_2^2 - \omega_1^2)}[-\omega_1^2(a_1 e^{-i\omega_1 t} + a_1^\dagger e^{i\omega_1 t}) - i\omega_2^2(a_2 e^{-i\omega_2 t} + a_2^\dagger e^{i\omega_2 t})], \\
v &= -i\omega_1(a_1 e^{-i\omega_1 t} - a_1^\dagger e^{i\omega_1 t}) + \omega_2(a_2 e^{-i\omega_2 t} - a_2^\dagger e^{i\omega_2 t}), \\
p_z &= \frac{1}{2(\omega_2^2 - \omega_1^2)}[i\omega_2^2 \omega_1(a_1 e^{-i\omega_1 t} - a_1^\dagger e^{i\omega_1 t}) + \omega_1^2 \omega_2(a_2 e^{-i\omega_2 t} - a_2^\dagger e^{i\omega_2 t})].
\end{aligned} \tag{30B.34}$$

This brings the Hamiltonian (30B.32) to the form

$$H = \omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 + \frac{1}{2}(\omega_1 + \omega_2), \tag{30B.35}$$

showing once more that the eigenstates all have a positive energy.

All results in this Appendix can immediately be taken over from quantum mechanics to quantum field theory. We simply replace the frequencies ω_0 , ω_1 and ω_2 by the momentum-dependent frequencies $\omega_0(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2}$, $\omega_1(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m_1^2}$ and $\omega_2(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m_2^2}$, and sum the expressions over all momenta, using the phase space integral formula $\sum_{\mathbf{p}} = V \int d^3p / (2\pi)^3$.

Then the quantum mechanical Green function (30B.3) turns into the quantum field-theoretic one:

$$G(x) = \theta(x_0) \int \frac{d^3p}{(2\pi)^3} \frac{e^{-i\omega_0(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_0(\mathbf{p})} + \theta(-x_0) \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\omega_0(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_0(\mathbf{p})}. \tag{30B.36}$$

Remember now that there is another, covariant way of expressing this Green function, namely in the Feynman way (7.146):

$$G_m^F(x - x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - m^2 + i\epsilon} e^{-ip(x-x')}, \tag{30B.37}$$

where we have used a superscript to indicate the Feynman $i\epsilon$ boundary condition and a subscript for the mass. Indeed, the p_0 -integral reproduces the Heaviside functions and forces the energy to be equal to the $\mathbf{p}$ -dependent values $\omega_0(\mathbf{p})$.

By the appropriate treatments of the poles in the energy integral, the positive Green function (30B.23) turns into the tachyon-free expression

$$\begin{aligned}
G^{\text{NT}}(x) &= \frac{\theta(x_0)}{m_2^2 - m_1^2} \int \frac{d^3p}{(2\pi)^3} \left(\frac{e^{-i\omega_1(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_1(\mathbf{p})} + \frac{e^{i\omega_2(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_2(\mathbf{p})} \right) \\
&+ \frac{\theta(-x_0)}{m_2^2 - m_1^2} \int \frac{d^3p}{(2\pi)^3} \left(\frac{e^{i\omega_1(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_1(\mathbf{p})} + \frac{e^{-i\omega_2(\mathbf{p})x_0 + i\mathbf{p}\mathbf{x}}}{2\omega_2(\mathbf{p})} \right).
\end{aligned} \tag{30B.38}$$

Also here exists another, covariant way of expressing the Green function, namely in the form:

$$\begin{aligned}
G^{\text{NT}}(x) &= \int \frac{d^4p}{(2\pi)^4} \frac{i}{(p^2 - m_1^2 + i\eta)(p^2 - m_2^2 - i\eta)} e^{-ipx} \\
&= \frac{1}{m_2^2 - m_1^2} \int \frac{d^4p}{(2\pi)^4} \left(\frac{i}{p^2 - m_1^2 + i\epsilon} e^{-ipx} + \frac{i}{p^2 - m_2^2 - i\epsilon} e^{ipx} \right).
\end{aligned} \tag{30B.39}$$

Again, the p_0 -integral reproduces the Heaviside functions and forces the energy to be equal to the $\mathbf{p}$ -dependent values $\omega_1(\mathbf{p})$ and $\omega_2(\mathbf{p})$.

After reversing the direction of the energy integral in the second expression, this can be rewritten as

$$G^{\text{NT}}(x) = \frac{1}{m_2^2 - m_1^2} \int \frac{d^4 p}{(2\pi)^4} \left(\frac{i}{p^2 - m_1^2 + i\epsilon} e^{-ipx} + \frac{i}{p^2 - m_2^2 + i\epsilon} e^{ipx} \right), \quad (30\text{B.40})$$

or as

$$G^{\text{NT}}(x) = \frac{1}{m_2^2 - m_1^2} [G_{m_1}^{\text{F}}(x) + G_{m_2}^{\text{F}}(-x)]. \quad (30\text{B.41})$$

Now the spectral decomposition has explicitly a sum over propagators which carry only physical, non-tachyonic states with positive norm. Since a perturbatively defined quantum gravity can be expanded via Wick's theorem into a sum of free-particle diagrams in $G^{\text{NT}}(x)$, all diagrams involve only physical propagators.

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*In order for the light
to shine so brightly,
the darkness must be present.*
FRANCIS BACON (1561-1626)

31

Purely Geometric Part of Dark Matter

Plots of orbital velocities of stars of galaxies as a function of their distance from the center show a great surprise: They do not decrease with distance in a way that would be expected from an ordinary gravitational field created by the visible masses. This lead F. Zwicky [1] in 1933 to postulate the existence of *dark matter*. In fact, the observed velocity curves ask for large amounts of invisible matter in each galaxy. The presently best theoretical fit to the data is shown in Fig. 31.1, and the reader is referred to the original publication dealing with this issue [2].

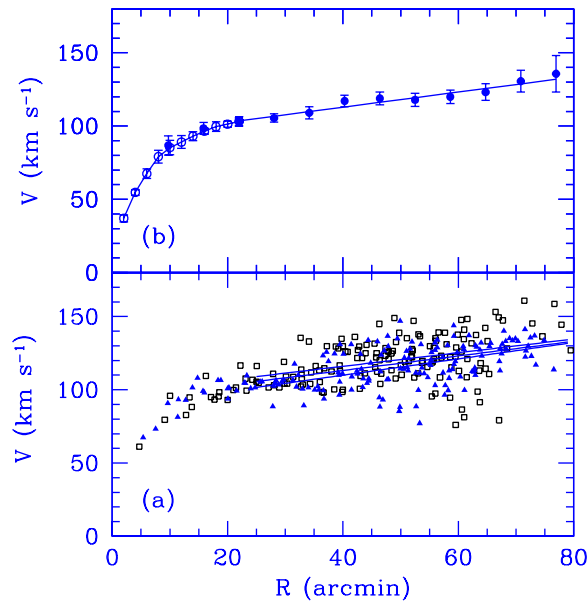


FIGURE 31.1 (a) Details of the fits to the velocity data. Filled triangles refer to the northern half, open squares to the southern half of the galaxy. Straight lines are the best linear fits for $R \geq 25$ arcmin to all data shown, once to the northern and once to the southern data set. (b) The straight line is the best linear fit to all unbinned data for $R > 25$ arcmin for the M33 rotation curve: Filled circles are from data displayed in (a), open circles follow Newton's theory, for comparison.

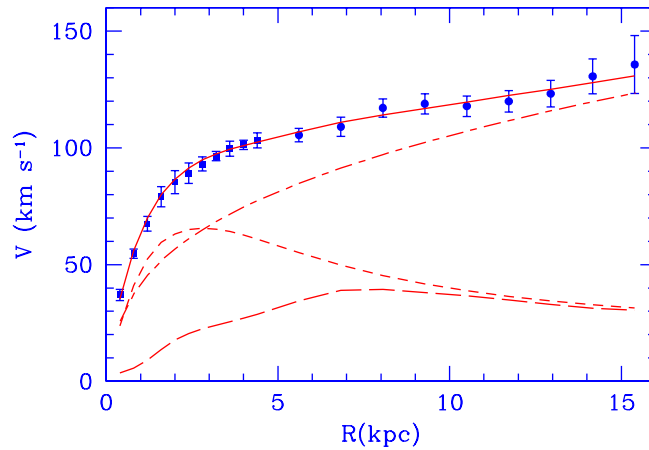


FIGURE 31.2 Velocity curve (points) of the galaxy M33 and comparison with a best fit model calculation (continuous line). Also shown is the halo contribution (dashed-dotted line), the stellar disk (short dashed line), and the gas contribution (long dashed line).

If a Friedmann model [3] is used to explain the evolution of the universe, one needs a large percentage of dark matter, roughly 23% of the mass energy of the universe. If dark matter is added to the so-called *dark energy*, which accounts for roughly 70% of the energy, one finds that the visible matter is practically negligible. See the contribution of the various components of matter in Fig. 31.3. This is the reason for ignoring visible atoms completely in the most extensive computer simulations of the evolution of cosmic structures [4], the so-called *Millennium Simulation*.

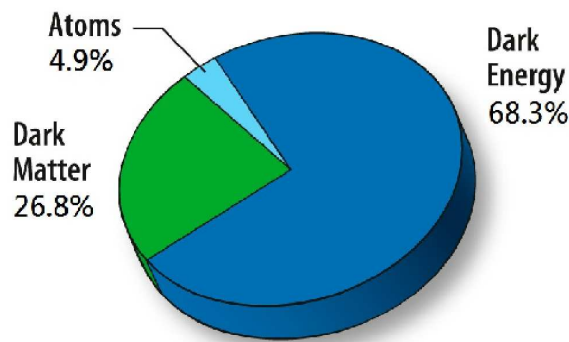


FIGURE 31.3 Various types of matter in the universe

In Fig. 31.4 we show the decomposition of the black-body radiation when the universe became first transparent. There are many speculations as to its composition. In this chapter we want to give the simplest possible explanation of at least part of it [5]. We argue that this part is not made of elementary particles, but of the singular worldlines and worldsheets in the solutions of *Einstein's vacuum field equation* $G_{\mu\nu} = 0$. In this way, the Einstein-Hilbert action governing space-

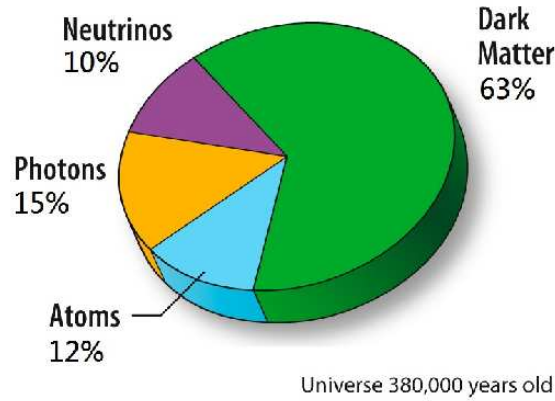


FIGURE 31.4 Various contributions to Dark Matter when the Universe became transparent (Credit: NASA/WMAP Science Team).

time also governs the fluctuations of these singular configurations of worldlines and worldsurfaces. Thus the spacetime action contains on the one hand the well-known action controlling the mechanics of relativistic point particles $-Mc \int ds$, on the other hand it contains the action used to describe elementary particles as closed bosonic “strings”.

Note that in the present context the “string” action appears in the physical number four of dimensions, such that it appears here in a novel physical context that is different from that in presently fashionable string theory where the unphysical number of 26 dimensions plays a special role.

Let us remember that all static electric fields in nature may be considered as originating from nontrivial solutions of the Poisson equation for the electric potential $\phi(x)$ as a function of $x = (t, \mathbf{x})$:

$$\Delta\phi(x) \equiv \nabla \cdot \nabla \phi(x) = 0. \quad (31.1)$$

The simplest of them has the form e/r , where $r = |\mathbf{x}|$. It is attributed to point-like electric charges, whose size e can be extracted from the pole strength of the singularity of the electric field $\mathbf{E}$ which points radially outward and has a strength e/r^2 . This becomes explicitly visible by performing an area integral over the $\mathbf{E}$ field around the singularity. Applying the famous Gauss integral theorem,

$$\int_V d^3x \nabla \cdot \mathbf{E} = \int_A d^2\mathbf{a} \cdot \mathbf{E}, \quad (31.2)$$

the area integral is equal to the volume integral over $\nabla \cdot \mathbf{E} = -\Delta\phi(x)$. Thus a field that solves the homogeneous Poisson equation can have a nonzero volume integral $\int_V d^3x \Delta\phi(x) = -4\pi e$. This fact can be expressed in a local way with the help of a Dirac-delta function $\delta^{(3)}(\mathbf{x})$ as

$$\Delta\phi(x) = -4\pi e \delta^{(3)}(\mathbf{x}). \quad (31.3)$$

In the sequel, it will be useful to re-express the Gauss theorem (31.2) in a one-dimensional form as

$$\int^R dr \partial_r r^2 E_r(r) = R^2 E_r(R). \quad (31.4)$$

This is valid for all R , in particular for small R , where $E_r(R) = 4\pi e/R^2$. Hence we can express the combination of Eqs. (31.2) and (31.2) in the radial form

$$\int d^3x \nabla \cdot \mathbf{E} = -4\pi \int^R dr r^2 \nabla \cdot \nabla e/r = 4\pi e \int^R dr \partial_r \delta(r). \quad (31.5)$$

Thus we find the electric charge e from the one-dimensional equation

$$e \int^R dr \partial_r \delta(r) = e. \quad (31.6)$$

This shows once more the radial part of the homogeneous Maxwell equation in the presence of a pointlike singularity: $\nabla \cdot \mathbf{E} = 4\pi e \delta^{(3)}(\mathbf{x})$.

For gravitational objects, the situation is quite similar. The Einstein equation in the vacuum, $G_{\mu\nu} = 0$, possesses simple nontrivial solutions in the form of the Schwarzschild metric defined by

$$ds^2 = B(r)c^2 dt^2 - A(r)dr^2 - r^2(d\theta^2 + \sin^2 \theta d\varphi^2), \quad (31.7)$$

with $B(r) = 1 - r_S/r$, $A(r) = 1/B(r)$, where $r_S \equiv 2G_N M/c^2$ is the Schwarzschild radius and G_N Newton's gravitational constant. Its Einstein tensor has the component

$$G_t^t = A'/A^2 r - (1 - A)/Ar^2, \quad (31.8)$$

which vanishes in the vacuum.

Let us now allow for singularities in spacetime and calculate the volume integral $\int_V d^3x \sqrt{-g} G_t^t$. Inserting (31.8) we find $\int_V d^3x \sqrt{B/A} [A'/Ar - (1 - A)/r^2]$. If this is evaluated with the gravitational singularities in the same way as in the electromagnetic case in Eqs. (31.2)–(31.5), we find that it is equal to $\int^R dr \partial_r (r - r/A) = (2G_N/c)M \int^R dr \partial_r \delta(r) = (2G_N/c)M$. Thus we obtain the nonzero integral

$$\int_V d^3x \sqrt{-g} G_t^t = \kappa c M, \quad (31.9)$$

where κ is defined in terms of the Planck length l_P , as

$$\kappa \equiv 8\pi l_P^2/\hbar = 8\pi G_N/c^3. \quad (31.10)$$

From (31.9) we identify the mass of the object as being M .

If the mass point moves through spacetime along a trajectory parametrized by $x^\mu(\tau)$, it has an energy-momentum tensor

$$\overset{m}{T}{}^{\mu\nu}(x) = Mc \int_{-\infty}^{\infty} d\tau \dot{x}^\mu(\tau) \dot{x}^\nu(\tau) \delta^{(4)}(x - x(\tau)), \quad (31.11)$$

where a dot denotes the τ -derivative.

We may integrate the associated solution of the homogeneous Einstein equation $G_{\mu\nu} = 0$ over spacetime, and find that its Einstein-Hilbert action

$$\mathcal{A}_{\text{EH}} = -\frac{1}{2\kappa} \int d^4x \sqrt{-g} R \quad (31.12)$$

vanishes. The situation is quite different, however, if we allow spacetime to be perforated by singularities. For line-like singularities, the Einstein-Hilbert action (31.12) will look as if it contains a δ -function-like source obeying $G^{\mu\nu} = \kappa \overset{\text{m}}{T}^{\mu}_{\mu}(x)$. If we insert here the equation of motion of a point particle $\dot{x}^2(\tau) = 1$, we arrive from the field equation $R = -G = -\kappa \overset{\text{m}}{T}^{\mu}_{\mu}(x) = -Mc \int d\tau \dot{x}(\tau)^2 \delta^{(4)}(x - x(\tau))$ at an action which is proportional to the classical action of a point-like particle:

$$\mathcal{A}_{\text{EH}}^{\text{worldline}} \propto -Mc \int ds. \quad (31.13)$$

A slight modification of (31.13), that is the same at the classical level, but different for fluctuating orbits, describes also the quantum physics of a spin-0 particle via a path integral over all orbits (see the discussion in Section 19.1 of the textbook [6], in particular Eq. (19.10)). Thus Einstein's action for a singular world line in spacetime can be used to define also the quantum physics of a spin-0 point particle.

In addition to pointlike singularities, the homogeneous Einstein equation will possess also surface-like singularities in spacetime. These may be parametrized by $x^\mu(\sigma, \tau)$, and their energy-momentum tensor has the form

$$T^{\mu\nu}(x) \propto \int_{-\infty}^{\infty} d\sigma d\tau (\dot{x}^\mu \dot{x}^\nu - x'^\mu x'^\nu) \delta^{(4)}(x - x(\sigma, \tau)), \quad (31.14)$$

where a prime denotes a σ -derivative. In the associated vanishing Einstein tensor, the δ -function on the surface manifests itself in the nonzero spacetime integral [7]

$$\int d^4x \sqrt{-g} G_{\mu}^{\mu} \propto \int d^2a \equiv \int_A d\sigma d\tau \sqrt{(\dot{x}x')^2 - \dot{x}'^2 x'^2}. \quad (31.15)$$

By analogy with the line-like case we obtain, for such a singular field configuration, an Einstein-Hilbert action (31.12)

$$\mathcal{A}_{\text{EH}}^{\text{worldsurface}} \propto -\frac{1}{2\kappa} \int_A d^2a = -\frac{\hbar}{16\pi l_{\text{P}}^2} \int_A d^2a. \quad (31.16)$$

The prefactor on the right-hand side has been expressed in terms of the Planck length l_{P} .

The important observation is now that, apart from a numerical proportionality factor of order unity, the right-hand side of Eq. (31.16) is precisely the Nambu-Goto action [8, 9] of a bosonic closed string in the true physical spacetime dimension four

$$\mathcal{A}_{\text{NG}} = -\frac{\hbar}{2\pi l_{\text{s}}^2} \int_A d^2a. \quad (31.17)$$

In this formula, l_s is the so-called string length parameter l_s . It measures the string tension, and corresponds in spacetime to a certain surface tension of the world-surface. This length scale can be related to the rather universal slope parameter $\alpha' = dl/dm^2$ of the Regge-trajectories [10]. These are found in plots of the angular momenta against the squares of the meson masses m^2 . The relation between the string length parameter l_s and slope parameter of the Regge theory is $l_s = \hbar c \sqrt{\alpha'}$. Note that now there is no extra mass parameter M , this being in contrast to the situation in world lines. The masses of the elementary particle come from the eigenmodes of the string vibrations.

The original string model was proposed to describe color-electric flux tubes and their Regge trajectories whose slopes α' lie around 1 GeV^{-2} . However, since the tubes are really fat objects, as fat as pions, only very long flux tubes are approximately line-like. Short tubes degenerate into spherical “MIT-bags” [11]. The flux-tube role of strings was therefore abandoned, and the action (31.17) was reinterpreted in a completely different fashion, as describing the fundamental particles of nature, assuming l_s to be of the order of l_P . Then the spin-2 particles of (31.17) would interact like gravitons and define Quantum Gravity. However, the ensuing “new string theory” [12] has been criticized by many authors [13]. One of its most embarrassing failures is that it has not produced any experimentally observable results. The particle spectra of its solutions have not matched the existing particle spectra.

The arising of the string action proposed here has a chance of curing this problem. If “strings” describe “dark matter”, there would be no need to reproduce other observed particle spectra. Instead, their celebrated virtue of extracting the interaction between gravitons from the properties of their spin-2 quanta can be used to fix the proportionality factor between the Einstein action (31.16) and the string action (31.17).

It must be kept in mind that just as $-Mc \int ds$ had to be modified for fluctuating paths [6] (recall Eq. (19.10) in that textbook), also the Nambu-Goto action (31.17) needs a modification for fluctuating surfaces. That was found by Polyakov [14] when studying the consequences of the conformal symmetry. He replaced the action (31.17) by a new action that is equal to (31.17) at the classical level, but contains in $D \neq 26$ dimensions another spin-0 field with a Liouville action.

Since the singularities of Einstein’s fields possess only gravitational interactions, their identification with “dark matter” seems very natural. All visible matter consists of singular solutions of the Maxwell equations as well as the field equations of the standard model. A grand-canonical ensemble of these and the singular solutions without matter sources explain the most important part of all matter in the Friedmann model of cosmological evolution.

But the main contribution to the energy comes from the above singularities of Einstein’s equation. Soon after the universe was created, the temperature was so high that the configurational entropy of the surfaces overwhelmed completely the impeding Boltzmann factors. Spacetime was filled with these surfaces in the same way as superfluid helium is filled with world-surfaces of vortex lines.

Vortex lines in superfluid helium are known to attract material particles such as frozen helium. This phenomenon provides us with an important tool to visualize vortex lines and tangles thereof [15]. In spacetime, we expect that any stable neutral particle will be attracted by its singularities. These could be the famous *wimps* (weakly interacting massive particles) of particle physics [16].

In helium above the temperature of the superfluid phase transition, these lie so densely packed that the superfluid behaves like a normal fluid [17, 18]. The Einstein-Hilbert action of such a singularity-filled turbulent geometry behaves like the action of a grand-canonical ensemble of world surfaces of a bosonic closed-string model.

Note once more that here these are two-dimensional objects living in four space-time dimensions. There is definitely a need to understand their spectrum by studying the associated Polyakov action. To be applicable in the physical dimension four one should not circumvent the accompanying Liouville field. Or one must find a way to take into account the fluctuations of the gravitational field around the field near the singular surface.

It should be realized that in the immediate neighborhood of line- and surface-like singularities, the curvature will be so high that Einstein's linear approximation $-(1/2\kappa)R$ to the Lagrangian must break down. It will have to be corrected by some nonlinear function of R . This starts out like Einstein's, but continues differently, similar to the action discussed in Chapter 29, that was suggested a long time ago [19]. Many modifications of this idea have meanwhile been investigated further [20].

After the big bang, the universe expanded and cooled down, so that large singular surfaces shrunk by emitting gravitational radiation. Their density decreased, and some phase transition made the cosmos homogeneous and isotropic on the large scale [21]. But it remained filled with gravitational radiation and small singular surfaces that had shrunk until their sizes reached the levels stabilized by quantum physics. The statistical mechanics of this cosmos can be described by analogy with a spacetime filled with superfluid helium. The specific heat of that is governed by the zero-mass phonons and by rotons. Recall that in this way Landau discovered the fundamental excitations called rotons [23], whose existence was deduced by him from the temperature behavior of the specific heat. In the universe, the role of rotons is played by the smallest surface-like singularities of the homogeneous Einstein equation. They must be there to satisfy the cosmological requirement of dark matter.

The situation can also be illustrated by a further analogy with many-body systems. The defects in a crystal, whose "atoms" have a lattice spacing l_P , simulate precisely the mathematics of a Riemann-Cartan spacetime, in which disclinations and dislocations define curvature and torsion [17, 18, 24]. Thus we may imagine a model of the universe as a "floppy world crystal" [25], a liquid-crystal-like phase [26] in which a first melting transition has led to correct gravitational $1/r$ -interactions between disclinations. The initial hot universe was filled with defects and thus it was in the "world-liquid"-phase of the "world crystal". After cooling down to the present liquid-crystal state, there remained plenty of residual defects around, which form our *dark matter*.

In the process of cooling down over a long time, the dark matter fraction can have decreased so that the expansion of the universe could have become faster and faster over the millenia. Thus it is well possible that the baby universe had so much dark-matter content that it practically did not expand at all for a long time. It would have been closer to the *steady-state universe* advocated in 1931 by Einstein and in the 1940's by Hoyle, Bondi, and Gold [35]. This would relief us from the absurd-sounding assumption that the entire universe came once out of a tiny beginning in which all matter of the world was compressed into a sphere of Planck radius.

We know that the cosmos is now filled with a cosmic microwave background (CMB) of photons of roughly 2.725 Kelvin, the remnants of the big bang. They contribute a constant $\Omega_{\text{rad}} h^2 = (2.47 \pm 0.01) \times 10^{-5}$ to the Friedmann equation of motion, where $h = 0.72 \pm 0.03$ is the Hubble parameter, defined in terms of the Hubble constant H by $h \equiv H/(100 \text{ km/Mpc sec})$. The symbol Ω denotes the energy density divided by the so-called critical density $\rho_c \equiv 3H^2/8\pi G_N = 1.88 \times 10^{-26} h^2 \text{ kg/m}^3$ [27]. The baryon density contributes $\Omega_{\text{rad}} h^2 = 0.0227 \pm 0.0006$, or 720 times as much, whereas the dark matter contributes $\Omega_{\text{dark}} h^2 = 0.104 \pm 0.006$, or 4210 as much. Let us assume, for a moment, that all massive strings are frozen out and that only the subsequently emitted gravitons form a thermal background [28]. Since the energy of massless states is proportional to T^4 , the temperature of this background would be $T_{\text{DMB}} \approx 4210^{1/4} \approx 8T_{\text{CMB}} \approx 22\text{K}$. We expect the presence of other singular solutions of Einstein's equation to change this result.

There is an alternative way of deriving the above-described properties of the fluctuating singular surfaces of Einstein's theory. One may rewrite Einstein's theory as a gauge theory [17, 18] and formulate it on a spacetime lattice [29]. Then the singular surfaces are built explicitly from plaquettes, as in lattice gauge theories of asymptotically-free nonabelian gauge theories [30]. In the abelian case, the surfaces are composed as shown in Ref. [31], for the nonabelian case, see [32]. An equivalent derivation could also be given in the framework of *loop gravity* [33]. But that would require a separate study beyond this chapter.

Summarizing we have seen that the Einstein-Hilbert action governs not only the classical physics of gravitational fields but also, via the fluctuations of its line- and surface-like singularities, the quantum physics of dark matter. A string-like action, derived from it for the fluctuating surface-like singularities, contains interacting spin-2 quanta that define a finite Quantum Gravity.

For other models of dark matter see [34].

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Note that in two papers written with K. Halperin [22], Huang manages to make his scalar field theory asymptotically free in the ultraviolet (though at the unpleasant cost of a sharp cutoff introducing forces of infinitely short range). This property allows him to deduce an effective *dark energy* in the baby universe. With our purely geometric tangles, such an effect may be reached using a lattice gauge formulation of Einstein's theory sketched at the end of the textbooks [17] and [18].

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