Charlie Harper

Analytic Methods in Physics



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Preface

This book is intended for undergraduate students who are majoring in physics (or other physical sciences), applied mathematics, or engineering. The goal of the book is to provide the essential mathematical physics background needed for the study of analytic mechanics and mechanical wave motion, heat and thermodynamics, electromagnetism, modern physics, and quantum mechanics. In addition, it is intended to provide the necessary background for advanced work in these areas. Numerous examples and illustrations are given throughout each chapter, and problems are included at the end of each chapter. Certain problems are used to introduce new material in a self-contained manner.

Throughout the book, the level of presentation is fairly uniform (with the possible exception of certain sections of chapters 2 and 12), and the included material should be readily accessible to undergraduate students who have a working knowledge of general physics and of differential and integral calculus. The desire to maintain a uniform level of presentation was used as a guide for the selection of topics to include (and exclude).

The material on essentials of vector spaces, essential algebraic structures, and exterior differential forms is invaluable for the study of physics today; the inclusion and presentation of this material at the undergraduate level are among the distinguishing features of this book.

Chapter 1 contains a standard treatment of vector analysis, fundamental physical quantities with SI units and dimensional analysis, and vector quantities in orthogonal curvilinear coordinates and coordinate transformations. Also, Maxwell's equations in both differential and integral forms are included, as well as an introduction of the notion of a gauge transformation.

In Chapter 2, a standard treatment of matrix analysis is presented. Then, essentials of vector spaces including notions of a function (mapping), a linear operator, eigenvalues and eigenfunctions, and the matrix representation of a linear operator are covered. Also, a brief introduction of topological spaces and elementary definitions of Hausdorff space, Banach space, Hilbert space, a manifold and topology is presented. The development on essential algebraic structures contains an elementary introduction to groups, rings, and fields as needed in mathematical physics. The primer on group theory in physics is required background for further study of applications of groups in physics.

Chapters 3-6 are standard treatments of functions of a complex variable, the calculus of residues, Fourier series, and Fourier transforms. These topics are introduced early so that these concepts will be available for use when needed in subsequent chapters, such as in Chapters 7 and 8.

Chapters 7 and 8 on ordinary and partial differentials contain a standard treatment of these subjects; in addition, algorithms for the numerical solutions of ordinary and partial differential equations are developed.

Chapter 9 on special functions begins with the Sturm-Liouville theory and orthogonal polynomials. It is shown that the completeness and orthogonality relations lead to the expansion of a function in terms of orthogonal polynomials or orthogonal functions; Fourier series, Legendre series, and the Hermite series are developed as examples of such expansions. The development of special functions via the power series solutions of appropriate ordinary differential equations follows the Sturm-Liouville theory. Also, the connections of special functions are discussed.

A brief and elementary introduction of integral equations is given in Chapter 10; this chapter ends with the famous Abel problem.

The introduction and applications of the calculus of variations and elementary functional analysis are given in Chapter 11. Hamilton's variational principle, Lagrangian and Hamiltonian mechanics are treated in some details. Also, the transition from classical mechanics to quantum mechanics in the Heisenberg picture, Schrödinger picture, and in the Feynman path integral approach is discussed.

Chapter 12 begins with a brief overview of differential geometry, differentiable manifold, and coordinate transformations in linear spaces. Then, a treatment of standard tensor analysis using indices ends with the Einstein equation in general relativity. This is followed by a coordinate free treatment of tensors involving exterior differential forms.

I am grateful to the many physics students who used many sections of the manuscript.

Charlie Harper

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Chapter 1

Vector Analysis

1.1 Introduction

1.1.1 Background

In valid expressions and equations involving physical quantities, the **dimension** (a certain combination of fundamental quantities) of each term must be the same; certain quantities such as the coefficient of friction are dimensionless. The **fundamental physical quantities**, definition of SI (système international) units, are (1) Length (meter, m); (2) Mass (kilogram, kg); (3) Time (second, s); (4) Temperature (Kelvin, K); (5) Amount of Substance (mole, mol); (6) Electric Current (Ampère, A); and (7) Luminous Intensity (candela, cd). Operational definitions for the seven fundamental quantities are given in Appendix I. Analyzing expressions and equations by use of concepts in this paragraph is called **dimensional analysis**.

Physical quantities that are not fundamental are referred to as **derived quantities**. The fundamental physical quantities in mechanics (the study of the motions of physical objects) are length, L, mass, M, and time, T. For example, 2 m/s + 3 cm/hr is a valid expression since the dimension of each term is length/time, L/T; the derived quantity in this case is speed.

A physical quantity that can be completely specified by giving its magnitude is a **scalar**. Here magnitude means a number and a unit; for example, "2 m" (a distance) is a magnitude. (For dimensionless quantities, only a number is required.). The following quantities are examples of scalars: mass, density, energy, and speed. Valid mathematical operations for scalars are the same as those for ordinary numbers and ordinary functions.

A physical quantity that can be completely specified by its magnitude and its direction is a vector. The quantity "2 m; West" (a displacement) is a vector since it has magnitude, 2 m, and direction, West. The following quantities are examples of vectors: velocity, acceleration, force, and momentum. In expressions and equations involving scalars and vectors, each term must be a scalar or each term must be a vector (e.g., all terms in an equation must be vectors if one term is a vector). Separate mathematical laws (rules) are needed for vector quantities since the mathematical laws for scalars are not, in general, valid for vector quantities. Modern vector analysis was developed by Gibbs¹ during the

¹Josiah Willard Gibbs (1839–1903), USA mathematician and physicist who formulated the theoretical foundation of physical chemistry and statistical mechanics, developed vector analysis, and conducted optical

period 1879-1884 and independently by Heaviside² during the period 1882-1888.

1.1.2 **Properties and Notations**

Boldface print is used in most textbooks to designate a vector quantity. In writing, the tradition is to place an arrow over a letter, \vec{A} (or \hat{A}). Note that the magnitude (also called the length or norm, $\|.\|$) of a vector, $|\mathbf{A}| = A$, is a scalar. The magnitude of a **unit vector** equals unity, $|\hat{\mathbf{A}}| = 1$; hence we may write $\mathbf{A} = A\hat{\mathbf{A}}$. A vector with zero magnitude, $|\mathbf{0}| = 0$, is a **null vector**.

An arrow is used to represent a vector quantity (e.g., see Fig. 1.1). The direction of the quantity is indicated by the head of the arrow, and the magnitude of the quantity is characterized by the length of the arrow. A basic property of a vector is that it may be moved parallel to itself (without rotation) without changing the vector.



Figure 1.1

In Fig. 1.1(a and b), vectors **B** and **A** are said to be **equal**, $\mathbf{B} = \mathbf{A}$, since they have the same length and direction, but they may not be equivalent. An understanding of the concept of vector equivalence is important in the study of mechanics and in other areas of physics. To be equivalent, vector quantities must produce identical mechanical effects. A horizontal force **F** acting on a wheel along a line through the axis of rotation (center of the wheel) tends to cause the wheel to translate; this force **F** acting along a line parallel to the axis of rotation will cause the wheel to rotate.

Vector $-\mathbf{A}$ is equal in magnitude to vector \mathbf{A} but opposite in direction (see Fig. 1.1b and c). Multiplication of a vector by a scalar, n, such that $n\mathbf{A} = \mathbf{A}n$ is shown in Fig. 1.1(d); here, an appropriate diagram could be developed for 0 < n < 1.

1.1.3 Geometric Addition of Vectors

The geometric addition of vectors is achieved by use of the following two steps:

- 1. Place the vectors heads to tail. Here the basic property of moving vectors is used.
- 2. Draw the vector from the tail of the first vector to the head of the last vector.

and thermodynamics research.

²Oliver Heaviside (1850–1925), British physicist who made contributions to electricity and magnetism and to the development of vector analysis. He predicted the existence of the ionized atmospheric layer now known as the ionosphere.

The **resultant vector** (sum vector or net vector) is the vector in step 2 of this rule. Numerical results for geometric addition are achieved by use of graph paper and a protractor or plain paper (using a metric ruler to scale lengths of vectors) and a protractor. Geometric addition of vectors is illustrated in Figs.1.2-1.4.





The commutative, $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$, and associative, $(\mathbf{C} + \mathbf{D}) + \mathbf{E} = \mathbf{C} + (\mathbf{D} + \mathbf{E})$, laws of addition are illustrated in Fig. 1.5.

Subtraction uses addition and a change in direction since $\mathbf{A} - \mathbf{B} = \mathbf{A} + (-\mathbf{B})$. The operation of subtraction is illustrated in Fig. 1.6.

Example 1 A particle travels 2 cm due North then 4 cm in a direction 60° West of North (see Fig. 1.7). By use of geometric addition of vectors, find the distance and displacement traveled.

Solution: See Fig. 1.7.



1.2 The Cartesian Coordinate System

1.2.1 Orthonormal Basis Vectors: i, j, k

An orthogonal basis for a three-dimensional vector space (see page 72) consists of a set of three mutually perpendicular vectors. In Fig. 1.8, the \mathbf{i} , \mathbf{j} , and \mathbf{k} set of vectors forms an orthonormal basis since \mathbf{i} , \mathbf{j} , and \mathbf{k} are mutually perpendicular unit vectors. The \mathbf{i} , \mathbf{j} , and \mathbf{k} basis vectors are universally understood to be unit vectors and the hat over the letters is not needed. This system is called a **Cartesian**³ coordinate system.

1.2.2 Rectangular Resolution of Vectors

The position of an object is completely specified by its **position vector** (sometimes called **radius vector**). A position vector is drawn from the origin of a coordinate system to the object in question. In mathematical physics, both the right- and left-handed Cartesian coordinate systems are used, and they are illustrated in Fig. 1.8. We, however, will use a right-hand system throughout this chapter.

The position vector, \mathbf{r} , of an object located at P(x, y, z) is shown in Fig. 1.9. In equation form, the position vector is written as

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k} \ . \tag{1.1}$$

Vectors, xi, yj, and zk are the three components of \mathbf{r} ; they are the vector representations of the projections of \mathbf{r} onto the three coordinate axes, respectively. Quantities x, y, and z are the magnitudes of the vector components in the three respective directions.

 $^{^{3}}$ René Descartes (1596–1650), French mathematician and philosopher; he is considered the originator of analytic geometry.



On using the Pythagorean⁴ theorem in Fig. 1.9, we find that

$$|\mathbf{r}|^2 = x^2 + y^2 + z^2 \tag{1.2}$$

where $|\mathbf{r}| = r$ is the magnitude of \mathbf{r} .

2

If the projections of an arbitrary vector **A** along the three axes of a Cartesian system have magnitudes A_x , A_y , and A_z , then vector **A** in terms of these three magnitudes may be written as

$$\mathbf{A} = A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k} \ . \tag{1.3}$$

In summary, we say that an arbitrary vector may be resolved into three components with one component along each of the three Cartesian axes. The magnitude (length or norm) of \mathbf{A} is given by

$$|\mathbf{A}| = \left(A_x^2 + A_y^2 + A_z^2\right)^{1/2} . \tag{1.4}$$

Note that $\mathbf{A}/|\mathbf{A}| = \hat{\mathbf{A}}$ is a unit vector in the direction of \mathbf{A} ; here we say that \mathbf{A} is normalized. The equality $\mathbf{A} = \mathbf{B}$ means that corresponding components are equal,

$$A_x = B_x, \quad A_y = B_y, \quad \text{and} \quad A_z = B_z.$$

⁴Pythagoras of Samos (circa 580-500 BC), Greek philosopher and mathematician.



In terms of scalar components, Newton's⁵ second law of motion becomes

$$\sum \mathbf{F} = m\mathbf{a} \Rightarrow \sum F_x = ma_x, \quad \sum F_y = ma_y, \text{ and } \sum F_z = ma_z.$$

Here, we note that one vector equation corresponds to three scalar equations.

1.2.3 Direction Cosines

The line segment from point O to point P makes angles α , β , and γ with the three coordinates axes in Fig. 1.9. Here we have

$$x = r \ell, \quad y = r m, \quad \text{and} \quad z = r n \tag{1.5}$$

where $\ell = \cos \alpha$, $m = \cos \beta$, and $n = \cos \gamma$. Quantities ℓ , m, and n are called **direction** cosines. Hence, the point P(x, y, z) may be located by giving its position vector, \mathbf{r} , or by specifying r (length \overline{OP}) and its direction cosines. Combining Eqs.(1.2 and 1.5), we find that

$$1 = \ell^2 + m^2 + n^2. \tag{1.6}$$

For an arbitrary vector **A**, we may write

$$\frac{\mathbf{A}}{|\mathbf{A}|} = \mathbf{i} \, \cos \, \alpha + \mathbf{j} \cos \, \beta + \mathbf{k} \cos \, \gamma. \tag{1.7}$$

Example 2 Find the direction cosines of the line segment from $P_1(-1, -4, 5)$ m to $P_2(3, -2, 2)$ m.

Solution: In general, we have

$$\ell = \cos \alpha = \Delta x/d$$
, $m = \cos \beta = \Delta y/d$, and $n = \cos \gamma = \Delta z/d$.

The distance from P_1 to P_2 is

$$d = \sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2}$$

= $\sqrt{(3+1)^2 + (-2+4)^2 + (2-5)^2}$
= 5.39 m.

⁵Sir Isaac Newton (1642–1727), English mathematician and natural philosopher (physicist) who is noted for his laws of mechanics, gravity, heat, and optics.

We therefore find that the direction cosines are

$$\ell = 4/5.39$$
, $m = 2/5.39$, and $n = -3/5.39$.

1.2.4 Vector Algebra

Addition The subject of vector algebra involves developing laws for the following two operation: (a) addition (subtraction) and (b) multiplication. The operation of addition is very simple and straightforward. To find the sum of to vectors **A** and **B**, add like components together; that is,

$$\mathbf{A} + \mathbf{B} = (A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k}) + (B_x \mathbf{i} + B_y \mathbf{j} + B_z \mathbf{k})$$
$$= (A_x + B_x) \mathbf{i} + (A_y + B_y) \mathbf{j} + (A_z + B_z) \mathbf{k}.$$
(1.8)

For subtraction, use a minus instead of plus in Eq.(1.8).

Example 3 By use of components, solve the problem in Example 1.

Solution: The components of d_1 and d_2 (see Fig. 1.10) are

$$d_1 = 2cm\mathbf{i}$$

$$d_2 = -4cm\cos 30^\circ \mathbf{i} + 4cm\sin 30^\circ \mathbf{j}$$

The displacement from the starting point is the sum of the above two vectors.

$$\mathbf{D} = \mathbf{d}_1 + \mathbf{d}_2$$
$$= -3.46cm\mathbf{i} + 4cm\mathbf{j}$$

The distance from the starting point is $|\mathbf{D}| = 5.29 cm$ and $\phi = 49.1^{\circ}$.







Figure 1.11:

Solution: Newton's second law of motion $(\sum \mathbf{F} = m\mathbf{a})$ is the appropriate law of mechanics for this problem.

On applying Newton's second law to this system at rest (see Fig. 1.11), we obtain

 $T_3 = 10N$ x-direction : $T_2 \cos 60^\circ - T_1 \cos 30^\circ = 0$ y-direction : $T_2 \sin 60^\circ + T_1 \sin 30^\circ = 10N$.

The results are $T_1 = 4.99N$, $T_2 = 8.66N$, and $T_3 = 10N$.

Example 5 Given $A = \mathbf{i} + 2\mathbf{j} + 3\mathbf{k}$ and $\mathbf{B} = 3\mathbf{i} + 2\mathbf{j} - \mathbf{k}$. Find (a) $|\mathbf{A}|$, (b) $\hat{\mathbf{A}}$, (c) $\mathbf{A} + \mathbf{B}$, and (d) $\mathbf{A} - \mathbf{B}$.

Solution:

Part A
$$|\mathbf{A}| = \sqrt{1^2 + 2^2 + 3^2} = 3.74;$$

Part B $\hat{\mathbf{A}} = \mathbf{A}/|\mathbf{A}| = (\mathbf{i} + 2\mathbf{j} + 3\mathbf{k})/3.74;$
Part C $\mathbf{A} + \mathbf{B} = (\mathbf{i} + 2\mathbf{j} + 3\mathbf{k}) + (3\mathbf{i} + 2\mathbf{j} - \mathbf{k}) = 4\mathbf{i} + 4\mathbf{j} + 2\mathbf{k};$ and
Part D $\mathbf{A} - \mathbf{B} = (\mathbf{i} + 2\mathbf{j} + 3\mathbf{k}) - (3\mathbf{i} + 2\mathbf{j} - \mathbf{k}) = -2\mathbf{i} + 4\mathbf{k}.$

Scalar Product Two kinds of products are defined for vectors, and they are called scalar product and vector product. The scalar product (also known as the dot product) of two vectors A and B is a scalar and is defined as follows:

$$\mathbf{A} \cdot \mathbf{B} \equiv |\mathbf{A}| |\mathbf{B}| \cos \theta$$

= $A_x B_x + A_y B_y + A_z B_z.$ (1.9)

In Eq.(1.9), θ is the smaller angle between **A** and **B** when they are placed tail to tail. Note that $\mathbf{i} \cdot \mathbf{i} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = 1$ since the angle between these three unit vectors is 0° and $\cos 0^\circ = 1$. Also, note that $\mathbf{i} \cdot \mathbf{j} = \mathbf{i} \cdot \mathbf{k} = \mathbf{k} \cdot \mathbf{j} = 0$ since the angle between these unit vectors is 90° and $\cos 90^\circ = 0$. By use of the definition in Eq.(1.9), it is clear that $\mathbf{A} \cdot \mathbf{B} = \mathbf{B} \cdot \mathbf{A}$ (commutative). The dot product of a vector **A** with itself is written as $\mathbf{A} \cdot \mathbf{A} = \mathbf{A}^2$ where $\mathbf{A}^2 = A_x^2 + A_y^2 + A_z^2$. The square of a vector is a scalar; vectors may appear to the first or second power only.



As can be seen in Fig. 1.12, the quantity $|\mathbf{B}| \cos \theta$ is the projection of **B** onto **A**. Hence the scalar product $\mathbf{A} \cdot \mathbf{B}$ equals $|\mathbf{A}|$ times the projection of **B** onto **A**. In summary, note that $\mathbf{A} \cdot \mathbf{B}$

- 1. is defined as $|\mathbf{A}| |\mathbf{B}| \cos \theta$;
- 2. equals $A_x B_x + A_y B_y + A_z B_z$; and
- 3. equals the projection of **B** onto **A** times $|\mathbf{A}|$.

The distributive property, $\mathbf{A} \cdot (\mathbf{B} + \mathbf{C}) = \mathbf{A} \cdot \mathbf{B} + \mathbf{A} \cdot \mathbf{C}$, of the dot product is illustrated by use of the diagram in Fig. 1.13 since $|\mathbf{A}|(b+c) = |\mathbf{A}|b + |\mathbf{A}|c$ for scalars. In Fig. 1.13, note that b + c, b and c are the projections of $\mathbf{B} + \mathbf{C}$, \mathbf{B} and \mathbf{C} onto \mathbf{A} respectively.



Figure 1.13

Example 6 Given $\mathbf{A} = \mathbf{i} + 2\mathbf{j} + 3\mathbf{k}$ and $\mathbf{B} = 3\mathbf{i} + 2\mathbf{j} + \mathbf{k}$. Find (a) $\mathbf{A} \cdot \mathbf{B}$ and (b) the smaller angle between the tails of \mathbf{A} and \mathbf{B} .

Solution:

Part A
$$\mathbf{A} \cdot \mathbf{B} = (\mathbf{i} + 2\mathbf{j} + 3\mathbf{k}) \cdot (3\mathbf{i} + 2\mathbf{j} + \mathbf{k}) = 10$$

Part B $\mathbf{A} \cdot \mathbf{B} = |\mathbf{A}| |\mathbf{B}| \cos \theta$
 $= \left(\sqrt{1^2 + 2^2 + 3^2}\right) \left(\sqrt{3^2 + 2^2 + 1^2}\right) \cos \theta = 14$
or $\cos \theta = 10/14 \Longrightarrow \theta = 44.4^\circ$.

The dot product is used throughout physics and is first encountered in general physics in connecting with the definition of the work done by a constant force. In equation form, this definition is

$$W \equiv \mathbf{F} \cdot \mathbf{D} \tag{1.10}$$

In Eq.(1.10), \mathbf{F} is a constant force acting on the object and \mathbf{D} is the displacement of the object.

Example 7 A constant force with magnitude 20N is applied to a 2 kg block at an angle of 30° above the horizontal. The coefficient of friction between the block and the horizontal table is 0.5. In moving the block 1.5 m to the right (see Fig. 1.14), calculate the work done by the (a) applied force and (b) frictional force.



Figure 1.14

Solution: The displacement of the block is 1.5 mi. The magnitude of the frictional force is $f_r = \mu N$ where N, the normal force, is obtained by summing all forces in the y-direction, $N = mg + 20N \sin 30^{\circ}$. The frictional force is always in the opposite direction of motion or intended motion. The frictional force is

$$\mathbf{f}_r = -\mu \left(mg + 20N\sin 30^\circ \right) \mathbf{i}.$$

Part A: The work done by the applied force is

$$W_F = (20N \cos 30^\circ \mathbf{i} - 20N \sin 30^\circ \mathbf{j}) \cdot (1.5 \ m\mathbf{i})$$

= 25.98 J (Newton meter = Joule, J).

Part B: The work done by the frictional force is

$$W_{f_r} = -0.5 (20N \sin 30^\circ + 19.6N) \mathbf{i} \cdot (1.5 \text{ mi})$$

= -22.2 J.

Example 8 Cauchy's Inequality. Note that

$$egin{aligned} \left(\mathbf{A} \cdot \mathbf{B}
ight) &= \left| \mathbf{A}
ight|^2 \left| \mathbf{B}
ight|^2 \cos heta \ &\leq \left| \mathbf{A}
ight|^2 \left| \mathbf{B}
ight|^2. \end{aligned}$$

The above inequality is referred to as the **Cauchy** (or **Cauchy-Schwartz**) inequality and is used throughout mathematical physics; for example, it is used in the derivation of the uncertainty principle.

Vector Product The vector product, often referred to as the cross product, of A and B is defined by

$$\mathbf{A} \times \mathbf{B} \equiv |\mathbf{A}| |\mathbf{B}| \sin \theta \,\, \hat{\mathbf{n}}. \tag{1.11}$$

In Eq.(1.11), θ is the smaller angle between **A** and **B** when they are placed tail to tail. Unit vector $\hat{\mathbf{n}}$ is perpendicular to the plane of **A** and **B** and is in the direction advanced by a right-hand woodscrew when it is turned from **A** to **B** (see Fig. 1.15). The cross product is not commutative because of the change in direction of $\hat{\mathbf{n}}$,

$$\mathbf{A} \times \mathbf{B} = -\mathbf{B} \times \mathbf{A}$$



Figure 1.15

The following cross products can be obtained from the definition in Eq.(1.11):

$$\mathbf{i} \times \mathbf{i} = \mathbf{j} \times \mathbf{j} = \mathbf{k} \times \mathbf{k} = \mathbf{0}.$$

The above equations result from the fact that the angle between these unit vectors is 0° and $\sin 0^{\circ} = 0$. Also, note that (see Fig. 1.16)

$$\mathbf{i} \times \mathbf{j} = \mathbf{k}, \ \mathbf{k} \times \mathbf{i} = \mathbf{j}, \ \text{and} \ \ \mathbf{j} \times \mathbf{k} = \mathbf{i}.$$

An alternate form of writing the three equations above is $\mathbf{i} \times \mathbf{j} = \mathbf{k}$ (cyclic, meaning cyclic permutation; also, see the mnemonic circle in Fig. 1.16).

In terms of the components of A and B, the cross product $\mathbf{A} \times \mathbf{B}$ may be written as

$$\mathbf{A} \times \mathbf{B} = (A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k}) \times (B_x \mathbf{i} + B_y \mathbf{j} + B_z \mathbf{k})$$

= $(A_y B_z - A_z B_y) \mathbf{i} - (A_x B_z - A_z B_x) \mathbf{j} + (A_x B_y - A_y B_x) \mathbf{k}$
= $\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$. (1.12)



Figure 1.16

Equation (1.12) results from use of the various cross products of the three unit-basis vectors. The resulting square array of quantities is called a **determinant**, and a discussion of determinants is given in Appendix II of this chapter. The distributive property for the cross product is valid, $\mathbf{A} \times (\mathbf{B} + \mathbf{C}) = \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C}$.

Example 9 Given $\mathbf{A} = \mathbf{i} + 2\mathbf{j} + 3\mathbf{k}$ and $\mathbf{B} = 3\mathbf{i} + 2\mathbf{j} + \mathbf{k}$. Find (a) $\mathbf{A} \times \mathbf{B}$ and (b) a unit vector perpendicular to both \mathbf{A} and \mathbf{B} .

Solution: Part A:

$$\mathbf{A} \times \mathbf{B} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 2 & 3 \\ 3 & 2 & 1 \end{vmatrix} = -4\mathbf{i} + 8\mathbf{j} - 4\mathbf{k}.$$

Part B: By definition, $\mathbf{A} \times \mathbf{B}$ is perpendicular to both \mathbf{A} and \mathbf{B} . A unit vector, $\hat{\mathbf{n}}$, in the direction of $\mathbf{A} \times \mathbf{B}$ is obtained as follows.

$$\hat{\mathbf{n}} = \frac{\mathbf{A} \times \mathbf{B}}{|\mathbf{A} \times \mathbf{B}|} = \frac{-4\mathbf{i} + 8\mathbf{j} - 4\mathbf{k}}{9.79}.$$

One may verify, using Cartesian components, the following results for triple vector and triple scalar products, respectively

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B} (\mathbf{A} \cdot \mathbf{C}) - \mathbf{C} (\mathbf{A} \cdot \mathbf{B})$$
(1.13)

and

$$\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix}.$$
(1.14)

Using properties of determinants (see Appendix II), it can be shown that the following result is valid for the triple scalar product.

$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = \mathbf{C} \cdot \mathbf{A} \times \mathbf{B} = \mathbf{B} \cdot \mathbf{C} \times \mathbf{A}$$
 (cyclic).

In the above equation, it is assumed that none of the vectors is the del operator (see page 27). If one or more of the vectors in the above equation is the del operator, the dot and the cross may be interchanged but the vectors may not (in general) be permuted.

In mechanics, torque is a twist or tendency of a force to cause rotation about a pivot point (or an axis), and it is defined by use of the vector product (see Fig. 1.17). In equation form, we write



Figure 1.17

In Eq.(1.15), **r** (not to be confused with position vector) is a vector from the pivot (or axis about which rotation is to occur) to the point of application of the force \mathbf{F} . If several forces act on the object, then the net torque is the vector sum of the torques produced by forces; it is given by

$$\operatorname{net} \mathbf{T} = \sum_{i=1}^{n} \mathbf{r}_{i} \times \mathbf{F}_{i}.$$

Angular momentum, L, is another physical quantity that is defined by use of the cross product; it may be written as

$$\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}. \tag{1.16}$$

In Eq.(1.16), \mathbf{r} (not to be confused with position vector or \mathbf{r} in the definition of torque) is the vector from the axis about which rotation takes place to the particle, and $\mathbf{p} \ (\mathbf{p} \equiv m\mathbf{v})$ is the linear momentum of the particle. The context of the problem determines which one of the three interpretations for \mathbf{r} is involved. In an inertial coordinate system, the total angular momentum of a system of particles about a point (or axis) is given by

$$\mathrm{net}\mathbf{L} = \sum_{i=1}^{n} \mathbf{r}_i \times \mathbf{p}_i.$$

Example 10 A force $\mathbf{F} = 5\mathbf{i} - 2\mathbf{k} N$ acts on an object at the point (0, 1, 1). Calculate the torque produced about the point (0, 2, 0).

Solution:

1.
$$\mathbf{r} = -\mathbf{j} + \mathbf{k} \mathbf{m}$$

2. $\mathbf{F} = 5\mathbf{i} - 2\mathbf{k} \mathbf{N}$
3. $\mathbf{T} = \mathbf{r} \times \mathbf{F} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & -1 & 1 \\ 5 & 0 & -2 \end{vmatrix} = 2\mathbf{i} + 5\mathbf{j} + 5\mathbf{k} \mathbf{J}$

(1.15)

Division by a Vector Since division is normally considered to be the inverse process of multiplication, one would naturally assume that two different kinds of division processes (corresponding to the two kinds of multiplication processes) exist for vectors. There, however, exists no unique definition for division by a vector. To understand the difficulty involved in developing a unique definition for division by a vector, consider the case of scalar multiplication $\alpha = \mathbf{A} \cdot \mathbf{B}$. Note that α/\mathbf{A} does not uniquely yield \mathbf{B} since we may write $\alpha = \mathbf{A} \cdot (\mathbf{B} + \mathbf{D})$ where \mathbf{D} is an arbitrary vector perpendicular to \mathbf{A} . Hence α/\mathbf{A} yields an arbitrary quotient. In a similar manner, one can show that the quotient of \mathbf{A}/\mathbf{B} is not unique if $\mathbf{A} = \mathbf{B} \times \mathbf{C}$.

1.3 Differentiation of Vector Functions

1.3.1 The Derivative of a Vector Function

A vector field $\mathbf{F}(s)$ assigns a vector to each point in the domain of s. Consider the vector field $\mathbf{F}(s)$ where s is a scalar variable. We say that \mathbf{F} is a function of s since each value of s yields a corresponding value for \mathbf{F} . The change in \mathbf{F} , $\Delta \mathbf{F}$, when s changes to $s + \Delta s$ (see Fig. 1.18) is given by

$$\Delta \mathbf{F} = \mathbf{F}(s + \Delta s) - \mathbf{F}(s).$$



Figure 1.18

If $\Delta \mathbf{F}/\Delta s$ approaches a limit as Δs approaches zero, this limit is called the derivative of **F** with respect to s; it is written as

$$\frac{dF}{ds} = \lim_{\Delta s \to 0} \left(\frac{\Delta F}{\Delta s} \right) = \lim_{\Delta s \to 0} \left[\frac{F(s + \Delta s) - F(s)}{\Delta s} \right]$$
$$= \mathbf{i} \frac{dF_x}{ds} + \mathbf{j} \frac{dF_y}{ds} + \mathbf{k} \frac{dF_z}{ds}.$$

Derivatives of Certain Vector Functions A summary of some useful relations involving

derivatives of vector functions is given below.

1.
$$\frac{d(\mathbf{a}\mathbf{A})}{ds} = a\frac{d\mathbf{A}}{ds}; \quad a = \text{ constant}$$

2.
$$\frac{d[b(s)\mathbf{A}(s)]}{ds} = b\frac{d\mathbf{A}}{ds} + \frac{db}{ds}\mathbf{A}$$

3.
$$\frac{d(\mathbf{A} + \mathbf{B})}{ds} = \frac{d\mathbf{A}}{ds} + \frac{d\mathbf{B}}{ds}$$

4.
$$\frac{d(\mathbf{A} \cdot \mathbf{B})}{ds} = \mathbf{A} \cdot \frac{d\mathbf{B}}{ds} + \frac{d\mathbf{A}}{ds} \cdot \mathbf{B}$$

5.
$$\frac{d(\mathbf{A} \times \mathbf{B})}{ds} = \mathbf{A} \times \frac{d\mathbf{B}}{ds} + \frac{d\mathbf{A}}{ds} \times \mathbf{B}$$

When time is the independent variable, the following relations often occur.

1.
$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \dot{\mathbf{r}}$$

2. $\mathbf{a} = \frac{d\mathbf{v}}{dt} = \ddot{\mathbf{r}} = \dot{\mathbf{v}}$
3. $\operatorname{net}\mathbf{F} = \frac{d\mathbf{p}}{dt} = m\mathbf{a}$

The Del Operator The del operator, ∇ , is a differential operator and is of immense importance in mathematical physics. It is defined by

$$\nabla \equiv \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}.$$
(1.17)

Information concerning the del operator and its use in mathematical physics will be given in various sections below. The del operator, also referred to as the **nabla operator**, is universally understood to be a vector quantity; hence, an arrow is not normally placed over this operator.

1.3.2 Concepts of Gradient, Divergence, and Curl

Let $\phi(x, y, z)$ be a single-valued continuous function in a certain region of space. If **r** is the position vector of an object located at P(x, y, z), then we have $\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$ and $d\mathbf{r} = dx\mathbf{i} + dy\mathbf{j} + dz\mathbf{k}$. The total differential of $\phi(x, y, z)$ is defined as

$$d\phi \equiv \frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy + \frac{\partial \phi}{\partial z} dz$$

= $\nabla \phi \cdot d\mathbf{r}$. (1.18)

The vector function $\nabla \phi$ is called the **gradient** of ϕ and is sometimes written as grad ϕ . On dividing both sides of Eq.(1.18) by dr, we obtain

$$\frac{d\phi}{dr} = \nabla \phi \cdot \frac{d\mathbf{r}}{dr} \quad \text{or} \quad \frac{d\phi}{du} = \nabla \phi \cdot \hat{\mathbf{u}} \quad \text{where} \quad \hat{\mathbf{u}} \equiv \frac{d\mathbf{u}}{du}.$$
(1.19)

In Eq.(1.19), the quantity $d\mathbf{r}/d\mathbf{r}$ is a unit vector in the direction of $d\mathbf{r}$; hence the change in ϕ in a particular direction equals $\nabla \phi$ dotted into a unit vector in that direction. Equation



Figure 1.19:

(1.19) is the definition of the directional derivative. Also, note that $\nabla \phi$ is a vector whose component in a particular direction, $\hat{\mathbf{u}}$ equals the directional derivative of ϕ with respect to u (see Fig. 1.19).

Example 11 Find the directional derivative of $\phi(x, y, z) = 2x^3 - 3yz + 6z$ at the point (2, 1, -3) in the direction of $\mathbf{A} = 4\mathbf{i} - 2\mathbf{j} + 4\mathbf{k}$.

Solution:

1.
$$\frac{d\phi}{du} = \nabla \phi \cdot \hat{\mathbf{u}} \quad \text{(the definition of directional derivative)}$$

2.
$$\nabla \phi = 6x^2 \mathbf{i} - 3z \mathbf{j} + (6 - 3y) \mathbf{k}$$

3.
$$\nabla \phi|_{2,1,-3} = 24 \mathbf{i} + 9 \mathbf{j} + 3 \mathbf{k}$$

4.
$$\hat{\mathbf{u}} = \frac{\mathbf{A}}{|\mathbf{A}|} = \frac{4\mathbf{i} - 2\mathbf{j} + 4\mathbf{k}}{6}$$

5.
$$\frac{d\phi}{du}|_{2,1,-3} = \nabla \phi \cdot \hat{\mathbf{u}} = (24\mathbf{i} + 9\mathbf{j} + 3\mathbf{k}) \cdot \frac{(4\mathbf{i} - 2\mathbf{j} + 4\mathbf{k})}{6} = 15.$$

Example 12 By use of the directional derivative, show that $\nabla r^n = nr^{n-2}\mathbf{r}$. Solution:

1.
$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$

2. $r = \sqrt{x^2 + y^2 + z^2}$
3. $\hat{\mathbf{r}} = \frac{\mathbf{r}}{r}$.

The magnitude of ∇r^n is given by the directional derivative of r^n which is

4.
$$\frac{dr^n}{dr} = nr^{n-1}.$$

The gradient of r^n equals the above magnitude times the unit vector \hat{r} ; the result is

5.
$$\nabla r^n = (nr^{n-1})\left(\frac{\mathbf{r}}{r}\right) = nr^{n-2}\mathbf{r}.$$

If $d\mathbf{r}$ is an arbitrary vector on the surface $\phi(x, y, z) = C$, then Eq.(1.18) becomes

$$d\phi = \nabla \phi \cdot d\mathbf{r} = 0.$$

In the above equation, note that the gradient of ϕ is perpendicular to the surface since $d\mathbf{r}$ is on the surface.

Example 13 Consider the surface $\phi = x^2 + y^2 - z = 1$; find a unit vector that is normal to this surface at point P(1, 1, 1).

Solution:

1. $\nabla \phi = 2x\mathbf{i} + 2y\mathbf{j} - \mathbf{k}$ 2. $\nabla \phi|_{1,1,1} = 2\mathbf{i} + 2\mathbf{j} - \mathbf{k}$; a vector normal to the surface at P(1,1,1)3. $\hat{\mathbf{u}} = \frac{\nabla \phi}{|\nabla \phi|} = \frac{2\mathbf{i} + 2\mathbf{j} - \mathbf{k}}{3}$; a unit vector normal to the surface at P(1,1,1).

Multiplication involving the ∇ operator is extremely useful in mathematical physics. Two products denoted by $\nabla \cdot F \equiv \operatorname{div} F$ and $\nabla \times F \equiv \operatorname{curl} F$ are called the **divergence** of Fand the **curl** of F, respectively. Their connections with physical problems will be revealed in later sections. Also, the scalar operator $\nabla \cdot \nabla = \nabla^2$ is very useful in mathematical physics; it is called the **Laplacian**⁶ operator. In equation form, it is

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$
 (1.20)

Equation (1.20) results from the fact that $\mathbf{i} \cdot \mathbf{j} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = 1$ and the dot products of the cross terms equal zero. Some important partial differential equations in mathematical physics that involve the Laplacian operator are given below.

Certain Important Equations Important equations involving the Laplacian operator that are used throughout the book are given below. These equations are called partial differential equations and are the subject of Chapter 8.

1.
$$\nabla^2 \phi = \begin{cases} -\rho/\epsilon_0$$
; Poisson's equation
0; Laplace's equation
2. $\nabla^2 \phi = \frac{1}{v^2} \frac{\partial^2 \phi}{\partial t^2}$; mechanical wave equation
3. $\nabla^2 \phi = \frac{1}{\sigma} \frac{\partial \phi}{\partial t}$; diffusion (or heat) equation
4. $\nabla^2 \phi + k^2 \phi = 0$; Helmholtz's equation
5. $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(x, y, z) \Psi$; Schrödinger's equation

The divergence and curl of F are given, respectively, by

$$\nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \quad \text{and} \quad \nabla \times \mathbf{F} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix}.$$
(1.21)

If at point P

$$\nabla \cdot \mathbf{V} \begin{cases} >0, \text{ then } \mathbf{V} \text{ has a source at } P \\ <0, \text{ then } \mathbf{V} \text{ has a sink at } P \\ =0, \text{ then } \mathbf{V} \text{ is said to be solenoidal.} \end{cases}$$
(1.22)

⁶Marquis Pierre Simon de Laplace (1749-1827), French mathematician and astronomer.

The vector **V** is classified as **irrotational** if $\nabla \times \mathbf{V} = \mathbf{0}$.

Special care must be exercised in treating vector operations when the differential operator ∇ is involved. Note that $\nabla \phi$ is a vector function, but $\phi \nabla$ is a vector operator; hence $\nabla \phi \neq \phi \nabla$ where $\phi(x, y, z)$.

Some Useful Relations Involving the Del Operator The relations below may be verified by writing the vectors in terms of their Cartesian components and carrying out the indicated operations.

- 1. $\nabla \cdot (\phi \mathbf{A}) = \mathbf{A} \cdot \nabla \phi + \phi \nabla \cdot \mathbf{A}$
- 2. $\nabla \times (\phi \mathbf{A}) = \phi \nabla \times \mathbf{A} \mathbf{A} \times \nabla \phi$
- 3. $\nabla \times \nabla \times \mathbf{A} = \nabla \nabla \cdot \mathbf{A} \nabla^2 \mathbf{A}$
- 4. $\nabla \cdot \mathbf{A} \times \mathbf{B} = \nabla \times \mathbf{A} \cdot \mathbf{B} = \mathbf{B} \cdot \nabla \times \mathbf{A} \mathbf{A} \cdot \nabla \times \mathbf{B}$
- 5. $\nabla \times (\mathbf{A} \times \mathbf{B}) = (\mathbf{B} \cdot \nabla)\mathbf{A} \mathbf{B}(\nabla \cdot \mathbf{A}) (\mathbf{A} \cdot \nabla)\mathbf{B} + \mathbf{A}(\nabla \cdot \mathbf{B})$

Example 14 Establish a physical meaning for the divergence of a vector by use of an illustration from hydrodynamics.



Figure 1.20:

Solution: Consider the flow indicated in Fig. 1.20 where $\mathbf{A} = \rho \mathbf{v}$ represents the mass of fluid flowing through a unit area normal to side ABOC per unit time. The density of the fluid is denoted by ρ , and \mathbf{v} is its velocity.

The y-component of \mathbf{A} through the area ABOC indicated in Fig. 1.20 per unit time is given by

 $A_{u}dxdz$.

The flow through the area DEFG per unit time may be represented by the following Taylor's expansion:

$$A_y(y+dy)dxdz = \left[A_y(y) + \frac{\partial A_y}{\partial y}dy + \dots\right]dxdz.$$

We will neglect higher-order terms in the above expansion. The net increase in the mass of the fluid inside the volume element $d\tau = dxdydz$ per unit time due to the flow through the two faces is

$$A_y dx dz - \left[A_y(y) + rac{\partial A_y}{\partial y} dy
ight] dx dz = -rac{\partial A_y}{\partial y} d au$$
 .

Similarly, the net increase in the mass of fluid per unit time due to the flow through BEFO and ADGC is

$$-\frac{\partial A_x}{\partial x}d au,$$

and the net increase in the mass of fluid per unit time due to the flow through FGCO and EDAB is

$$-\frac{\partial A_z}{\partial z}d\tau$$

The total increase in the mass of fluid per unit volume per unit time due to the excess of inward flow over the outward flow is

$$-\frac{\partial A_x}{\partial x} - \frac{\partial A_y}{\partial y} - \frac{\partial A_z}{\partial z} = -\nabla \cdot \mathbf{A}.$$

The above equation represents the rate of increase of the density of the fluid inside of the volume element $d\tau$. We may, therefore, write

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{A} \,. \tag{1.23}$$

Equation (1.23) is the **continuity equation**. For an incompressible fluid, we have

$$\frac{\partial \rho}{dt} = 0$$
 or $\nabla \cdot \mathbf{A} = 0$ (solenoidal). (1.24)

In this case, the excess of outward flow over inward flow is zero (no source is present). The physical interpretation of the curl of a vector is connected with the rotation (or circulation) of a vector field; its full meaning will be made clear by its use in later sections.

1.4 Integration of Vector Functions

We begin this Section on the integration of vector functions with an explanation of the various symbols of integration that will be used throughout the book. The notations $d\lambda$, $d\sigma$, and $d\tau$ will be used to represent an element of length, area, and volume respectively. In an integrand, these elements of length, area, and volume will be used to indicate single, double, and triple integrals respectively. The corresponding integrals are denoted by

$$\int_{A}^{B} (...) d\lambda \quad \text{(line integral from } A \text{ to } B)$$

$$\oint (...) d\lambda \quad \text{(line integral around a closed path)}$$

$$\int (...) d\sigma \quad \text{(integral over an open surface)}$$

$$\oint (...) d\sigma \quad \text{(integral over a closed surface)}$$

$$\int (...) d\tau \quad \text{(volume integral, triple integral)}.$$

The above differential elements in Cartesian coordinates represent (a) $d\lambda = dx, dy$, or dz; (b) $d\sigma = dxdy, dxdz$, or dydz; and (c) $d\tau = dxdydz$. In addition to $d\lambda$, dr will be used to denote line (or single) integral. A surface that encloses a volume is said to be closed; an open surface does not enclose a volume. An integral with a small circle through its center is used to indicate integration around a closed path or a closed surface, depending on the differential element in the integrand. An element of surface may be represented as a vector quantity, $d\sigma = \hat{\mathbf{n}} d\sigma$ where $\hat{\mathbf{n}}$ is a unit vector that is normal to the surface (also, called a **unit normal**).

1.4.1 Line Integrals

A vector field $\mathbf{F}(x, y, z)$ assigns a vector to each point of its domain. The **line integral** (tangential line integral), I_{λ} , of a vector field \mathbf{F} along a continuous curve C from A to B (see Fig. 1.21) is defined as the definite integral of the projection of \mathbf{F} onto an element of the tangent vector to the curve at point P(x, y, z).



In equation form, we write

$$I_{\lambda} = \int_{A}^{B} \mathbf{F} \cdot d\mathbf{r}.$$
 (1.25)

In Eq.(1.25), $d\mathbf{r}$ (tangent to the path) is an element of displacement at P(x, y, z). Note that the line integral from B to A is the negative of that from A to B. The work done by a variable force $\mathbf{F}(x, y, z)$ in moving an object from A to B is defined as

$$W \equiv \int_{A}^{B} \mathbf{F} \cdot d\mathbf{r}$$

Example 15 Calculate the work done by the force $\mathbf{F} = 2y\mathbf{i} + xy\mathbf{j} N$ in moving an object along a straight line from A(0,0,0) to B(2,1,0) m.

Solution:

$$W = \int_{A}^{B} \mathbf{F} \cdot d\mathbf{r}$$

= $\int (2x\mathbf{i} + xy\mathbf{j}) \cdot (dx\mathbf{i} + dy\mathbf{j} + dz\mathbf{k})$
= $\int (2ydx + xydy)$
= $\int_{0}^{2} xdx + 2\int_{0}^{1} y^{2}dy$ (since the equation for the path is $x = 2y$)
= 2.67 J.

Example 16 Show that the work done on an object of mass m by a net force during a displacement from A to B equals the change in the kinetic energy of the object.

Solution: The work is given by

$$\begin{split} W &= \int_{A}^{B} \operatorname{net} \mathbf{F} \cdot d\mathbf{r} \\ &= m \int_{A}^{B} \frac{d\mathbf{v}}{dt} \cdot d\mathbf{r} \quad (\text{by use of Newton's second law}) \\ &= m \int_{A}^{B} \frac{d\mathbf{v}}{dt} \cdot \mathbf{v} dt \quad (\text{since } \mathbf{v} = d\mathbf{r}/dt) \\ &= \frac{m}{2} \int_{A}^{B} d(\mathbf{v} \cdot \mathbf{v}) \quad (\text{since } d(\mathbf{v} \cdot \mathbf{v})/dt = 2\mathbf{v} \cdot d\mathbf{v}/dt) \\ &= \frac{m}{2} (v_{B}^{2} - v_{A}^{2}) \quad (\text{the work-energy theorem of mechanics}) \\ &= \Delta K \quad (\text{change in kinetic energy}). \end{split}$$

The total energy of a mechanical system is conserved if the force (field) is given by $\mathbf{F} = -\nabla \phi(x, y, z)$ where ϕ is a single-valued continuous function with continuous derivatives (a smooth function); the smooth function ϕ is referred to as the potential energy of the system. The system is said to be a conservative force system (or conservative system) since its total energy is constant.

Example 17 If $\mathbf{F} = -\nabla \phi$, show that the total energy of the system is conserved (constant).

Solution: Work now becomes

$$W = \int_{A}^{B} \mathbf{F} \cdot d\mathbf{r}$$

= $-\int_{A}^{B} \nabla \phi \cdot d\mathbf{r}$
= $\int_{A}^{B} d\phi$
= $-\phi_{B} - \phi_{A}$
= $K_{B} - K_{A}$ (by us of the result in the previous Example).

We obtain the conservation of energy principle (the total mechanical energy is constant) by rearranging terms: $K_A + \phi_A = K_B + \phi_B$.

In a conservative system, the **potential energy** of a particle located at A(x, y, z) relative to a fixed point $B(x_0, y_0, z_0)$ where the potential energy may be set to zero (the reference level) is defined by

$$\phi(x, y, z) = \int_{A}^{B} \mathbf{F} \cdot d\mathbf{r}.$$
 (1.27)

For a conservative system, note that

$$W = \oint \mathbf{F} \cdot d\mathbf{r} = \oint \nabla \phi \cdot d\mathbf{r} = \oint d\phi = 0.$$

The circle in the integral means integration around a closed path. Since the potential energy is a smooth function, we have $\nabla \times \mathbf{F} = -\nabla \times \nabla \phi = 0$. In summary, we find that a **conservative mechanical system** is characterized by the following three equivalent equations.

1.
$$\mathbf{F} = -\nabla \phi$$
;
2. $\nabla \times \mathbf{F} = 0$; and
3. $W = \oint \mathbf{F} \cdot d\mathbf{r} = 0$.

Care is required with the third equation above since conservative force systems are a subset of forces for which the equation is valid.

1.4.2 The Divergence Theorem Due to Gauss

The normal surface integral of the vector field $\mathbf{F}(x, y, z)$ over a closed boundary is defined as the surface (double) integral of the projection of $\mathbf{F}(x, y, z)$ onto a unit normal to the surface at point P(x, y, z), and it is written as

$$I_{\sigma} = \oint \mathbf{F} \cdot d\sigma = \oint \mathbf{F} \cdot \hat{\mathbf{n}} d\sigma.$$
(1.28)

In Eq.(1.28), $d\sigma$ is an element of the boundary surface, $\hat{\mathbf{n}}$ is a unit outward normal to this element of area, and the circle through the integral sign means (double) integration around a closed surface.

The sign convention for a unit normal to a surface is as follows: (a) For a closed surface (a surface which encloses a volume), the outward normal is defined to be positive. (b) For an open surface, the right-hand woodscrew rule is used. The direction of rotation of the woodscrew is the same as that in which the periphery is traversed, and the direction of the normal is the direction advanced by the woodscrew.

The divergence theorem due to Gauss⁷ is as follows: The normal surface integral of a vector field \mathbf{F} over the boundary of a closed simply-connected surface (a surface without holes and can be shrunk to a point) of arbitrary shape equals the volume integral of the divergence of \mathbf{F} taken throughout the enclosed volume. In equation form, we write

$$\oint \mathbf{F} \cdot d\sigma = \int \nabla \cdot \mathbf{F} d\tau. \tag{1.29}$$

To prove this theorem, we first expand the right-hand side of Eq.(1.29) and obtain

$$\int \nabla \cdot \mathbf{F} d\tau = \int \left[\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right] dx dy dz.$$
(1.30)

The theorem is valid for an arbitrarily shaped closed surface. We, however, choose the volume in Fig. 1.22 for convenience; we obtain the following results:



$d\sigma_1$	$= -\mathbf{k}dxdy$ (bottom)	$d\sigma_4 = -\mathbf{i} dy dz$ (back)
$d\sigma_2$	= i dy dz (front)	$d\sigma_5 = \mathbf{k} dx dy \ (\mathrm{top})$
$d\sigma_3$	$= -\mathbf{j}dxdz$ (left)	$d\sigma_6 = \mathbf{j} dx dz$ (right)

 $^{^{7}}$ Carl Friedrich Gauss (1777–1855), German mathematician, physicist, and astronomer. He is known for major contributions in each of the three disciplines.

Integrating the last term on the right-hand side of Eq.(1.30) with respect to z from z' to z'', we obtain

$$\int_{z'}^{z''} \frac{\partial F_z}{\partial z} dx dy dz = \int [F_z(x, y, z'') - F_z(x, y, z')] dx dy$$
$$= \int_{\sigma_5} F_z(x, y, z'') dx dy - \int_{\sigma_1} F_z(x, y, z') dx dy.$$
(1.31)

Note that

 $\hat{\mathbf{n}}_1 \cdot \mathbf{k} d\sigma_1 = dx dy$ (bottom) and $\hat{\mathbf{n}}_5 \cdot \mathbf{k} d\sigma_5 = dx dy$ (top). (1.32)

On substituting Eq.(1.32) into Eq.(1.31), we may write

$$\int_{z'}^{z''} \frac{\partial F_z}{\partial z} dx dy dz = \int_{\sigma_5} F_z(x, y, z'') \hat{\mathbf{n}}_5 \cdot \mathbf{k} d\sigma_5 + \int_{\sigma_1} F_z(x, y, z') \hat{\mathbf{n}}_1 \cdot \mathbf{k} d\sigma_1$$
$$= \oint F_z \mathbf{k} \cdot \hat{\mathbf{n}} d\sigma. \tag{1.33}$$

The above equation results from the fact that the integrals over the sides equal zero since **k** is perpendicular to $d\sigma_2$, $d\sigma_3$, $d\sigma_4$, and $d\sigma_6$. Similarly, it can be shown that

$$\int \frac{\partial F_x}{\partial x} d\tau = \oint F_x \mathbf{i} \cdot \hat{\mathbf{n}} d\sigma \tag{1.34}$$

and

$$\int \frac{\partial F_y}{\partial y} d\tau = \oint F_y \mathbf{j} \cdot \hat{\mathbf{n}} d\sigma.$$
(1.35)

Combining Eqs.(1.33-1.35) proves the theorem. The result is

$$\oint \mathbf{F} \cdot d\sigma = \int \nabla \cdot \mathbf{F} d\tau. \tag{1.29'}$$

Example 18 By use of the divergence theorem due to Gauss, obtain the integral form for Maxwell's first equation.

Solution: The fundamental equations in electromagnetism, Maxwell's equations, may be written in compact form by use of the divergence and curl of vector quantities. In partial differential equation form, the four Maxwell⁸ equations (in the absence of matter) in SI units are

⁸James Clark Maxwell (1831–1879), British physicists who made fundamental contributions to electromagnetic theory and to the kinetic theory of gases. He was appointed the first Cavendish Professor of Physics at Cambridge in 1871.

1.
$$\nabla \cdot \mathbf{D} = \rho$$
 (Gauss's Law)
2. $\nabla \cdot \mathbf{B} = 0$ (no free magnetic poles)
3. $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ (Faraday's Law)
4. $\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$ (Ampère's Law)

In Maxwell's equations, (a) the displacement vector \mathbf{D} is related to the electric field intensity vector, $\mathbf{D} = \epsilon_0 \mathbf{E}$ where $\epsilon_0 = 8.85 \times 10^{-12} \mathrm{C}^2 \mathrm{N}^{-1} \mathrm{m}^{-2}$ is the permittivity of free space; (b) the magnetic induction vector \mathbf{B} is related to the magnetic intensity vector, $\mathbf{B} = \mu_0 \mathbf{H}$ where $\mu_0 = 4\pi \times 10^{-7} \mathrm{NA}^{-2}$ is the permeability of free space; (c) \mathbf{J} is current density; and (d) ρ is volume charge density (in a vacuum, $\rho = 0$ and $\mathbf{J} = \mathbf{0}$). Maxwell's equations plus the Lorentz⁹ force law, $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$, represent a complete theory for electromagnetism. By use of Maxwell's first equation in differential form and the divergence theorem due to Gauss, we may write (letting $\mathbf{F} = \epsilon_0 \mathbf{E}$, electric field intensity)

$$\oint \mathbf{E} \cdot d\sigma = \int \nabla \cdot \mathbf{E} d\tau$$

$$= \frac{1}{\epsilon_0} \int \rho d\tau \quad \text{(by us of Maxwell's first equation)}$$

$$= \frac{q_{\text{enclosed}}}{\epsilon_0}.$$

In electrostatics, the above equation is called **Gauss's law** (Maxwell's first equation in integral form), and the arbitrarily shaped hypothetical surface σ is known as a **Gaussian surface**.

Gauss's law, for example, may be used to find the electric field at a distance r from a charge q (see Fig. 1.23). For convenience, we let σ be a spherical surface enclosing the total charge q and obtain

$$E \oint d\sigma = E4\pi r^2$$
$$= \frac{1}{\epsilon_0} \int \rho d\tau = \frac{q}{\epsilon_0}.$$

Solving the above equation for E, we obtain the usual expression for the field of a point charge at distance r from the charge q.

Example 19 By use of the divergence theorem, obtain the integral form for Maxwell's second equation.

Solution: On letting $\mathbf{F} = \mathbf{B}$ (magnetic induction vector) in the divergence theorem and using the differential form of Maxwell's second equation, we obtain $\oint \mathbf{B} \cdot d\sigma = 0$ which is the integral form of Maxwell's second equation (Gauss's law in magnetism).

⁹Hendrik Antoon Lorentz (1853–1928), Dutch physicist who made fundamental contributions to electromagnetic theory and special relativity. He shared the 1902 Nobel prize in physics with Peter Zeeman (1865–1943).



Figure 1.23: Gaussian surface

Example 20 Develop a relation for the magnetic vector potential and for the electric potential.

Solution : Since $\nabla \cdot \mathbf{B} = 0$ (solenoidal, no source or sink; no free magnetic poles), the magnetic induction vector \mathbf{B} can be expressed as the curl of a vector because the divergence of the curl of a vector equals zero; we may write $\mathbf{B} = \nabla \times \mathbf{A}$ where \mathbf{A} is the magnetic vector potential.

By use of Maxwell's third equation and the relation for the vector potential, we may write

$$abla imes \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = -\frac{\partial (
abla imes \mathbf{A})}{\partial t}.$$

The above equation may be written in the form

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = \mathbf{0}.$$

Since the electromagnetic field is a conservative force field, we obtain

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \varphi \quad \text{or} \quad \mathbf{E} = -\nabla \varphi - \frac{\partial \mathbf{A}}{\partial t}.$$

In the above equations, φ is the electric (scalar) potential. Note that the above equations for **B** and **E** do not determine the scalar and vector potentials uniquely since for an arbitrary function f(x, y, z, t) the following equations

$$\varphi \rightarrow \varphi' = \varphi + \frac{\partial f}{\partial t}$$
 and $\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} - \nabla f$

leave **E** and **B** unchanged. The above transformation is known as a **gauge transformation of the second kind**. (A gauge transformation of the first kind involves invariance of the Lagrangian density in quantum field theory.)

In the **Coulomb**¹⁰ gauge (also called the radiative gauge) where $\nabla \cdot \mathbf{A} = 0$, the divergence of \mathbf{E} in the above equation leads to **Poisson's equation** as follows.

¹⁰Charles Augustin de Coulomb (1736–1806), French physicist who made fundamental contributions to electricity and magnetism.
$$\nabla \cdot \mathbf{E} = -\nabla \cdot \left(\nabla \varphi + \frac{\partial \mathbf{A}}{\partial t} \right)$$

= $-\nabla^2 \varphi - \frac{\partial (\nabla \cdot \mathbf{A})}{\partial t}$
= $-\nabla^2 \varphi$ (Coulomb gauge: $\nabla \cdot \mathbf{A} = 0$)
= $\frac{\rho}{\epsilon_0}$ (by use of Maxwell's first equation).

Example 21 An application of the divergence theorem to the problem of heat conduction. Here we consider the problem of the transfer of heat through an object by means of conduction. We assume that (a) the temperature, T = T(x, y, z, t), within the object is a finite and continuous function; (b) through any point, a surface on which the temperature is everywhere the same (isothermal surface) may be drawn; (c) the temperature gradient, ∇T , and the direction of heat flow are normal to the isothermal surface at the point in question; (d) ∇T is a finite and continuous function and is in the direction of increasing T; and (e) the rate of heat flow per unit area across the isothermal surface, F, is given by $\mathbf{F} = -k\nabla T$ (Fourier's Law) where k is called the thermal conductivity of the substance under investigation and the negative sign indicates that the heat flows from points at higher temperatures to points at lower temperatures.

Solution : If σ is an arbitrary closed surface drawn entirely within a certain region of the object under investigation, then the total amount of heat flowing out of σ in time Δt is given by

$$Q = -\Delta t \oint k \nabla T \cdot \hat{\mathbf{n}} d\sigma$$
$$= -\Delta t \int \nabla \cdot (k \nabla T) d\tau.$$

We have used the divergence theorem to obtain the last equation. The quantity

$$Q = -\Delta t \int c \rho \frac{\partial T}{\partial t} d\tau$$

is another representation of the amount of heat flowing out of σ in time Δt provided c is the specific heat of the object, ρ is the density of the object, and $\partial T/\partial t$ is the rate of increase in temperature within σ . Equating the two expressions for the heat flow, we obtain

$$\int \left[c\rho \frac{\partial T}{\partial t} - \nabla \cdot (k\nabla T) \right] d\tau = 0.$$

Since the volume is arbitrary, the above equation implies that

$$c\rho \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T).$$

The above equation is the heat conduction equation and was first developed by Fourier¹¹ in 1822.

1.4.3 Green's Theorem

The theorem due to $Green^{12}$ is an important corollary of the divergence theorem, and it has numerous applications in various branches of physics.

Let ψ and ϕ be two smooth scalar functions of position within a certain region bounded by a closed surface σ . On applying the divergence theorem to $\psi \nabla \phi$ in this region, we obtain

$$\oint \psi \nabla \phi \cdot d\sigma = \int \nabla \cdot (\psi \nabla \phi) d\tau$$
$$= \int [\psi \nabla \cdot \nabla \phi + \nabla \psi \cdot \nabla \phi] d\tau$$
$$= \int [\psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi] d\tau.$$

The above equation may be written in the form

$$\oint \psi \frac{\partial \phi}{\partial u} d\sigma = \int [\psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi] d\tau.$$
(1.36)

Equation (1.36) is known as **Green's theorem in the first form**. A second form of Green's theorem is obtained when the following two equations are considered.

$$\nabla \cdot (\psi \nabla \phi) = \psi \nabla \cdot \nabla \phi + \nabla \psi \cdot \nabla \phi$$

and

$$\nabla \cdot (\phi \nabla \psi) = \phi \nabla \cdot \nabla \psi + \nabla \phi \cdot \nabla \psi.$$

On subtracting the second equation from the first equation and integrating over an arbitrary volume, we obtain

$$\int \nabla \cdot (\psi \nabla \phi - \phi \nabla \psi) d\tau = \int [\psi \nabla^2 \phi - \phi \nabla^2 \psi] d\tau.$$

¹¹Baron Jean Baptiste Joseph Fourier (1768–1830), French mathematician and physicist who formulated a method for analyzing periodic functions and studied heat conduction.

¹²George Green (1793-1841), English mathematician and physicist.

Converting the left-hand side of the above equation to a surface integral by use of the divergence theorem, we obtain

$$\oint \left[\psi \frac{\partial \phi}{\partial u} - \phi \frac{\partial \psi}{\partial u}\right] d\sigma = \int [\psi \nabla^2 \phi - \phi \nabla^2 \psi] d\tau.$$
(1.37)

Equation (1.37) is the second form of Green's theorem.

1.4.4 The Curl Theorem Due to Stokes

A third and equally important theorem involving integrals of vector functions is the curl theorem due to Stokes¹³. The curl theorem is as follows: If the vector field \mathbf{F} is a smooth function, the line integral of \mathbf{F} around a closed curve λ equals the normal surface integral of curl \mathbf{F} over an open surface bounded by λ . In equation form, we write

$$\oint \mathbf{F} \cdot d\lambda = \int \nabla \times \mathbf{F} \cdot d\sigma.$$
(1.38)

To prove the curl theorem, we first expand the right-hand side of Eq.(1.38); it becomes

$$\int \nabla \times \mathbf{F} \cdot \hat{\mathbf{n}} d\sigma - \int \hat{\mathbf{n}} \cdot [\nabla \times \mathbf{i} F_x + \nabla \times \mathbf{j} F_y + \nabla \times \mathbf{k} F_z] d\sigma$$

The first integral on the right-hand side of the above equation reduces to

$$\int \hat{\mathbf{n}} \cdot (\nabla \times \mathbf{i} F_x) d\sigma = \int \left[\hat{\mathbf{n}} \cdot \mathbf{j} \frac{\partial F_x}{\partial z} - \hat{\mathbf{n}} \cdot \mathbf{k} \frac{\partial F_x}{\partial y} \right] d\sigma.$$
(1.39)

Note that the projection of $d\sigma$ onto the x-y-plane (see Fig. 1.24) leads to

$$\hat{\mathbf{n}} \cdot \mathbf{k} d\sigma = dx dy. \tag{1.40}$$

Let the line segment from P_1 to P_2 be the intersection of the surface σ with a plane that is parallel to the x-z-plane at a distance x from the origin (see Fig. 1.24). Along the strip from P_1 to P_2 , we have

$$dF_x = \frac{\partial F_x}{\partial y} dy + \frac{\partial F_x}{\partial z} dz$$
 and $d\mathbf{r} = dy\mathbf{j} + dz\mathbf{k}$.

The vector $d\mathbf{r}$ is tangent to the segment from P_1 to P_2 at A and perpendicular to $\hat{\mathbf{n}}$. We may therefore write

$$d\mathbf{r} \cdot \hat{\mathbf{n}} = 0 = dy \hat{\mathbf{n}} \cdot \mathbf{j} + dz \hat{\mathbf{n}} \cdot \mathbf{k}$$

or $\hat{\mathbf{n}} \cdot \mathbf{j} = -\frac{dz}{dy} \hat{\mathbf{n}} \cdot \mathbf{k} = -\frac{dz}{dy} \left(\frac{dxdy}{d\sigma}\right)$
or $\hat{\mathbf{n}} \cdot \mathbf{j} d\sigma = -dxdz.$ (1.41)

 $^{^{13}}$ Sir George Gabriel Stokes (1819–1903), British mathematician and physicist known for his study of hydrodynamics.





Figure 1.24

On substituting Eqs.(1.40 and 1.41) into Eq.(1.39), we obtain

$$\int \hat{\mathbf{n}} \cdot (\nabla \times \mathbf{i} F_x) d\sigma = -\int \left[\frac{\partial F_x}{\partial z} dz + \frac{\partial F_x}{\partial y} dy \right] dx$$
$$= -\int dx \int dF_x$$
$$= -\int [F_x(x, y_2, z_2) - F_x(x, y_1, z_1)] dx.$$

The sense of the periphery at P_1 is positive, $dx = d\lambda_x$; at P_2 , $\hat{\mathbf{n}}$ is negative, $dx = -d\lambda_x$ (see Fig. 1.24). Hence the equation reduces to

$$\int \hat{\mathbf{n}} \cdot (\nabla \times \mathbf{i} F_x) d\sigma = \int F_x(x, y_2, z_2) d\lambda_x + \int F_x(x, y_1, z_1) d\lambda_x$$
$$= \oint F_x d\lambda_x.$$

In the above equation, the first integral on the right-hand side is on the back part, and the second integral in on the front part. In a manner similarly to that leading to the above equation, we find that

$$\int \hat{\mathbf{n}} \cdot (\nabla \times \mathbf{j} F_y) d\sigma = \oint F_y d\lambda_y$$

and

$$\int \mathbf{\hat{n}} \cdot (\nabla \times \mathbf{k} F_z) d\sigma = \oint F_z d\lambda_z$$

Combining the above three equations, we obtain

$$\oint \mathbf{F} \cdot d\lambda = \int \nabla \times \mathbf{F} \cdot d\sigma, \qquad (1.38')$$

and the theorem is proved. The curl theorem is extremely useful in potential theory and in other areas of mathematical physics.

Example 22 By use of the curl theorem, obtain the integral form for Maxwell's third equation, Faraday's¹⁴ law of electromagnetic induction.

Solution : On letting $\mathbf{F} = \mathbf{E}$ (electric field intensity) in the curl theorem, we obtain

$$\oint \mathbf{E} \cdot d\lambda = \int \nabla \times \mathbf{E} \cdot d\sigma$$

$$= -\frac{\partial}{\partial t} \int \mathbf{B} \cdot d\sigma \quad (\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t \quad \text{Maxwell's third equation})$$

$$= -\frac{\partial \Phi_B}{\partial t} \quad \text{where} \quad \Phi_B \equiv \int \mathbf{B} \cdot d\sigma \quad \text{(total magnetic flux)}.$$

Example 23 By use of the curl theorem, obtain the integral form for Maxwell's fourth equation, the Ampère¹⁵-Maxwell law.

Solution : On letting $\mathbf{F} = \mathbf{B}$ (magnetic induction vector) in the curl theorem, we obtain

$$\oint \mathbf{B} \cdot d\lambda = \int \nabla \times \mathbf{B} \cdot d\sigma$$
$$= \mu_0 \int \mathbf{J} \cdot d\sigma + \mu_0 \epsilon_0 \int \frac{\partial \mathbf{E}}{\partial t} \cdot d\sigma$$
$$= \mu_0 I + \mu_0 \epsilon_0 \frac{\partial \Phi_E}{\partial t}.$$

The second line results from use of Maxwell's fourth equation. In the third line, Φ_E is total electric flux and I is current; they are respectively given by

$$\Phi_E = \int \mathbf{E} \cdot d\sigma$$
 and $I \equiv \int \mathbf{J} \cdot d\sigma$.

1.5 Orthogonal Curvilinear Coordinates

1.5.1 Introduction

Thus far, our presentation has made exclusive use of the right-hand Cartesian coordinate system. Often the solution of a physical problem is made easier by first selecting an appropriate coordinate system. In general, it is easier to solve a problem involving spherical

 $^{^{14}}$ Michael Faraday (1791–1867), English scientist who laid the foundations of classical field theory (despite little formal education).

¹⁵André Marie Ampère (1775–1836), French physicist and mathematician who is known for his work in electricity and magnetism.

geometry by use of spherical coordinates than by use of Cartesian coordinates. It is therefore desirable to develop a procedure for making the transformation from Cartesian coordinates to other coordinate systems. This Section is devoted to transformations from Cartesian coordinates to other orthogonal coordinate systems. Note, however, that the various basic relations in previous sections involving vectors and vector fields remain valid in other orthogonal coordinate systems.

Let the position of a point in space be completely described by $P(u^1, u^2, u^3)$, where u^1, u^2 and u^3 are three single-valued functions of position. For $u^i = \text{constant} (i = 1, 2, 3)$, the u^i are three surfaces that intersect at P. These surfaces are called **coordinate surfaces**, and the three curves of intersection are called **coordinate lines**. Tangents to the coordinate lines at are called **coordinate axes**. If the relative orientation of the coordinate surfaces changes from point to point, the u^i are called **general curvilinear coordinates**. If the three surfaces are everywhere mutually perpendicular, the u^i are referred to as **orthogonal curvilinear coordinates**.

It is assumed that the following transformations exist.

$$x^1 = f_1(u^1, u^2, u^3);$$
 $x^2 = f_2(u^1, u^2, u^3);$ and $x^3 = f_3(u^1, u^2, u^3)$

and

$$u^1 = F_1(x^1, x^2, x^3);$$
 $u^2 = F_2(x^1, x^2, x^3);$ and $u^3 = F_3(x^1, x^2, x^3).$

In the above equations, the following notation has been used: $x = x^1, y = x^2$, and $z = x^3$. The position vector of a point P is a function of the u^i , $\mathbf{r} = \mathbf{r}(u^1, u^2, u^3)$. An element of displacement is given by

$$egin{aligned} d\mathbf{r} &= rac{\partial \mathbf{r}}{\partial u^1} du^1 + rac{\partial \mathbf{r}}{\partial u^2} du^2 + rac{\partial \mathbf{r}}{\partial u^3} du^3 \ &= \sum_{i=1}^3 rac{\partial \mathbf{r}}{\partial u^i} du^i \equiv d\mathbf{s}. \end{aligned}$$

The square of an element of length is an invariant (same for all coordinate systems) and is given by

$$ds^{2} = d\mathbf{r} \cdot d\mathbf{r} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial \mathbf{r}}{\partial u^{i}} \cdot \frac{\partial \mathbf{r}}{\partial u^{j}} du^{i} du^{j}.$$
(1.42)

Note that the $\partial \mathbf{r}/\partial u^i$ are tangent to the u^i respectively, since $\partial \mathbf{r}/\partial u^1$ means u^2 and u^3 are held constant and $\mathbf{r} = \mathbf{r}(u^1)$ is constrained to move along the u^1 surface. Let the three coordinate axes be represented by \mathbf{a}_i where $\mathbf{a}_i = \partial \mathbf{r}/\partial u^i$ (see Fig. 1.25). Equation (1.42) becomes

$$ds^{2} = \sum_{i=1}^{3} \sum_{j=1}^{3} \mathbf{a}_{i} \cdot \mathbf{a}_{j} du^{i} du^{j} = \sum_{i=1}^{3} \sum_{j=1}^{3} g_{ij} du^{i} du^{j}.$$
 (1.43)

The quantities $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j = g_{ji}$ are called **metric coefficients**, and they characterize the relative nature of the space. More information on the g_{ij} may be found in Chapter 12.



Figure 1.25

In orthogonal curvilinear coordinate systems, $\mathbf{a}_i \cdot \mathbf{a}_j = 0$ for $i \neq j$, and the square of an element of length becomes

$$\begin{aligned} ds^2 &= ds_1^2 + ds_2^2 + ds_3^2 \\ &= g_{11}(du^1)^2 + g_{22}(du^2)^2 + g_{33}(du^3)^2. \end{aligned}$$

Note that $du^2 = du^3 = 0$ when the element of length ds is along u^1 ; we may therefore write

$$egin{aligned} &ds_1 = \sqrt{g_{11}} du^1 = h_1 du^1; \ &ds_2 = \sqrt{g_{22}} du^2 = h_2 du^2; \ & ext{ and } \ &ds_3 = \sqrt{g_{33}} du^3 = h_3 du^3. \end{aligned}$$

In the above equations, the scale factors h_i are given by $\sqrt{g_{ii}}$.

We now develop a scheme for determining g_{ii} when the x^i are known. In Cartesian coordinates, $g_{11} = g_{22} = g_{33} = 1$ and $ds^2 = (dx^1)^2 + (dx^2)^2 + (dx^3)^2$; in terms of the u^i , we write

$$ds^{2} = \sum_{k=1}^{3} dx^{k} dx^{k}$$

= $\sum_{k=1}^{3} \left[\left(\sum_{i=1}^{3} \frac{\partial x^{k}}{\partial u^{i}} du^{i} \right) \left(\sum_{j=1}^{3} \frac{\partial x^{k}}{\partial u^{j}} du^{j} \right) \right]$
= $\sum_{i=1}^{3} \sum_{j=1}^{3} \left(\sum_{k=1}^{3} \frac{\partial x^{k}}{\partial u^{i}} \frac{\partial x^{k}}{\partial u^{j}} \right) du^{i} du^{j}.$ (1.44)

On comparing Eq.(1.43) with Eq.(1.44), we note that

$$g_{ii} = \sum_{k=1}^{3} \left(\frac{\partial x^k}{\partial u^i}\right)^2. \tag{1.45}$$

Elements of area and volume are respectively given by

$$d\sigma_{ij} = h_i h_j du^i du^j$$
 and $d\tau = h_1 h_2 h_3 du^1 du^2 du^3$.

Expressions for the gradient, divergence, curl, and Laplacian in orthogonal curvilinear coordinates will now be developed.

1.5.2 The Gradient in Orthogonal Curvilinear Coordinates

Since $d\psi/ds$ is the component of $\nabla\psi$ in the ds direction (see page 27), $\nabla\psi$ is given by

$$\nabla \psi = \hat{\mathbf{e}}_1 \frac{\partial \psi}{\partial s_1} + \hat{\mathbf{e}}_2 \frac{\partial \psi}{\partial s_2} + \hat{\mathbf{e}}_3 \frac{\partial \psi}{\partial s_3}$$
$$= \frac{\hat{\mathbf{e}}_1}{h_1} \frac{\partial \psi}{\partial u^1} + \frac{\hat{\mathbf{e}}_2}{h_2} \frac{\partial \psi}{\partial u^2} + \frac{\hat{\mathbf{e}}_3}{h_3} \frac{\partial \psi}{\partial u^3}.$$
(1.46)

In Eq.(1.46), unit vectors $\hat{\mathbf{e}}_i$ are along $d\mathbf{s}_i$ respectively. Note that (a) $\hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2 = \hat{\mathbf{e}}_3$ (cyclic); (b) $\hat{\mathbf{e}}_i = h_i \nabla u^i$; and (c) $\nabla \cdot (\hat{\mathbf{e}}_1/h_2h_3) = \nabla \cdot \nabla u^2 \times \nabla u^3 = 0$; the last equality results form interchanging the cross and the dot and noting that the curl of the gradient equals zero. Also, this last equality provided motivation for writing the arbitrary vector \mathbf{V} in the form given in the first equation in the next Section.

1.5.3 Divergence and Curl in Orthogonal Curvilinear Coordinates

An arbitrary vector \mathbf{V} in terms of components may be written as

$$\begin{aligned} \mathbf{V} &= \hat{\mathbf{e}}_1 V_1 + \hat{\mathbf{e}}_2 V_2 + \hat{\mathbf{e}}_3 V_3 \\ &= \frac{\hat{\mathbf{e}}_1}{h_2 h_3} (h_2 h_3 V_1) + \frac{\hat{\mathbf{e}}_2}{h_1 h_3} (h_1 h_3 V_2) + \frac{\hat{\mathbf{e}}_3}{h_1 h_2} (h_1 h_2 V_3). \end{aligned}$$

Concept (c) in the previous Section was the motivation for writing V in the form given in the last step above. The divergence of V is given by

$$\nabla \cdot \mathbf{V} = \frac{\hat{\mathbf{e}}_1}{h_2 h_3} \cdot \nabla (h_2 h_3 V_1) + \frac{\hat{\mathbf{e}}_2}{h_1 h_3} \cdot \nabla (h_1 h_3 V_2) + \frac{\hat{\mathbf{e}}_3}{h_1 h_2} \cdot \nabla (h_1 h_2 V_3)$$
$$= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial (h_2 h_3 V_1)}{\partial u^1} + \frac{\partial (h_1 h_3 V_2)}{\partial u^2} + \frac{\partial (h_1 h_2 V_3)}{\partial u^3} \right]. \tag{1.47}$$

The expression for the divergence in terms of curvilinear coordinates, Eq.(1.47), results from use of the relation $\nabla \cdot (\phi \mathbf{A}) = \mathbf{A} \cdot \nabla \phi + \phi \nabla \cdot \mathbf{A}$ and use of concepts at the end of the previous Section.

In a similar manner to that used to derive the expression for the divergence in terms of curvilinear coordinates, the curl of V may be written in the form

$$\nabla \times \mathbf{V} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \hat{\mathbf{e}}_1 & h_2 \hat{\mathbf{e}}_2 & h_3 \hat{\mathbf{e}}_3 \\ \frac{\partial}{\partial u^1} & \frac{\partial}{\partial u^2} & \frac{\partial}{\partial u^3} \\ h_1 V_1 & h_2 V_2 & h_3 V_3 \end{vmatrix}.$$
(1.48)

1.5.4 The Laplacian in Orthogonal Curvilinear Coordinates

The Laplacian in orthogonal curvilinear coordinates is given by

$$\nabla^{2}\psi = \nabla \cdot \nabla\psi$$

$$= \nabla \cdot \left[\frac{\hat{\mathbf{e}}_{1}}{h_{1}}\frac{\partial\psi}{\partial u^{1}} + \frac{\hat{\mathbf{e}}_{2}}{h_{2}}\frac{\partial\psi}{\partial u^{2}} + \frac{\hat{\mathbf{e}}_{3}}{h_{3}}\frac{\partial\psi}{\partial u^{3}}\right]$$

$$= \frac{1}{h_{1}h_{2}h_{3}}\left[\frac{\partial}{\partial u^{1}}\left(\frac{h_{2}h_{3}}{h_{1}}\frac{\partial\psi}{\partial u^{1}}\right) + \frac{\partial}{\partial u^{2}}\left(\frac{h_{1}h_{3}}{h_{2}}\frac{\partial\psi}{\partial u^{2}}\right)$$

$$+ \frac{\partial}{\partial u^{3}}\left(\frac{h_{1}h_{2}}{h_{3}}\frac{\partial\psi}{\partial u^{3}}\right)\right].$$
(1.49)

The essential task in determining explicit forms for the gradient, divergence, curl, and Laplacian in specific orthogonal curvilinear coordinates is that of calculating the scale factors h_i which are related to the metric coefficients.

In the following three Sections, we give the details for three extremely useful coordinate transformations.

1.5.5 Plane Polar Coordinates (r, θ)

In plane polar (or simply polar) coordinates, we have $x = r \cos \theta$ and $y = r \sin \theta$ (see Fig. 1.26).



Figure 1.26

1.5.6 Right Circular Cylindrical Coordinates (ρ, ϕ, z)



Figure 1.27

For right circular cylindrical (or simply cylindrical) coordinates, we have $x = \rho \cos \phi$, $y = \rho \sin \phi$, and z = z (see Fig. 1.27).

1.5.7 Spherical Polar Coordinates (r, θ, ϕ)

In spherical polar (or simply spherical) coordinates, we have $\rho = r \sin \theta$, $x = \rho \cos \phi$, $y = \rho \sin \phi$, and $z = r \cos \theta$ (see Fig. 1.28).



Example 24 Find the g_{ii} (metric coefficients) and h_i (scale factors) for cylindrical coordinates.

Solution : The required transformation is $x, y, z \to \rho, \phi, z$. From Fig. 1.27, we have

$$u^1 = \rho, \ u^2 = \phi, \ \text{and} \ \ u^3 = z.$$

Also, we have

$$x = x^{1} = \rho \cos \phi, \ y = x^{2} = \rho \sin \phi, \ \text{and} \ z = x^{3} = z.$$

By use of equation for the g_{ii} (see Eq.(1.45)), we obtain

$$g_{11} = \sum_{k=1}^{3} \left(\frac{\partial x^{k}}{\partial u^{1}}\right)^{2} = \left[\frac{\partial(\rho\cos\phi)}{\partial\rho}\right]^{2} + \left[\frac{\partial(\rho\sin\phi)}{\partial\rho}\right]^{2} + \left[\frac{\partial(z)}{\partial\rho}\right]^{2} \\ = \cos^{2}\phi + \sin^{2}\phi = 1 = h_{1}^{2};$$

$$g_{22} = \sum_{k=1}^{3} \left(\frac{\partial x^{k}}{\partial u^{2}}\right)^{2} = \left[\frac{\partial(\rho\cos\phi)}{\partial\phi}\right]^{2} + \left[\frac{\partial(\rho\sin\phi)}{\partial\phi}\right]^{2} + \left[\frac{\partial(z)}{\partial\phi}\right]^{2} = \rho^{2}\sin^{2}\phi + \rho^{2}\cos^{2} = \rho^{2} = h_{2}^{2};$$

$$g_{33} = \sum_{k=1}^{3} \left(\frac{\partial x^{k}}{\partial u^{3}}\right) = \left[\frac{\partial(\rho\cos\phi)}{\partial z}\right]^{2} + \left[\frac{\partial(\rho\sin\phi)}{\partial z}\right]^{2} + \left[\frac{\partial(z)}{\partial z}\right]^{2} = 1 = h_{3}^{2}.$$

The scale factors for cylindrical coordinates are $h_1 = 1$, $h_2 = \rho$, and $h_3 = 1$.

Similarly, it can be shown that the scale factors for spherical coordinates are $h_1 = 1$, $h_2 = r$, and $h_3 = r \sin \theta$.

1.6 Problems

1.1 The pressure at any depth h in a fluid at rest is given by $P_h = P_0 + \rho hx$ where ρ is the density of the fluid. By use of dimensionless analysis, determine the dimension of the quantity represented by x; what is the name of this physical quantity?

1.2 Find A + B and A - B for A = 2i - j + k and B = i - 3j - 5k. 1.3 Consider two points $P_1(-1, -4, 5)$ and $P_2(3, -2, 2)$.

- (a) Calculate the distance from P_1 to P_2 .
- (b) Calculate the direction cosines for the line connecting P_1 and P_2 .
- (c) Determine the equation of the line connecting P_1 and P_2 .
- 1.4 Find a unit vector in the direction of $\mathbf{A} = 4\mathbf{i} + 3\mathbf{k}$.
- 1.5 Show that $\mathbf{A} = \mathbf{i} + 4\mathbf{j} + 3\mathbf{k}$ and $\mathbf{B} = 4\mathbf{i} + 2\mathbf{j} 4\mathbf{k}$ are perpendicular.
- 1.6 Determine the smaller angle between the tails of 2i and 3i + 4j.
- 1.7 Determine if $\mathbf{A} = \mathbf{i} + \mathbf{j} + \mathbf{k}$ and $\mathbf{B} = 3\mathbf{i} + \mathbf{k}$ satisfy the Cauchy inequality.
- 1.8 Find a unit vector perpendicular to $\mathbf{i} 2\mathbf{j} 3\mathbf{k}$ and $\mathbf{i} + 2\mathbf{j} \mathbf{k}$.

1.9 Find the projection of $8\mathbf{i} + \mathbf{j}$ in the direction of $\mathbf{i} + 2\mathbf{j} - 2\mathbf{k}$.

1.10 Show that $\mathbf{A} = 2\mathbf{i} - \mathbf{j} + \mathbf{k}$, $\mathbf{B} = \mathbf{i} - 3\mathbf{j} - 5\mathbf{k}$, and $\mathbf{C} = 3\mathbf{i} - 4\mathbf{j} - 4\mathbf{k}$ form the sides of a right triangle.

1.11 By use of the determinant form, calculate $\mathbf{k} \times \mathbf{i}$.

1.12 Calculate $\mathbf{A} \cdot \mathbf{B} \times \mathbf{C}$ if $\mathbf{A} = 2\mathbf{i}, \mathbf{B} = 3\mathbf{j}$, and $\mathbf{C} = 4\mathbf{k}$.

1.13 Compute $(\mathbf{A} \times \mathbf{B}) \times \mathbf{C}$ and $\mathbf{A} \times (\mathbf{B} \times \mathbf{C})$ directly for $\mathbf{A} = 2\mathbf{i} + 2\mathbf{j}$, $\mathbf{B} = 8\mathbf{i}$, and $\mathbf{C} = 3\mathbf{i} - \mathbf{j} + \mathbf{k}$.

1.14 Write down the three scalar equations corresponding to the Lorentz force law, $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$.

1.15 By use of Cartesian components, show that

(a)
$$\mathbf{A} \cdot \mathbf{B} \times \mathbf{C} = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix}$$
 and
(b) $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B}).$

1.16 By use of Cartesian components, show that

(a)
$$\nabla \cdot (\phi \mathbf{A}) = \mathbf{A} \cdot \nabla \phi + \phi \nabla \cdot \mathbf{A},$$

(b) $\nabla \times (\phi \mathbf{A}) = \phi \nabla \times \mathbf{A} - \mathbf{A} \times \nabla \phi,$
(c) $\nabla \times \nabla \times \mathbf{A} = \nabla \nabla \cdot \mathbf{A} - \nabla^2 \mathbf{A}.$

1.17 By use of Cartesian components, show that

(a)
$$\nabla \cdot \mathbf{r} = 3$$
,
(b) $\nabla \times \mathbf{r} = \mathbf{0}$, and
(c) $\nabla r^n = nr^{n-2}\mathbf{r}$.

1.18 Given: $\mathbf{A} = x^2 y \mathbf{i} + (x - y) \mathbf{k}$, $\mathbf{B} = x \mathbf{i}$, and $\phi = x y^2 z^3$. Find

(a) div **B**,
(b) Curl **A**, and
(c) grad φ.

1.19 If $\nabla^2 \phi = 0$, show that $\nabla \phi$ is both solenoidal and irrotational.

1.20 If **A** is irrotational, show that $\mathbf{A} \times \mathbf{r}$ is solenoidal.

1.21 Find the directional derivative of $\phi(x, y, z) = 2x^3 - 3yz$ at the point (2,1,3) in the direction parallel to the vector with components given by (2, 1, -2).

1.22 Find a unit normal to the surface $\phi = x^2 + yz = C$ at the point (2, 1, 1).

1.23 Compute the line integral along the line segment joining (0,0,0) and (1,2,4) if $\mathbf{A} = x^2 \mathbf{i} + y \mathbf{j} + (xz - y) \mathbf{k}$.

1.24 By use of Maxwell's equations for a vacuum, show that

$$\nabla^2 E_x = \epsilon_0 \mu_0 \frac{\partial^2 E_x}{\partial t^2}, \quad \nabla^2 E_y = \epsilon_0 \mu_0 \frac{\partial^2 E_y}{\partial t^2}, \quad \text{and} \quad \nabla^2 E_z = \epsilon_0 \mu_0 \frac{\partial^2 E_z}{\partial t^2}$$

1.25 In Maxwell's electromagnetic theory, choose the vector and scalar potentials (A and φ) such that

$$\nabla \cdot \mathbf{A} + \frac{\partial \varphi}{\partial t} = 0$$
 (Lorentz gauge condition)

and show that

(a)
$$\nabla^2 \mathbf{A} - \epsilon_0 \mu_0 \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu_0 \mathbf{J}$$
 and
(b) $\nabla^2 \varphi - \epsilon_0 \mu_0 \frac{\partial^2 \varphi}{\partial t^2} = -\frac{\rho}{\epsilon_0}.$

The above equations may be written in the following compact forms

$$\square^2 \mathbf{A} = -\mu_0 \mathbf{J}$$
 and $\square^2 \varphi = \frac{\rho}{\epsilon_0}$

where the d'Alembertian¹⁶ operator \square^2 is defined by

$$\Box^2 = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}.$$

Here Maxwell's equations have been reduced to the study of equations for the vector and scalar potential.

1.26 By use of Stokes' theorem, prove that $\nabla \times \nabla V = \mathbf{0}$.

1.27 By use of Green's theorem, establish the conditions for

$$\int \chi \nabla^2 \psi d\tau = \int \psi \nabla^2 \chi d\tau$$

 $^{^{16}}$ Jean Le Rond d'Alembert (1717–1783), French mathematician and physicist who was one of the leading scientists of his time.

where χ and ψ are scalar functions of x, y, and z. 1.28 In the divergence theorem, let $\mathbf{F} = \phi \mathbf{C}$ (where \mathbf{C} is an arbitrary constant vector) and show that

$$\oint \phi \hat{\mathbf{n}} d\sigma = \int \nabla \phi d\tau.$$

1.29 If σ is a closed surface which bounds a volume τ , prove that

(a)
$$\oint \hat{\mathbf{n}} d\sigma = \mathbf{0}$$
,
(b) $\int \nabla \cdot \hat{\mathbf{n}} d\tau = \sigma$, and
(c) $\int \nabla \times \hat{\mathbf{n}} d\tau = \mathbf{0}$.

1.30 In the divergence theorem, let $\mathbf{F} = \mathbf{B} \times \mathbf{C}$ (where \mathbf{C} is an arbitrary constant vector) and show that

$$\oint \hat{\mathbf{n}} \times \mathbf{B} d\sigma = \int \nabla \times \mathbf{B} d\tau.$$

1.31 Show that the derivative of angular momentum with respect to time equals torque. 1.32 Show that $\mathbf{F} = xy^2\mathbf{i} + x^3y\mathbf{j}$ is not a conservative force field.

1.33 Show that the force in Problem 1.32 is inconsistent with $\mathbf{F} = -\nabla \phi$.

1.34 (a) Modify the force in Problem 1.32 so that it becomes a conservative force and find the expression for the corresponding potential energy. (b) Show that this potential energy leads to the force in Part (a).

1.35 The gravitational force on mass m at distance r from the center of the Earth is

$$\mathbf{F} = -G rac{m M_E}{r^2} \hat{\mathbf{r}} \; .$$

(a) Show that the gravitational force field is conservative. (b) Obtain the expression for the gravitational potential energy. (c) Repeat Parts (a) and (b) for the Coulomb force law. 1.36 If \mathbf{v} is the velocity of a particle whose constant angular velocity is ω , show that $\nabla \times \mathbf{v} = 2\omega$. (*Hint*: Draw a detailed diagram for the problem.)

1.37 At time t the position vector of a moving particle is $\mathbf{r} = \mathbf{A} \cos \omega t + \mathbf{B} \sin \omega t$ where **A** and **B** are constant vectors and ω is a constant scalar. (a) Find the velocity of the particle at time t. (b) Show that $\mathbf{r} \times \mathbf{v}$ equals a constant vector. (c) Show that the acceleration is directed toward the origin and is proportional to the displacement (simple harmonic motion, SHM).

1.38 Suppose the radius vector for a particle moving in a plane is given by $\mathbf{r} = r(t)\hat{\mathbf{r}}$ with polar coordinates (r, θ) where $|\hat{\mathbf{r}}| = 1$. (a) Show that the velocity of this particle is given by

$$\mathbf{v} = \frac{dr}{dt}\mathbf{\hat{r}} + r\frac{d\theta}{dt}\mathbf{\hat{T}}$$

where $\hat{\mathbf{T}} = -\mathbf{i}\sin\theta + \mathbf{j}\cos\theta$. (b) Show that the acceleration of this particle is given by

$$\mathbf{a} = \left[\frac{d^2r}{dt^2} - r\left(\frac{d\theta}{dt}\right)^2\right]\hat{\mathbf{r}} + \left[r\frac{d^2\theta}{dt^2} + 2\frac{dr}{dt}\frac{d\theta}{dt}\right]\hat{\mathbf{T}}.$$

(c) Identify the radial and tangential components of the velocity and acceleration, respectively. Identify the centripetal acceleration. The Coriolis¹⁷ acceleration is given by $2(dr/dt)(d\theta/dt)\hat{\mathbf{T}}$.

1.39 A force with x, y, and z components of 3, 4, and 12 N, respectively, displaces an object from the point (1, 2, 3) to (2, -3, 1). Calculate the work done by this force.

1.40 A force with magnitude 6 N acts through the point P(4, -1, 7) in the same direction as the vector with components (9, 6, -2). Calculate the torque of this force about the point A(1, -3, 2).

1.41 Two particles of mass m collide elastically. The initial momentum of particle one is \mathbf{p}_1 and its momentum after collision is \mathbf{q}_1 . Particle two is initially at rest. By use of (a) conservation of kinetic energy, (b) conservation of momentum, and (c) the dot product, show that the angle between the two particles after collision is 90°. (*Hint*: Write kinetic energy in terms of the momentum squared, e.g., $KE = \mathbf{p}^2/2m$).

1.42 A particle with initial momentum p_1 **i** explodes into two pieces. Piece one moves vertically upward such that $q_1 = 1.5p_1$ where \mathbf{q}_1 is the momentum of piece one after the explosion. By use of the conservation of momentum principle, calculate the final momentum of piece two after the explosion, q_2 .

1.43 Supply the steps that lead to Eq.(1.48).

1.44 Write down Laplace's equation in cylindrical coordinates.

1.45 For spherical coordinates, calculate the scale factors and write down Laplace's equation. 1.46 In spherical coordinates where $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, and $z = r \cos \theta$, we find that

$$\frac{\partial}{\partial z} = \cos\theta \frac{\partial}{\partial r} - \frac{1}{r}\sin\theta \frac{\partial}{\partial \theta}.$$

By use of the change of variables rule, express $\partial/\partial x$ and $\partial/\partial y$ in spherical polar coordinates.

1.7 Appendix I: Système International (SI) Units

The following seven physical quantities are fundamental in the SI system of units:

- 1. Length meter (m)
- 2. Mass kilogram (kg)
- 3. Time second (s)
- 4. Temperature Kelvin (K); K means degree Kelvin
- 5. Amount of Substance mole (mol)
- 6. Electric Current Ampère (A)
- 7. Luminous Intensity candela (cd)

 $^{^{17}}$ Gustave Gaspard de Coriolis (1792–1843), French mathematician and scientist who is best known for the Coroilis force.

Definitions

- 1. Meter is the distance traveled by light in vacuum during 1/299, 792, 458 second. The speed of light is a fundamental constant $c \equiv 299, 792, 458$ m/s. (1983)
- Kilogram is the mass that equals the mass of the Platinum-Iridium alloy cylinder that is kept at the International bureau of Weights and Measures at Sèvres, France. (1989)
- 3. Second is the duration of 9, 192, 631, 770 periods of the radiation corresponding to transitions between the two hyperfine levels of the ground state of Cesium-133. (1967)
- 4. Ampère is the constant current in two straight parallel conductors (of infinite length with negligible cross section and 1 m apart in a vacuum) that produces a force per unit length of 2×10^{-7} N/m. (1947)
- 5. Kelvin is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water which is approximately 0.01° C. (1967)
- 6. Mole is the amount of substance which contains as many elementary entities as there are atoms in 0.012 kg of Carbon-12. (1971)
- 7. Candela is the luminous intensity (in the perpendicular direction) of a surface of 1/600,000 square meter of a blackbody at the temperature of freezing Platinum under a pressure of 101,325 N/m. (1967)

1.8 Appendix II: Properties of Determinants

1.8.1 Introduction

This appendix is devoted to a summary of some essential properties of determinants. A **de-terminant** is a square array of quantities called elements which may be combined according to the rules given below. In symbolic form, we write

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 & \dots & r_1 \\ a_2 & b_2 & c_2 & \dots & r_2 \\ \vdots & \vdots & \vdots & & \vdots \\ a_n & b_n & c_n & \dots & r_n \end{vmatrix}$$

The order of the above determinant is n. The value of the determinant in terms of the elements $a_i, b_j, \ldots, r_{\ell}$ is defined as

$$\Delta = \sum_{i,j,\dots,\ell}^{n} \epsilon_{ij\dots\ell} a_i b_j \dots r_{\ell}$$
(A1.1)

where the Levi-Civita¹⁸ symbol, $\epsilon_{ij...\ell}$, has the following property:

$$\epsilon_{ij\ldots\ell} = \begin{cases} +1 & \text{for an even permutation of } (i, j, \ldots, \ell) \\ -1 & \text{for an odd permutation of } (i, j, \ldots, \ell) \\ 0 & \text{if an index in repeated.} \end{cases}$$
(A1.2)

For example,

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } ijk = 123, \ 231, \ 312\\ -1 & \text{if } ijk = 321, \ 213, \ 132\\ 0 & \text{otherwise.} \end{cases}$$

On applying Eq.(A1.1) to a third-order determinant

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix},$$

we obtain

$$\Delta = \sum_{ijk}^{3} \epsilon_{ijk} a_i b_j c_k$$

=
$$\sum_{jk}^{3} (\epsilon_{1jk} a_1 b_j c_k + \epsilon_{2jk} a_2 b_j c_k + \epsilon_{3jk} a_3 b_j c_k).$$
 (A1.3)

Equation (A1.3) reduces to

$$\Delta = \sum_{k}^{3} (\epsilon_{11k} a_1 b_1 c_k + \epsilon_{12k} a_1 b_2 c_k + \epsilon_{13k} a_1 b_3 c_k + \epsilon_{21k} a_2 b_1 c_k + \epsilon_{22k} a_2 b_2 c_k + \epsilon_{23k} a_2 b_3 c_k + \epsilon_{31k} a_3 b_1 c_k + \epsilon_{32k} a_3 b_2 c_k + \epsilon_{33k} a_3 b_3 c_k).$$
(A1.4)

Since $\epsilon_{11k} = \epsilon_{22k} = \epsilon_{33k} = 0$, Eq.(A1.4) becomes

$$\Delta = \epsilon_{121}a_1b_2c_1 + \epsilon_{122}a_1b_2c_2 + \epsilon_{123}a_1b_2c_3 + \epsilon_{131}a_1b_3c_1 + \epsilon_{132}a_1b_3c_2 + \epsilon_{133}a_1b_3c_3 + \epsilon_{211}a_2b_1c_1 + \epsilon_{212}a_2b_1c_2 + \epsilon_{213}a_2b_1c_3 + \epsilon_{231}a_2b_3c_1 + \epsilon_{232}a_2b_3c_2 + \epsilon_{233}a_2b_3c_3 + \epsilon_{311}a_3b_1c_1 + \epsilon_{312}a_3b_1c_2 + \epsilon_{313}a_3b_1c_3 + \epsilon_{321}a_3b_2c_1 + \epsilon_{322}a_3b_2c_2 + \epsilon_{323}a_3b_2c_3.$$
(A1.5)

With the aid of Eq.(A1.2), Eq.(A1.5) reduces to

$$\Delta = a_1 b_2 c_3 - a_1 b_3 c_2 - a_2 b_1 c_3 + a_2 b_3 c_1 + a_3 b_1 c_2 - a_3 b_2 c_1 \tag{A1.6}$$

¹⁸Tullio Levi-Civita (1872–1941), Italian mathematician and physicist who is best known for his work on tensor calculus. He was a student of Ricci.

The following scheme may be used to obtain the result in Eq.(A1.6): (a) Copy the first two columns on the left of the determinant. (b) The first positive term results from the product of the three elements along the main diagonal in the original determinant; the second positive term results from the product of the three elements along a line parallel to and above the main diagonal; and the third positive term results from the product of the three elements along a parallel line above the previous line. (c) The first negative term results from the product of the three elements along a diagonal starting with c_1 and ending with a_3 ; subsequent negative terms result from products along lines parallel to and below the previous line.

The result from this scheme is, of course, the same as that in Eq.(A1.6) and is written as

$$\Delta = a_1 b_2 c_3 + b_1 c_2 a_3 + c_1 a_2 b_3 - (c_1 b_2 a_3 + a_1 c_2 b_3 + b_1 a_2 c_3).$$

1.8.2 The Laplace Development by Minors

The result in Eq.(A1.6) may be written in the form

$$\Delta = a_1(b_2c_3 - b_3c_2) - a_2(b_1c_3 - b_3c_1) + a_3(b_1c_2 - b_2c_1)$$

= $a_1 \begin{vmatrix} b_2 & c_2 \\ b_3 & c_3 \end{vmatrix} - a_2 \begin{vmatrix} b_1 & c_1 \\ b_3 & c_3 \end{vmatrix} + a_3 \begin{vmatrix} b_1 & c_1 \\ b_2 & c_2 \end{vmatrix}$ (A1.7)

where
$$\begin{vmatrix} b_2 & c_2 \\ b_3 & c_3 \end{vmatrix} = b_2 c_3 - b_3 c_2.$$

The procedure of expressing Δ in the form given in Eq.(A1.7) may be generalized to obtain the value of an *n*th-order determinant. In Eq.(A1.7), it is seen that the expansion of a third-order determinant is expressed as a linear combination of the product of an element and a second-order determinant. Careful examination of Eq.(A1.7) reveals that the second-order determinant is the determinant obtained by omitting the elements in the row and column in which the multiplying element (the element in front of the second-order determinant) appears in the original determinant. The resulting second-order determinant is called a **minor**. Thus the minor of a_1 is obtained in the following manner: eliminate the row and column containing a_1 .

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$
 out

The minor of a_1 is therefore

$$\begin{vmatrix} b_2 & c_2 \\ b_3 & c_3 \end{vmatrix}.$$

In the general *n*th-order determinant, the sign $(-1)^{i+j}$ is associated with the minor of the element in the *i*th row and the *j*th column. The minor with its sign $(-1)^{i+j}$ is called the **cofactor**. For the general determinant

$$|A| = \det A = \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & & & \vdots \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix}$$

the value in terms of cofactors is given by

$$|A| = \sum_{j=1}^{n} a_{ij} A^{ij}$$
 for any *i*. (A1.8)

The relation in Eq.(A1.8) is called the **Laplace development**. Expanding it along the first row gives i = 1. For example,

$$|A| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$$
 becomes $|A| = \sum_{j=1}^{2} a_{ij} A^{ij} = a_{11} A^{11} + a_{12} A^{12}$

where

$$A^{11} = (-1)^{1+1} |a_{22}| = a_{22}$$
 and $A^{12} = (-1)^{1+2} |a_{21}| = -a_{21}$. (A1.9)

On substituting Eq.(A1.9) into the expression for |A|, we obtain the expected result

$$|A| = a_{11}a_{22} - a_{12}a_{21}.$$

Unlike matrices (see page 60), determinants may be evaluated to yield a number.

1.9 Summary of Some Properties of Determinants

The following are properties of determinants which may be readily proved.

1. The value of a determinant is not changed if corresponding rows and columns are interchanged.

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix}.$$

2. If a multiple of one column is added (row by row) to another column or if a multiple of one row is added (column by column) to another row, the value of the determinant is unchanged.

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 + kb_1 & b_1 & c_1 \\ a_2 + kb_2 & b_2 & c_2 \\ a_3 + kb_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 + \ell a_3 & b_1 + \ell b_3 & c_1 + \ell c_3 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}.$$

3. If each element of a column or row is zero, the value of the determinant is zero.

$$\Delta = \begin{vmatrix} 0 & b_1 & c_1 \\ 0 & b_2 & c_2 \\ 0 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ 0 & 0 & 0 \\ a_3 & b_3 & c_3 \end{vmatrix} = 0.$$

4. If two columns or rows are identical, the value of the determinant is zero.

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_1 & b_1 & c_1 \end{vmatrix} = \begin{vmatrix} c_1 & c_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = 0.$$

5. If two column or rows are proportional, the value of the determinant is zero.

$$\Delta = \begin{vmatrix} a_1 & ka_1 & c_1 \\ a_2 & ka_2 & c_2 \\ a_3 & ka_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ \ell a_2 & \ell b_2 & \ell c_2 \end{vmatrix} = 0.$$

6. If two column or rows are interchanged, the sign of the determinant is changed.

$$\Delta = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = - \begin{vmatrix} c_1 & b_1 & a_1 \\ c_2 & b_2 & a_2 \\ c_3 & b_3 & a_3 \end{vmatrix} = \begin{vmatrix} c_2 & b_2 & a_2 \\ c_1 & b_1 & a_1 \\ c_3 & b_3 & a_3 \end{vmatrix}.$$

7. If each element of a column or row is multiplied by the same number, the resulting determinant is multiplied by that same number.

$$\Delta = \begin{vmatrix} a_1 & b_1 & kc_1 \\ a_2 & b_2 & kc_2 \\ a_3 & b_3 & kc_3 \end{vmatrix} = \begin{vmatrix} ka_1 & kb_1 & kc_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = k \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

Chapter 2

Modern Algebraic Methods in Physics

2.1 Introduction

In modern (abstract) algebra, arithmetic operations are generalized and applied to objects other than real numbers. As with most of pure mathematics, modern algebra is normally presented as an axiomatic study consisting of theorems and proofs. This axiomatic approach to the subject may well be responsible for long delays in the use of newly developed modern algebraic concepts in physics. It is now clearly recognized that certain elements of modern algebra are invaluable in mathematical physics. Many excellent texts on modern (abstract) algebra exist, and we make no attempt at an axiomatic presentation. The presentation in this chapter is intended to define, explain, and give examples of certain modern algebraic concepts that are use through mathematical physics and will be used in subsequent chapters of this book.

In quantum mechanics and certain other areas of physics, physical quantities are represented by linear operators on a vector space. While this approach may seem far removed from an experimental process, it makes possible the development of these subject areas by use of rigorous mathematical procedures. Moreover, agreement between calculated results obtained by use of this formal (or abstract) approach with experimentally measured values has given credence to this formulation. Mathematical operations involving linear operators are often carried out by use of matrices since linear operators may be represented by matrices. Hence a knowledge of vector spaces, linear operators, and matrix analysis is required in many areas of physics. An introductory presentation of matrix analysis with examples is given in the next Section. Then, basic concepts of vector spaces, including topological spaces, are explained, and definitions of groups, rings, fields, and algebras are given. A study of some of the material in the section on topological spaces may be deferred until it is actually needed in Chapters 11 and 12.

2.2 Matrix Analysis

The term "matrix" was introduced by Cayley¹, and matrix theory was developed by Cayley, Hamilton², and Sylvester³ in the study of simultaneous linear equations.

Matrices were rarely used by physicists prior to 1925. Today, matrices are used in most areas of physics. A matrix is a rectangular array of quantities,

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}$$
(2.1)

where the a_{ij} are elements (of the *i*th row and *j*th column); they may be real or complex numbers or functions. When i = j, the element is a diagonal element, and the element is off-diagonal when $i \neq j$. The above general matrix A has m rows and n columns and is a matrix of order $m \times n$ (m by n). If m = n, the matrix is a square matrix. The main diagonal of a square matrix consists of the elements $a_{11}, a_{22}, \ldots, a_{nn}$.

The row matrix is written as

$$A = (a_{11} \ a_{12} \ \dots \ a_{1n}),$$

and the column matrix is written as

$$A = \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix}.$$

Two matrices, A and B, of the same order are said to be **equal** iff (if and only if) $a_{ij} = b_{ij}$ for all *i* and *j* (the symbol \forall is often used by mathematicians to mean "for all"). For example, x = 2 for A = B where

$$A = \begin{pmatrix} x \\ 1 \end{pmatrix}$$
 and $B = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$.

If $a_{ij} = 0$ for all *i* and *j* $(\forall i, j)$, then *A* is said to be a **null matrix**. For example, the 2×2 null matrix is given by

$$A = \left(\begin{array}{cc} 0 & 0\\ 0 & 0 \end{array}\right).$$

The multiplication of a matrix A by a scalar k is given by $kA = ka_{ij}$ for all i and j; for example,

$$2\left(\begin{array}{cc}1&2\\3&1\end{array}\right)=\left(\begin{array}{cc}2&4\\6&2\end{array}\right)$$

Note that k may be negative and/or a fraction as well as complex.

 $^{^{1}}$ Arthur Cayley (1821–1895), English mathematician who made important contributions to advance pure mathematics.

 $^{^{2}}$ Sir William Rowan Hamilton (1805–1865), Irish mathematician who made important contributions in mathematics and physics.

³James Joseph Sylvester (1814–1897), English mathematician who is known for his use of matrix theory to study higher dimensional geometry. He coined the term discriminant.

2.2.1 Matrix Operations

Matrix Addition The operation of addition (or subtraction) for two matrices is defined iff they have the same order. For two $n \times m$ matrices A and B, addition (subtraction) is defined as

$$C = A \pm B \tag{2.2}$$

where $c_{ij} = a_{ij} \pm b_{ij}$ for all *i* and *j*; for example,

$$\begin{pmatrix} 3 & 1 & 4 \\ 4 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 2 \\ 3 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 2 & 2 & 2 \\ 1 & 0 & -1 \end{pmatrix}.$$

Also, the following laws are valid for addition (subtraction) of matrices of the same order:

Commutative law:
$$A + B = B + A$$

Associative law: $(A + B) + C = A + (B + C)$.

Matrix Multiplication For matrices A and B, two kinds of products are defined; they are called the matrix product, AB, and the direct product, $A \otimes B$.

Elements of C in the matrix product C = AB are obtained by use of the following definition:

$$c_{ij} = \sum_{k=1}^{s} a_{ik} b_{kj}$$
(2.3)

where the orders of A, B, and C are $n \times s, s \times m$, and $n \times m$, respectively. Note that the matrix product is defined for conformable matrices only; this means that the number of columns of A must equal the number of rows of B. As is clear from the above definition of the matrix product, the commutative law of multiplication is not, in general, valid for the matrix product, $AB \neq BA$. The associative law of multiplication, however, is valid for the matrix product, A(BC) = (AB)C.

Consider

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$
 and $B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$.

Here the matrix products become

$$AB = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$
$$= \begin{pmatrix} a_{11}b_{11} + a_{12}b_{12} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}$$

and

$$BA = \begin{pmatrix} b_{11}a_{11} + b_{12}a_{22} & b_{11}a_{11} + b_{11}a_{22} \\ b_{21}a_{11} + b_{22}a_{12} & b_{21}a_{12} + b_{22}a_{22} \end{pmatrix}.$$

For example,

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 2 & 3 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 2 & 3 \end{pmatrix} \quad \text{and}$$
$$\begin{pmatrix} 0 & 0 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 3 \end{pmatrix}.$$

In this example, note that the matrix product is not commutative. Consider the following system of linear equations:

$$3x + y + 2z = 3$$

$$2x - 3y - z = -3$$

$$x + 2y + z = 4.$$

In matrix form, the above system of three linear equations may be written as

$$\begin{pmatrix} 3 & 1 & 2 \\ 2 & -3 & -1 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 3 \\ -3 \\ 4 \end{pmatrix}.$$

The direct product (also called tensor product) is defined for general matrices. If A is an $n \times n$ matrix and B is an $m \times m$ matrix, then the **direct product** $A \otimes B$ is an $nm \times nm$ matrix and is defined by

$$C = A \otimes B$$
 where $C_{ik,jp} = a_{ij}b_{kp}$. (2.4)

If

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$
 and $B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$,

then

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}$$
$$= \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}.$$

Consider the following two matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

The direct product $\sigma_1 \otimes \sigma_3$ is given by

$$\sigma_1 \otimes \sigma_3 = \begin{pmatrix} 0 \times \sigma_3 & 1 \times \sigma_3 \\ 1 \times \sigma_3 & 0 \times \sigma_3 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

Division by a Matrix The operation of division is not defined for matrices. The notion of the inverse of a square matrix, discussed below, is introduced to serve a similar purpose. The Derivative of a Matrix The derivative of a matrix respect to a variable s equals the derivative of each element with respect to s separately; for example,

$$\frac{d}{dx} \left(\begin{array}{ccc} x & x^3 & 2 \\ e^{-x} & 0 & 3x^2 \end{array} \right) = \left(\begin{array}{ccc} 1 & 3x^2 & 0 \\ -e^{-x} & 0 & 6x \end{array} \right).$$

The Integral of a Matrix The integral of a matrix with respect to a variable s equals the integral of each element with respect to s separately; for example,

$$\int \left(\begin{array}{ccc} x & x^3 & 2 \\ e^{-x} & 0 & 3x^2 \end{array}\right) dx = \left(\begin{array}{ccc} x^2/2 & x^4/4 & 2x \\ -e^{-x} & c & x^3 \end{array}\right) + \left(\begin{array}{ccc} c_1 & c_2 & c_3 \\ c_4 & 0 & c_5 \end{array}\right).$$

Partitioned Matrices Thus far, we have assumed that the elements of matrices are numbers or functions. The elements, however, may themselves be matrices. That is to say, a matrix may be partitioned. The following is one way of partitioning a 3×3 matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} & \vdots & a_{13} \\ a_{21} & a_{22} & \vdots & a_{23} \\ \cdots & \cdots & \cdots & \cdots \\ a_{31} & a_{32} & \vdots & a_{33} \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

The indicated b's are called **submatrices**. For partitioned matrices, the usual operations are valid.

2.2.2 Properties of Arbitrary Matrices

The Transpose of a Matrix The transpose of an arbitrary matrix A is written as A^{T} and is obtained by interchanging corresponding rows and columns of A; if we write $A = a_{ij}$, then $A^{T} = a_{ji}$. For example,

$$A = \begin{pmatrix} 1 & -1 & 2 \\ 3 & 0 & 1 \end{pmatrix}$$
 and $A^T = \begin{pmatrix} 1 & 3 \\ -1 & 0 \\ 2 & 1 \end{pmatrix}$.

Note that the transpose (operator) operation reverses the order of matrix multiplication, $(AB)^T = B^T A^T$.

The Complex Conjugate of a Matrix For z = x + iy, x is the real part and y is the imaginary part of z. The quantity i is given by $i = \sqrt{-1}$. The complex conjugate A^* of an arbitrary matrix A is formed by taking the complex conjugate (changing the sign of the imaginary part) of each element; hence we have $A^* = a_{ij}^*$. For example,

$$A = \begin{pmatrix} 2+3i & 4-5i \\ 3 & 4i \end{pmatrix} \quad \text{and} \quad A^* = \begin{pmatrix} 2-3i & 4+5i \\ 3 & -4i \end{pmatrix}.$$

If $A^* = A$, then A is a real matrix.

The Hermitian Conjugate of a Matrix The Hermitian⁴ conjugate A^{\dagger} (also known as the Hermitian operator, A^{H}) of an arbitrary matrix A is obtained by taking the complex conjugate of the matrix (each element) and then the transpose of the complex conjugate matrix. For example,

$$A = \begin{pmatrix} 2+3i & 4-5i \\ 3 & 4i \end{pmatrix}$$
$$A^{\dagger} = \begin{pmatrix} 2-3i & 4+5i \\ 3 & -4i \end{pmatrix}^{T} = \begin{pmatrix} 2-3i & 3 \\ 4+5i & -4i \end{pmatrix}.$$

The Hermitian operation reverses the order of matrix multiplication, $(AB)^{\dagger} = B^{\dagger}A^{\dagger}$.

2.2.3 Special Square Matrices

The Identity Matrix A matrix defined by $I = \delta_{ij}$ where IA = AI is called an identity matrix. Elements of the Kronecker⁵ delta, δ_{ij} , have the following property:

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j. \end{cases}$$
(2.5)

The 3×3 unit matrix is given by

$$I = \left(\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right) \,.$$

Diagonal Matrices The diagonal alignment of elements in a matrix extending from the upper left to the lower right is called the **principal** or **main diagonal**. The diagonal matrix is given by $D = d_{ij}\delta_{ij}$. The following is an example of a 3×3 diagonal matrix:

$$D = \left(\begin{array}{rrr} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 4 \end{array}\right) \,.$$

Singular Matrices If det|A| = 0, then A is said to be a singular matrix. For example,

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$
 or $\det |A| = 0.$

Cofactor Matrices The cofactor matrix is written as A^C and is defined by $A^C = A^{ij}$. The *ij*-th element of the cofactor of A^{ij} is the determinant of a submatrix obtained by striking the *i*th row and the *j*th column of A and choosing the sign $(-1)^{i+j}$. For example,

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \quad \text{and} \quad A^{c} = \begin{pmatrix} A^{11} & A^{12} & A^{13} \\ A^{21} & A^{22} & A^{23} \\ A^{31} & A^{32} & A^{33} \end{pmatrix}$$

⁴Charles Hermite (1822–1901), French mathematician who is known for his work in number theory, algebra, and the theory of equations.

⁵Leopold Kronecker (1823–1891), German mathematician who was an advocate of the reduction of all mathematics to arguments involving only integers and finite number of steps. He is known for the remark "God created the integers, all else is the result of man".

where

$$\begin{split} A^{11} &= (-1)^{1+1} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix}, \quad A^{12} &= (-1)^{1+2} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix}, \\ A^{13} &= (-1)^{1+3} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}, \quad A^{21} &= (-1)^{2+1} \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix}, \\ A^{22} &= (-1)^{2+2} \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix}, \quad A^{23} &= (-1)^{2+3} \begin{vmatrix} a_{11} & a_{12} \\ a_{31} & a_{32} \end{vmatrix}, \\ A^{31} &= (-1)^{3+1} \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix}, \quad A^{32} &= (-1)^{3+2} \begin{vmatrix} a_{11} & a_{13} \\ a_{21} & a_{23} \end{vmatrix}, \quad \text{and} \\ A^{33} &= (-1)^{3+3} \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}. \end{split}$$

Adjoint and Self-Adjoint Matrices The adjoint of a matrix is written as adjA (or A^{CT}); it is defined as the cofactor transpose. For example,

$$A = \begin{pmatrix} 1 & 3 \\ 2 & 1 \end{pmatrix}, \quad A^C = \begin{pmatrix} 1 & -2 \\ -3 & 1 \end{pmatrix}, \quad A^{CT} = \begin{pmatrix} 1 & -3 \\ -2 & 1 \end{pmatrix}.$$

If adjA = A, then A is said to be **self-adjoint**. For example,

$$A = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A^C = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \text{ and}$$
$$A^{CT} = \operatorname{adj} A = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = A.$$

Symmetric and Antisymmetric Matrices If the transpose of A equals $A(A^T = A)$, then A is said to by a symmetric matrix. For example,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 and $\sigma_1^T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_1.$

If $A^T = -A$, then A is referred to as an antisymmetric matrix (skew matrix). For example,

$$\sigma_2 = \left(egin{array}{cc} 0 & -i \ i & 0 \end{array}
ight) \quad ext{ and } \quad \sigma_2^T = \left(egin{array}{cc} 0 & i \ -i & 0 \end{array}
ight) = -\sigma_2.$$

Hermitian Matrices If the Hermitian conjugate of A equals A, $A^{\dagger} = A$, then A is said to be a **Hermitian matrix**. For example,

$$\sigma_2 = \left(egin{array}{cc} 0 & -i \ i & 0 \end{array}
ight) \quad ext{ and } \quad \sigma_2^* = \left(egin{array}{cc} 0 & i \ -i & 0 \end{array}
ight);$$

hence we have

$$(\sigma_2^*)^T = \sigma_2^\dagger = \left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right) = \sigma_2.$$

In quantum mechanics, observables are represented by Hermitian operators, i.e. Hermitian matrices.

Unitary Matrices If $AA^{\dagger} = I$, then A is defined to be a unitary matrix. For example,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (\sigma_1^*)^T = \sigma_1^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{and}$$
$$\sigma_1 \sigma_1^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I.$$

Orthogonal Matrices If $AA^T = I$, then A is said to be an **orthogonal matrix**. For example,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_1^T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \text{ and}$$
$$\sigma_1 \sigma_1^T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I.$$

The Trace of a Matrix The trace of a matrix is the sum of its diagonal elements and is written as

$$\mathrm{Tr}A = \sum_{k} a_{kk}.$$
 (2.6)

For example,

$$A = \left(egin{array}{cc} 2 & 4 \ 3 & 7 \end{array}
ight) \qquad ext{and} \qquad ext{Tr} A = 2 + 7 = 9$$

The Inverse of a Matrix For the **inverse matrix** A^{-1} , it is required that $AA^{-1} = I$. Now, we develop the explicit expression for A^{-1} . In the Laplace development for the value of a determinant by use of minors (see Appendix II of Chapter 1), we have

$$|A| = \sum_{j=1}^{n} a_{ij} A^{ij}$$
 or $|A| \, \delta_{ij} = \sum_{j=1}^{n} a_{ij} A^{kj}$.

Let $b_{jk} = A^{kj}$; that is to say, $B = A^{CT}$. The above equation becomes

$$|A| \,\delta_{ij} = \sum_{j=1}^{n} a_{ij} b_{jk} \quad \text{or} \quad I \,|A| = AB = AA^{CT} \quad \text{where} \quad \delta_{ik} = I.$$

On dividing the above equation by |A|, we obtain

$$I = A \left[\frac{A^{CT}}{|A|} \right]. \tag{2.7}$$

The quantity in brackets must be A^{-1} since $AA^{-1} = I$.

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Example 25 Find the inverse of

$$A = \left(\begin{array}{cc} 1 & 3\\ 2 & 1 \end{array}\right).$$

Solution : For A, we have |A| = 1 - 6 = -5,

$$A^{C} = \begin{pmatrix} A^{11} & A^{12} \\ A^{21} & A^{22} \end{pmatrix} = \begin{pmatrix} 1 & -2 \\ -3 & 1 \end{pmatrix} \text{ and } A^{CT} = \begin{pmatrix} 1 & -3 \\ -2 & 1 \end{pmatrix}.$$

The inverse of A is therefore

$$A^{-1} = \frac{A^{CT}}{|A|} = -\frac{1}{5} \begin{pmatrix} 1 & -3 \\ -2 & 1 \end{pmatrix}.$$

The above equation for A^{-1} is correct since $AA^{-1} = I$.

Example 26 By use of the matrix method, solve the following system of linear equations:

$$x + 3y = 2$$

 $2x + y = 3$

Solution : In matrix form we write this system of equations as AX = C where

$$A = \begin{pmatrix} 1 & 3 \\ 2 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} x \\ y \end{pmatrix}, \text{ and } C = \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$

The solution of AX = C is

$$X = A^{-1}C = rac{A^{CT}}{|A|}$$
 where $|A| = -5$ and $A^{CT} = \begin{pmatrix} 1 & -3 \\ -2 & 1 \end{pmatrix}$.

We therefore find that

$$X = \begin{pmatrix} x \\ y \end{pmatrix} = -\frac{1}{5} \begin{pmatrix} 1 & -3 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 7/5 \\ 1/5 \end{pmatrix}.$$

The solutions are x = 7/5 and y = 1/5.

For a system of linear equations involving n variables and m equations AX = C, the following three possible outcomes exist: (a) A unique solution exists, and the system is called consistent. (b) Multiple solutions exist or the system has an infinite number of solutions, and the system is said to be undetermined. (c) No solution exists, and the system is called inconsistent.

2.2.4 The Eigenvalue Problem

The importance of eigenvalue problems in mathematical physics cannot be overemphasized. The mathematical development of linear operators and eigenvalue equations is presented on page 73. In general, it is assumed that associated with each linear operator is a set of functions and corresponding numbers such that $Au_i = \lambda_i u_i$ where A (also written as \hat{A} and can be put in matrix form) is a linear operator, u_i are eigenfunctions, and λ_i are known as eigenvalues. The matrix form of an eigenvalue equation is $AX = \lambda IX$ or $(A - \lambda)X = 0$ where A is represented by a square matrix; the condition for a nontrivial solution of this equation is

$$|A - \lambda I| = 0. \tag{2.8}$$

The above equation is called the secular equation (or characteristic equation) of A. The eigenvalues are just the roots of the secular equation and are obtained by expanding the determinant

$$|A - \lambda I| = \begin{vmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} - \lambda \end{vmatrix}.$$
 (2.9)

Example 27 Find the eigenvalues of

$$A = \left(\begin{array}{cc} 3 & 1 \\ 2 & 2 \end{array}\right).$$

Solution : In this case the secular equation reduces to

$$\begin{vmatrix} 3-\lambda & 1\\ 2 & 2-\lambda \end{vmatrix} = (3-\lambda)(2-\lambda) - 2$$
$$= (\lambda-1)(\lambda-4)$$
$$= 0.$$

The eigenvalues are $\lambda = 1$ and $\lambda = 4$.

The secular equation may be written as $|A - \lambda I| = 0 = \phi(\lambda)$ where $\phi(\lambda)$ is the *n*th degree polynomial (*n*th degree matrix) which can be represented as

$$\phi(\lambda) = \phi_0 I + \phi_1 \lambda + \ldots + \phi_{n-1} \lambda^{n-1} + \phi_n \lambda^n.$$
(2.10)

The well-known **Cayley-Hamilton theorem** states that $\lambda = A$ satisfies the above *n*th degree polynomial. Loosely stated, we say that a matrix satisfies its own characteristic equation, $\phi(\lambda) = 0$.

Example 28 Illustrate the Cayley-Hamilton theorem for matrix A where

$$A = \left(\begin{array}{rrr} 1 & 2 & 0 \\ 2 & -1 & 0 \\ 0 & 0 & 1 \end{array}\right).$$

Solution : For matrix A, we have

$$\phi(\lambda) = \begin{vmatrix} 1 - \lambda & 2 & 0 \\ 2 & -1 - \lambda & 0 \\ 0 & 0 & 1 - \lambda \end{vmatrix} = -5 + 5\lambda + \lambda^2 - \lambda^3.$$

The corresponding third-degree polynomial (third-degree matrix) is

$$\phi(\lambda) = \phi_0 I + \phi_1 \lambda + \phi_2 \lambda^2 + \phi_3 \lambda^3$$

where $\phi_0 = -5, \phi_1 = 5, \phi_2 = 1$, and $\phi_3 = -1$. By use of the Cayley-Hamilton theorem, we may write

$$\begin{split} \phi(\lambda) &= \phi_0 I + \phi_1 A + \phi_2 A^2 + \phi_3 A^3 = 0 \\ &= \begin{pmatrix} -5 & 0 & 0 \\ 0 & -5 & 0 \\ 0 & 0 & -5 \end{pmatrix} + \begin{pmatrix} 5 & 10 & 0 \\ 10 & -5 & 0 \\ 0 & 0 & 5 \end{pmatrix} + \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &+ \begin{pmatrix} -5 & -10 & 0 \\ -10 & 5 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \end{split}$$

2.2.5 Rotations in Two and Three Dimensions

Consider the rotation of the two-dimensional Cartesian system in Fig. 2.1 where

$$\beta = \theta$$
 since $\theta + \gamma = \pi/2$ and $\gamma + \beta = \pi/2$.



Figure 2.1

The relations between the prime and unprime axes are

$$x' = x \cos \theta + (\ell_1 + \ell_2) \sin \theta = x \cos \theta + y \sin \theta$$

and

$$y' = (y - \ell_2)\cos\theta = y\cos\theta - x\sin\theta$$

In matrix form, the above equations may be written as

$$\begin{pmatrix} x'\\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta\\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x\\ y \end{pmatrix} \quad \text{or} \quad X' = R_2 X.$$

In the above equation, we have

$$X' = \begin{pmatrix} x' \\ y' \end{pmatrix}, \quad R_2 = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \quad \text{and} \quad X = \begin{pmatrix} x \\ y \end{pmatrix}.$$

The matrix R_2 is called the 2×2 rotation matrix.

The above transformation equations may be written as

$$x'_i = \sum_{j=1}^2 \lambda_{ij} x_j \quad (i = 1, 2).$$

In the above equations, we have

$$x \to x_1, y \to x_2, x' \to x'_1, y' \to x'_2, \text{ and } \lambda_{ij} = \cos(x'_i, x_j).$$

In three dimensions, we have

$$x'_{i} = \sum_{j=1}^{3} \lambda_{ij} x_{j}$$
 where $\lambda_{ij} = \cos(x'_{i}, x_{j})$ $(i, j = 1, 2, 3).$

Example 29 Find the transformation equations for a 90° rotation about the x_3 -axis (see Fig. 2.2).

Solution : Here the elements, λ_{ij} , of the rotation matrix are given by

$$\begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The second matrix results from the following relations:

$$\begin{array}{ll} \lambda_{11} = \cos(x_1', x_1) = \cos(\pi/2) = 0 & \lambda_{23} = \cos(x_2', x_3) = \cos(\pi/2) = 0 \\ \lambda_{12} = \cos(x_1', x_2) = \cos 0^\circ = 1 & \lambda_{31} = \cos(x_3', x_1) = \cos(\pi/2) = 0 \\ \lambda_{13} = \cos(x_1', x_3) = \cos(\pi/2) = 0 & \lambda_{32} = \cos(x_3', x_2) = \cos(\pi/2) = 0 \\ \lambda_{21} = \cos(x_2', x_1) = \cos \pi = -1 & \lambda_{33} = \cos(x_3', x_3) = \cos 0^\circ = 1 \\ \lambda_{22} = \cos(x_2', x_2) = \cos(\pi/2) = 0 \end{array}$$

In matrix form, the transformation equations become

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_2 \\ -x_1 \\ x_3 \end{pmatrix}.$$

From the above equations, we have $x'_1 = x_2, x'_2 = -x_1$, and $x'_3 = x_3$.



2.3 Essentials of Vector Spaces

2.3.1 Basic Definitions

A vector space (over the real numbers) is a nonempty set, a collection of well-defined objects, V for which the operations of addition and scalar multiplication are valid. The operation of addition is a rule that assigns to every pair of elements $u, w \in V$ (the symbol \in is used by mathematicians to means "is an element of" or "is in") a third element $u+w \in V$. The operation of scalar multiplication is a rule that assigns to each real number $a \in \mathbb{R}$ (where \mathbb{R} is the set of all real numbers) and each element $u \in V$ and $b \in \mathbb{R}$; quantities u, w, and a are as above.

The Operation of Addition

- 1. Closure: $u + w \in V$
- 2. Associative law: (u+v) + w = u + (v+w)
- 3. Commutative law: u + v = v + u
- 4. Existence of a zero element: u + 0 = u and 0 + u = u
- 5. Existence of negatives: u + (-u) = 0 and -u + u = 0

The Operation of Scalar Multiplication

6. Closure: a(u + w), (a + b)u, and abu ∈ V
7. a(u + w) = au + aw; (a + b)u = au + bu
(ab)u = a(bu); 0u = 0; and 1u = u

The above properties for scalar multiplication may be extended to complex numbers. The elements of V are called **vectors**. The term "vector", in this context, is used in an abstract mathematical sense; it is the generalization of a physical vector discussed in Chapter 1 to cases of arbitrary dimensions.

If

$$\sum_{i=1}^{n} a_i u_i = 0 \tag{2.11}$$

implies that $a_i = 0$ for all *i*, then the set of vectors $\{u_i\}$ is said to be linearly independent; here $\{a_i\}$ is a set of scalars.

A subset $S = \{u_1, u_2, \dots, u_n\}$ of V is a **basis** iff:

- 1. the elements of S are linearly independent and
- 2. every element of V can be expressed as a linear combination of the elements of S.

We may write

$$w = a_1 u_1 + a_2 u_2 + \ldots + a_n u_n$$
 where $\{a_i\} \in \mathbb{R}$ and $w \in V$. (2.12)

For example, the i, j, k unit vectors described in Chapter 1 are the basis for the threedimensional Cartesian space (a three-dimensional vector space).

A vector space V is said to be *n*-dimensional, $\dim V = n$, if it contains a maximum of *n* linearly independent vectors. A vector space is called **infinite-dimensional** if there exists an arbitrarily large (but denumerable) number of linearly independent vectors in the space.

2.3.2 Mapping and Linear Operators

A function (or mapping), $f : A \mapsto B$, from a set A into a set B is a rule that assigns to each element $a \in A$ an element $b \in B$, b = f(a). A pictorial representation of the map $f : A \mapsto B$ is given in Fig. 2.3.



Figure 2.3

In Fig. 2.4, the composite map $g \circ f$ of the maps $f : A \mapsto B$ and $g : B \mapsto C$ is illustrated. The composition of maps is read from right to left since it means map f then map g. The map $f : A \mapsto B$ is said to be **one-to-one** (**injective**, **faithful**, or **1-1**) if each element of B has at most one element of A mapped into it. This map is called **onto** (**surjective**) if each element of B has at least one element of A mapped into it. A map that is both 1-1 and onto is referred to as **bijective**.



A function T which transforms (or maps) elements in vector space V into elements in vector space $W, T: V \mapsto W$, is a **linear function** if T(u+v) = T(u) + T(v) and T(au) = aT(u) are valid for all $u, v \in V$ and for all $a \in \mathbb{R}$. The set of all linear functions on the vector space V is a vector space V^* with the same dimension as V, i.e. $\dim V = \dim V^*$. The vector space V^* is called the **dual** of the vector space V.

The case $T: V \mapsto V$ is referred to as a **linear operator** on V. The number λ is an **eigenvalue** (characteristic value) of the linear operator T if there exists a nonzero vector u (called the **eigenfunction** or **eigenvector** of T) in V for which $T(u)=\lambda u$. In mathematical physics, (a) linear operators are normally differential operators; (b) eigenvalue equations are differential equations; and (c) eigenfunctions (solutions) form a vector space and satisfy certain imposed boundary conditions.

Example 30 Show that the linear operator T may be represented by a matrix.

Solution: Consider some basis vectors $e_i = \{e_1, e_2, \dots, e_s\}$ in the vector space V and note that the transformation to a new basis e'_i may be written as

$$e_i' = Te_i = \sum_{j=i}^s T_{ji}e_j.$$

The last step in the above equation results from the fact that e'_i can be expanded in terms of the original basis, e_i . By use of the definition of a basis and use of the above equation, an arbitrary vector u in V may be written as

$$u = \sum_{i=1}^{s} u_i e_i;$$
 therefore $Tu = \sum_{i=1}^{s} u_i Te_i = \sum_{j=1}^{s} \left\{ \sum_{i=1}^{s} T_{ji} u_i \right\} e_j = u'.$

From the above equation, it is clear that

$$u_j' = \sum_{i=1}^s T_{ji} u_i.$$

In terms of the original basis, the above equation relates the transformed components u'_j to the original components. The set of coefficients T_{ji} (*j*-th row and *i*-th column) form

the matrix representation for the linear operator T. The matrix representation of a linear operator is consistent with the fact that matrix multiplication is not in general commutative, as can be shown from the definition on page 61.

In order for two $n \times n$ matrices A and B to represent the same linear operator T, they must be related by $A = S^{-1}BS$ where S is an invertible $n \times n$ matrix; here, we say that A is **similar** to B, and the previous equation is called a **similarity transformation**.

Example 31 A Quantum Mechanical Illustration of a Linear Operator. Show that the commutator of x and p_x equals $i\hbar$; that is to say, show that $[x, p_x] = i\hbar$ where the operator $x \to x$ and the operator $\mathbf{p} \to -i\hbar\nabla$ or $p_x \to -i\hbar\partial/\partial x$.

Solution: Linear operators, in contrast to ordinary numbers and functions, do not always commute; that is to say, AB is not always equal BA where A and B are linear operators. The difference AB - BA is symbolically written as [A, B] and is called the **commutator** of A and B.

In quantum mechanics, linear operators that are Hermitian play a central role, and it is understood that simultaneous specification of the physical quantities represented by two noncommuting Hermitian linear operators, $[A, B] \neq 0$, cannot be made (uncertainty principle). The value of the commutator $[x, p_x]$ is obtained by operating on some function $\psi(x)$; we obtain

$$[x, p_x]\psi = (xp_x - p_x x)\psi = -i\hbar\left\{\frac{\partial\psi}{\partial x} - \frac{\partial(x\psi)}{\partial x}\right\} = i\hbar\psi$$

or
$$[x, p_x] = i\hbar$$
.

The linear function $T: V \mapsto W$ is said to be a **homomorphism** if the following two conditions are satisfied for all $u, v \in V$:

1.
$$T(u+v) = T(u) + T(v)$$

2.
$$T(uv) = T(u)T(v).$$

An isomorphism $T: V \mapsto W$ from V to W is a homomorphism that is 1-1 and onto W. In this case, V and W are said to be isomorphic. Isomorphism means that the properties of V and W are indistinguishable even though the vectors of V and W are different. That is to say, $T: V \mapsto W$ is 1-1 if it is not possible for two distinct vectors in V to be assigned the same vector in W by the linear transformation T; also, note that $\dim V = \dim W$ and that every n-dimensional vector space is isomorphic to \mathbb{R}^n , an n-tuple of real numbers (x^1, x^2, \ldots, x^n) . An isomorphism of a vector space onto itself is called an **automorphism**.

2.3.3 Inner Product and Norm

The inner product on V, denoted by \langle , \rangle , is a function which assigns to each pair of vectors in V a real number satisfying the following four conditions.

- 1. $\langle u, u \rangle \ge 0$ where $\langle u, u \rangle = 0$ iff u = 0;
- 2. $\langle u, w \rangle = \langle w, u \rangle;$
- 3. $\langle u, w + v \rangle = \langle u, w \rangle + \langle u, v \rangle$; and
- 4. $a \langle u, w \rangle = \langle au, w \rangle$ where $a \in \mathbb{R}$.

Operationally, the inner product of two vectors $u, w \in \mathbb{R}^n$ is defined as

$$\langle u, w \rangle = \sum_{i=1}^{n} u_i w_i. \tag{2.13}$$

If the inner product of two vectors equals zero, $\langle u, w \rangle = 0$, the vectors are said to be **orthogonal**. In \mathbb{R}^3 , the inner product equals the dot product to two vectors as defined in Chapter 1.

The function $\|\cdot\|: V \mapsto \mathbb{R}$ is a **norm** on V if the map satisfies the following properties.

- 1. ||au|| = a ||u|| for all $u \in V$ and for all $a \in \mathbb{R}$;
- 2. $||u+w|| \le ||u|| + ||w||$ for all $u, w \in V$; and
- 3. ||u|| > 0 for $u \in V$ and $u \neq 0$.

A vector space with a norm defined on it is called a **normed vector space**. The norm of a vector u is defined to be the real number given by

$$\|u\| = \sqrt{\langle u, u \rangle}.\tag{2.14}$$

When ||u|| = 1, u is called a **unit vector**. The norm on \mathbb{R}^n is called the Euclidean⁶ norm, and the normed space $(\mathbb{R}^n, ||\cdot||)$ is an n-dimensional Euclidean space.

2.3.4 The Legendre Transformation

The Legendre⁷ transformation is a very useful mathematical tool for changing an independent variable of a function without altering the mathematical or physical contents of the function. The Legendre transformation transforms functions on a vector space to functions on the dual space. Here we illustrate the Legendre transformation method by considering a function y = f(x) such that f''(x) > 0 (a convex function).

The objective of the Legendre transform is accomplished by noting that the curve y(x) may be represented as the envelop of a family of tangents (see Fig. 2.5b). The equation $\phi = \phi(p)$, where p = dy/dx is the slope of an arbitrary tangent, completely represents y(x) in Fig. 2.5a. The equation of the arbitrary tangent in Fig 2.5a is

$$y(x) = px + \phi(p).$$

⁶Euclid (circa 365–275 BC), Greek mathematician whose treatment of elementary plane geometry serves as the basis for most beginning courses on the subject.

⁷Adrien Marie Legendre (1752–1833), French mathematician who is known for his work on number theory and elliptic integrals. He invented the method of least squares.


Figure 2.5

The function $\phi(p)$ is called the **Legendre transform** of y(x), and it contains the same mathematical and physical information as y(x). The above equation is normally written as

$$\phi(p) = y(x) - xp = y(x) - x \frac{dy}{dx}$$
 where $p = \frac{dy}{dx}$.

If $p \neq dy/dx$, then the Legendre transformation of y(x) to $\phi(p)$ cannot be made. In simple terms, the Legendre transformation may be stated as follows:

new function = old function - (old variable)
$$\left[\frac{d(\text{old function})}{d(\text{old variable})}\right]$$
.

2.3.5 Topological Spaces

The purpose of this Section is to give appropriate definitions and explanation of concepts needed in the discussion of Lie groups and in Chapter 12. It is placed here because the material is an extension of elementary concepts of vector spaces. The study of this particular subsection may be deferred until needed (e.g., used as a reference as needed). We begin with a some definitions from the theory of sets. A set with no elements is called an **empty** set (or null set), denoted by \emptyset . The intersection of two sets A and B is, in symbolic form, written as $A \cap B$ (A intersects B), and the union of A and B is denoted by $A \cup B$ (A union B). These operations are illustrated in Fig. 2.6.





Figure 2.6

Elements of $A \cup B$ are the points that belong to at least one of sets A and B, and elements of $A \cap B$ are the points that belong to both A and B. A set of points in a metric space (see the definition below) M is defined to be **closed** if the set contains all its limit points in M; here, the null set is taken to be closed, and the whole of M is closed. For example, the set of points $0 \le x \le 1$ on the Euclidean line is closed, denoted with brackets [0, 1]. A set of points in a metric space M is said to be **open** in M if every point of the set has a neighborhood consisting of points of the set alone; here, the null set is regarded as being open. The set of points 0 < x < 1 on the Euclidean line is neither open nor closed, denoted with brackets [0, 1).

Let X be a nonempty set and T be a collection of subsets of X such that the following are valid.

- 1. Both the empty set and X itself are in T, i.e. $\emptyset, X \in T$.
- 2. The collection T is closed under finite intersections; if $t_1, t_2, \ldots, t_n \in T$, then $t_1 \cap t_2 \cap \ldots \cap t_n \in T$.
- 3. The collection T is closed under arbitrary unions; if each $a \in I$ and $t_a \in T$, then $\bigcup_{a \in I} t_a \in T$. (It holds that unions of any collection of subsets of T are in T.)

The pair of objects (X, T), often written as X, is called a **topological space** (or space). The set X is said to be the **underlying set**, and the collection T is called the **topology** on the set X. Topology is a study of continuity; more precisely, it is a study of properties that are invariant under continuous deformation. A collection of subsets of X, $\{x_i\}$, is said to **cover** X if the unions of $\{x_i\}$ are contained in X such that each point of X is in one of the subsets. The elements of T are called (even defined as) **open sets** (If all the points of a set are themselves elements of the set, the set is said to be **closed**.), and the elements of X for a manifold are its points. A **manifold** is the extension of curves and surfaces to arbitrary dimensions. An n-dimensional manifold (n-dimensional space) is locally like \mathbb{R}^n (or Euclidean space), but it may be very different from \mathbb{R}^n globally.

A topological space X is called Hausdorff⁸ space (also known as separated space) if, in addition to the above three conditions, the following condition is satisfied: If a and b are any two distinct points of X, then there exists a pair of open sets O_a and O_b such that $O_a \cap O_b$ for $a \in O_a$ and $b \in O_b$. The space $X = \mathbb{R}^n$ is a Hausdorff space. A space X is said to be compact if every infinite sequence of points $t_1, t_2, \ldots, (t_i \in X)$ contains a subsequence of points that converges to a point such that the point is in X. For example, a sphere and a torus in Euclidean space are contained in a finite portion of the space and would be classified as compact. A paraboloid in Euclidean space, however, would not be compact.

A chart (an open piece of surface) C of the set X is defined as a subset t of X together with a continuous invertible map $f: t \mapsto \mathbb{R}^n$ called the **coordinate function**. The subset t corresponds to a local region being like \mathbb{R}^n for a manifold, and f may be considered the introduction of local coordinates. Two charts C_1 and C_2 with overlapping neighbourhoods and coordinate functions f_1 and f_2 are said to be **compatible** if the composition map

⁸Felix Hausdorff (1869–1942), German mathematician known for the introduction of fractional dimensions in connection with small-scale structure of mathematical shapes.

 $f_1 \circ f_2^{-1}$ is differentiable. An **atlas** (system of charts) is a set of compatible charts covering X. A **differentiable manifold** M is a Hausdorff topological space with an atlas.

A metric space (X, d) is a topological space where the open sets are provided by a distance function $d(x, y), d: X \times X \mapsto \mathbb{R}$, with the following properties for $x, y, z \in X$. (In this section, the distance function, d(x, y), should not be confused with the letter for the differential "d".)

- 1. $d(x,y) \ge 0$ and d(x,y) = 0 iff x = y;
- 2. d(x, y) = d(y, x);
- 3. $d(x, z) \le d(x, y) + d(y, z)$.

For $x = (x_1, x_2, ...)$ and $y = (y_1, y_2, ...)$, note that

$$d(x,y) = \|x-y\| = \sum_{i=1}^{\infty} (x_i - y_i)^{1/2}.$$
(2.15)

In a metric space (X, d), a sequence a_1, a_2, \ldots of points of X is called a **Cauchy⁹** sequence if for each $\epsilon > 0$ there is a positive integer N such that $d(a_n, a_m) < \epsilon$ whenever n, m > N. A metric space X is called **complete** if every Cauchy sequence in X converges to a point in X.

As previously explained, a normed space $(V, \|\cdot\|)$ is a vector space V together with a norm $\|\cdot\|$ defined on it. A complete normed vector space with either real or complex numbers as scalars is called a **Banach**¹⁰ space.

An inner product space (V, \langle , \rangle) is a vector space V together with an inner product \langle , \rangle defined on it. A complete inner product space is called a **Hilbert**¹¹ space and is extremely important in many areas of physics, including quantum mechanics.

Thus far, the notations used are those preferred by mathematicians. In quantum physics, a vector in Hilbert space, the state of a system, may be denoted by $|\psi\rangle$, and the inner product (ψ, ϕ) is written as $\langle \psi | \phi \rangle$ where $|\phi\rangle$ is called the **ket vector** and $\langle \psi |$, a vector in the dual space, is called the **bra vector**. This latter notation is due to Dirac¹². In Dirac notation, the following relations are valid.

- 1. $\langle \psi | a\phi \rangle = a \langle \psi | \phi \rangle;$
- 2. $\langle a\psi | \phi \rangle = a^* \langle \psi | \phi \rangle$,
- 3. $\langle \psi | \phi \rangle^{\dagger} = \langle \phi | \psi \rangle;$
- 4. $\langle \psi | \psi \rangle = \|\psi\|$; and

¹¹David Hilbert (1862–1943), German mathematician known for his work in algebraic number theory, functional analysis, mathematical physics, and the calculus of variations. In 1895, he became Professor of Mathematics at the University of Gottingen, where he remained for the rest of his life.

¹²Paul Adrien Maurice Dirac (1902–1984), English physicist who made fundamental contributions to the development of quantum mechanics. In 1933, he shared the Nobel Prize for physics with Erwin Schrödinger.

⁹Augustin Louis Cauchy (1789–1857), French mathematician and mathematical physicist known for his work in geometry, complex variable theory, and differential equations.

 $^{^{10}}$ Stefan Banach (1892–1945), Polish mathematician known for his work in functional analysis and topological spaces.

5. $\langle \psi_{n'} | A \psi_n \rangle = \langle A^{\dagger} \psi_{n'} | \psi_n \rangle$ for operator A.

In terms of the Schrödinger notation, we have

$$egin{aligned} &\langle\psi|\;\phi
angle&=\int_{-\infty}^{\infty}\psi^{*}(x)\phi(x)dx \quad ext{ and } \ &\langle A
angle&=\int_{-\infty}^{\infty}\psi^{*}(x,t)A\psi(x,t)dx=\langle\psi|\;A\psi
angle\,. \end{aligned}$$

The average (expectation value) of an observable represented by the Hermitian operator A for a system in state $\psi(x,t)$ is denoted by $\langle A \rangle$.

2.3.6 Manifolds

The basic ideas of topology evolved during the mid-19th century as a result of studies in algebra and analytic geometry. **Topology** is concerned with those properties of geometric figures that are invariant under continuous transformations (deformations). Two figures are topologically equivalent if one can be deformed into the other by such processes as bending, stretching, and/or twisting (but not tearing, cutting, or folding); it is for this reason that topology is sometimes referred to as "rubber-sheet geometry". For example, the following figures are topologically identical, i.e. **homeomorphic**: (a) circle and square, (b) sphere and cylinder, and (c) torus (doughnut shape) and cup. **Homotopy** is the theory of the relation between topologically identical spaces.

Geometry (figures) may be reduced to the following three points of view:

- 1. point set figures are consider sets of points having such properties as being open, closed, and compact;
- 2. complexes (combinatorial) figures are combinations of simple figures (simplexes) joined together in a regular manner (e.g., points + line segments = triangles);
- 3. analytic geometry here, one assigns equations to geometrical figures; (e.g., x+y=1 is a straight line); and
- 4. manifolds coordinates have no intrinsic geometric meaning, and the description of figures is independent of the choice of coordinates. The main task in the theory of manifolds is the search for geometric invariances.

Physical problems generally involve continuous spaces (e.g., 3-D space, 4-D space-time, and phase space), and these spaces have their characteristic geometric properties. In differential geometry, a systematic study of common properties of spaces is made. The definition of a differentiable manifold (or simply a manifold) is a mathematical definition of space. More precisely, a **manifold** is a topological space in which some neighborhood of each point is like \mathbb{R}^n (Euclidean space). Globally (taken as a whole), a manifold may be different from \mathbb{R}^n ; for example, a one-dimensional manifold is a straight line which is locally and globally like \mathbb{R}^1 . A circle S^1 , however, is locally like \mathbb{R}^1 , but it is not like \mathbb{R}^1 globally. (Here, S^1 is not related to the S used in the following.) The definitions in this subsection are background material for Chapter 12.

2.4 Essential Algebraic Structures

2.4.1 Definition of a Group

In modern (abstract) algebra, the main idea is to abstract from algebra its basic properties and study the subject in terms of these properties. A group is one of the simplest and most basic as well as the most widely studied algebraic structure. We begin the introduction of the theory of groups with the definition of a binary operation. A closed **binary operation** \star on a set S is a rule that assigns to each ordered pair of elements (a, b)in S (also written as $a, b \in S$) some (since it could be a or b) element in S. Ordered pair allows for the possibility that (a, b) and (b, a) could be assigned a different element. Typical binary operations are + (addition) and \cdot or \times (multiplication). When the binary operation is multiplication, the notation ab is normally used for $a \cdot b$ or $a \times b$. A **group** $\langle G, \star \rangle$ is a set of distinct elements G such that the following axioms hold.

1. The binary operation is closed: $a \star b \in G$ for all $a, b \in G$;

- 2. The binary operation is associative: $(a \star b) \star c = a \star (b \star c)$ for all $a, b, c \in G$;
- 3. There is an identity element e in G such that: $e \star a = a \star e = a$ for all $a \in G$; and
- 4. There is an inverse element a^{-1} in G such that: $a^{-1} \star a = a \star a^{-1} = e$ for all $a \in G$.

The notation $\langle G, \star \rangle$ is normally written as G. The symbol E is often used for e (the identity); use of e or E for the identity element is for the German word *Einheit* which means unity. The set of all real integers with addition as the operation (0 is the identity element and -a is the inverse) is a group. The set of all positive real integers, excluding zero, with addition as the operation is not a group since there is no identity element or inverse element.

If G is finite (i.e., it contains a finite number of elements), then G is said to be a finite group, and the number of elements of G is called its order; otherwise G is an infinite group. If the elements of an infinite group are denumerable, the group is called discrete; for example, the set of all integers is a discrete group. An infinite group is said to be a continuous group if the elements are nondenumerable (e.g., the set of all real numbers). The elements of a continuous group are characterized by a set of real parameters such that at least one of the parameters varies continuously over a certain interval. In addition, continuity conditions are imposed on the elements of the group manifold.

A nonempty subset H of the group G that is closed under the same operation as G and is itself a group is called a **subgroup** of G. Note that a group always has at least two subgroups, the identity and the group itself. A group with no subgroups except itself and the identity is called a **simple group**. The Jordan-Hölder theorem (stated in 1869) shows that simple groups are the foundation for all groups. If all the elements of a group can be found by taking powers of a single element, the group is said to be a **cyclic group** $\{a, a^2, a^3, \ldots, a^n \equiv e\}$. The algebraic structure for which axiom 4 above does not hold is called a **semigroup**; for example, the set of all positive integers, including zero, is a semigroup. Semigroups have many applications in computer science.

Let *H* be a subgroup of *G*. The sets of elements of the form aH for all $a \in G$ are called **left cosets** of *H* in *G*, and the sets of elements Ha for all $a \in G$ are called the **right cosets** of *H* in *G*. Note that cosets are not, in general, groups.

A group G is **abelian**¹³ if its binary operation is commutative, $a \star b = b \star a$. Since ordinary multiplication is used, all cyclic groups must be abelian. Addition is the binary operation for the abelian group whose elements are all the real integers where e = 0 and $a^{-1} = -a$ for all $a \in G$. A group G is non-abelian (with or without the dash) if its binary operation is not commutative, $a \star b \neq b \star a$. When matrix multiplication is the binary operation, the corresponding groups are typically non-abelian groups.

Element a of group G is said to be **conjugate** to an element $b \in G$ if there exist an element $c \in G$ such that $a = cbc^{-1}$. Note that if elements a and b are conjugate to element c, then a and b are conjugate to each other (i.e., a, b, and c are conjugate elements). The concept of **class** refers to elements that are all conjugate to each other and is useful when treating groups with large numbers of elements. If H is a subgroup of G, then the set of elements aha^{-1} for any $a \in G$ and all $h \in H$ is a subgroup of G called the **conjugate subgroup** of H in G. If $aha^{-1} = H$ for all $a \in G$ and all $h \in H$, then H is said to be an **invariant subgroup** in G; note that a second definition of invariant subgroup may be written as aH = Ha (the left coset equals the right coset) for all $a \in G$. A map of group G onto group G', $\phi : G \mapsto G'$, is a **homomorphism** if the following condition holds.

$$\phi(ab) = \phi(a)\phi(b) \quad \text{for all} \ a, b \in G. \tag{2.16}$$

The operation on the left-hand side of Eq. (2.16) takes place in G and the operation on the right-hand side takes place in G'. An **isomorphism** is a homomorphism that is one to one. Equation (2.16) expresses the relation between the binary operations of the two groups (the structures of the two groups). As is discussed below, these two concepts are extremely useful when applying group theory the physical problems.

2.4.2 Definitions of Rings and Fields

In this subsection, we consider algebraic structures involving two binary operations. The integers and real numbers with addition and multiplication as the binary operations are such structures. Consider the set $\langle R, +, \times \rangle$ with addition and multiplication as the two binary operations in R. The set R is called a **ring** if R is an abelian group with respect to addition and is a semigroup with respect to multiplication; that is to say, $\langle R, +, \times \rangle$ is a ring if the following three conditions are satisfied:

- 1. $\langle R, + \rangle$ is an abelian group with zero;
- 2. $\langle R, + \rangle$ is closed (there may be a unit); and
- 3. multiplication distributes over addition,

a(b+c) = ab + ac and (b+c)a = ba + ca for all $a, b, c \in R$.

A ring consisting of a single element 0 is called a zero ring. A field is a set $\langle F, +, \times \rangle$ such that the following conditions are satisfied:

 $^{^{13}}$ Niels Henrik Abel (1802–1829), Norwegian mathematician who was instrumental in establishing mathematical analysis on a rigorous basis. At the age of 18, he earned wide recognition with his first paper. (Now, it is common to use a small "a" in the word abelian.)

- 1. $\langle F, + \rangle$ is an abelian group;
- 2. $\langle F, + \rangle$ excluding zero, forms a group; and
- 3. multiplication distributes over addition,

a(b+c) = ab + ac and (b+c)a = ba + ca for all $a, b, c \in F$.

Note that a field is a ring, but not all rings are fields. The real, rational, and complex numbers are familiar fields generally used in mathematical physics.

An **algebra** consists of a vector space V over a field F together with a binary operation of multiplication on the set of vectors of V such that the following conditions are satisfied for all $a \in F$ and for all $\alpha, \beta, \gamma \in V$.

1.
$$(a\alpha)\beta = a(\alpha\beta) = \alpha(a\beta);$$

- 2. $(\alpha + \beta)\gamma = \alpha\gamma + \beta\gamma$; and
- 3. $\alpha(\beta + \gamma) = \alpha\beta + \alpha\gamma$.

If (in addition to the above three conditions) the following fourth condition is valid, then V is said to be an **associative algebra** over F.

4. $(\alpha\beta)\gamma = \alpha(\beta\gamma)$ for all $\alpha,\beta,\gamma \in V$.

The algebra V over a field F is a **division algebra** over F if V has a unity for multiplication and contains a multiplicative inverse of each non-zero element.

2.4.3 A Primer on Group Theory in Physics

This subsection is devoted to the basic definitions and essential concepts of group theory needed in physics. From the point of view of mathematical physics, the basic idea of group theory is a result of comparisons of numerous examples occurring in different subjects such as (a) groups of geometric transformations, (b) groups of numbers, and (c) groups of permutations. Groups in these three areas all obey the same four basic axioms, and theorems in abstract group theory apply to all groups independent of the branch of mathematics or area of physics in which the groups occur. In physics, the meaning of the group elements is ascertained (the expression "put in by hand" is often used) from some physical situation (e.g., a conservation law). The two basic approaches in the study of groups are (a) combinatorial: determining the properties of a group by finding all the subgroups of a group and (b) mapping: a homomorphism of group G onto group G' that is one to one (an isomorphism) which means that properties of G may be found from properties of G', even if the elements of the two groups have very different meaning.

Concepts of symmetry and invariance permeate many problems in most areas of physics, and group theory is a tool for the systematic study of these concepts. Applications of the mathematical theory of groups, however, seems almost an impossible task because of the extremely large number of groups used in various areas of chemistry and physics. It is, therefore, extremely useful to understand how to determine the number of distinct (non-isomorphic) groups that exists for a given order n. In this connection, the group multiplication table (group table or Cayley table) is useful. In a multiplication table,

- 1. we list the group elements across the top and down the left side and
- 2. each element may appear only once in each row and in each column (e.g., the elements in each row and in each column are distinct).

The general multiplication table is given below.

×	e	a	b	с	d	
e	e	a	b	c	d	
a	a	a^2	ab	ac	ad	• • •
b	b	ba	b^2	bc	bd	• • •
с	c	ca	cb	c^2	cd	•••
d	d	da	db	dc	d^2	•••
:	:	:	:	:	÷	·

General Multiplication Table

We now give a summary of the first six cases.

- 1. n = 1; there is only one distinct structure: a group having only the identity $\{e\}$.
- n = 2; there is only one distinct structure: a group with elements {e, a} where a² = e; for example, {1, -1}.
- 3. n = 3; there is only one distinct structure: a cyclic group with elements $\{a, a^2, a^3 \equiv e\}$.
- 4. n = 4; there are two distinct groups:
 - (a) a cyclic group with elements $\{e, a, b, c\}$ where $a^2 = b, a^3 = c$, and $a^4 = e$ and

(b) a noncyclic group with elements $\{a, a^2, a^3, a^4 \equiv e\}$ where ab = c, bc = a, ca = b, and $a^2 = b^2 = c^2 = e$; this group is known as the group V (Viergruppe) or Klein 4-group.

- 5. n = 5; there is only one distinct structure: a cyclic group with elements $\{a, a^2, a^3, a^4, a^5 \equiv e\}$.
- 6. n = 6; there are two distinct groups:
 - (a) a cyclic group with elements $\{a, a^2, a^3, a^4, a^5, a^6 \equiv e\}$ and
 - (b) a noncyclic and non-abelian group with elements $\{a, b, c, d, f, e\}$ where
 - $a^3 = b^3 = e, c^2 = d^2 = f^2 = e, a^2 = b, ac = f, ca = d, bc = d, \dots$

Although tedious, it is possible to extend the above analysis to higher values of n. The simplest nontrivial group has elements $\{e, a\}$; this is an abelian group with ordinary multiplication as the group operation. The multiplication table for G_2 with elements $\{e, a\}$ is given below. The Multiplication Table for Group G_2

×	e	a	
e	e	a	
a	a	e	

The abelian group G_4 with elements $\{e, a, b, c\}$ and ordinary multiplication as the operation has the multiplication table given below.

The Multiplication Table for Group G_4

×	e	a	b	с
e	e	a	b	с
a	a	e	с	b
b	b	c	a	e
с	С	b	e	a

A group with elements $\{1, -1, i, -i\}$ is an isomorphism onto G_4 .

Quaternions were introduced by Hamilton, and they form a four-dimensional vector space over the real numbers with basis vectors denoted by 1, i, j, k. A quaternion is a vector x = a+bi+cj+dk where a, b, c, and d are real. The algebraic operations for quaternions are ordinary addition, scalar multiplication, and quaternion multiplication. The **quaternion product** of any two basis vectors is defined by the requirement that 1 acts as the identity and that

1.
$$i^2 = j^2 = k^2 = -1$$
; (i.e., *i*, *j*, and *k* are imaginary) and

2.
$$ij = -ji = k$$
; $jk = -kj = i$; and $ki = -ik = j$

The quaternion group Q_8 is the set $\{1, -1, i, -i, j, -j, k, -k\}$ with the multiplication table given as follows.

_ ×	1	-1	i	-i	j	-j	k	-k
1	1	-1	i	-i	j	-j	k	-k
-1	-1	1	-i	i	-j	j	-k	k
i	i	$-\overline{i}$	-1	1	k	-k	-j	j
-i	-i	i	1	-1	-k	k	j	-j
j	j	-j	-k	k	-1	1	i	-i
-j	-j	j	k	-k	1	-1	-i	i
k	k	-k	j	-j	-i	i	-1	1
-k	-k	k	-j	j	i	-i	1	-1

The Multiplication Table for the Quaternion Group Q_8

Also, the quaternion group may be defined by use of the following matrices with matrix multiplication as the group operation.

$$q_{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, q_{2} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, q_{3} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}, q_{4} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix},$$
$$q_{5} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, q_{6} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, q_{7} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, q_{8} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

The Symmetry Group The set of all transformations that preserve the distances between all pairs of points of an object and that bring the object into coincidence with itself characterizes the symmetry of the object. Each of these transformations is called a symmetry transformation, and the set of all such transformations forms a group called the symmetry group of the object. Symmetry transformations are composed of the following three fundamental types of transformations: (a) rotation through a definite angle about some axis, (b) reflection (or inversion), and (c) translation (parallel displacement).

The first systematic application of group theory in chemistry and physics involved the development of the 32 point groups and 230 space groups, symmetry groups, which characterize crystal symmetries. The **point groups** are composed of combinations of rotations and reflections (or inversions) about a fixed origin (a point; hence the name point groups) that leave a crystal lattice unchanged. The **space groups** are composed of combinations of rotations of rotations, reflections (or inversions), and translations that leave the crystal invariant.

The Symmetric Group Group theory evolved from the study of finite permutations. A **permutation** of the set $\{a_1, a_2, \ldots, a_n\}$ is a one to one mapping of the set onto itself (e.g., $123 \rightarrow 132$); the set S_n of all permutations and the operation of composition of mappings form a group called the **symmetric group** of degree n. The order of the symmetric group is the number of ways of arranging n objects which is n!. A subgroup of S_n is called a **permutation group**. Every finite group may be written as a permutation group since every finite group is isomorphic to a permutation group of its elements. The symmetric group is widely used in various areas of physics such as quantum mechanics, atomic structure and identical particles, nuclear physics, and elementary particle theory. In addition, the symmetric group plays an important role in the study of continuous groups.

Lie Groups Lie¹⁴ developed the theory of continuous transformation groups and their role in the theory of differential equations. While the theory of finite groups is some what self contained, the theory of Lie groups (i.e., continuous groups) is a fundamental tool in other areas such as differential topology and differential geometry, number theory, differential equations, quantum mechanics, and elementary particle physics. A Lie group is a group as well as an *n*-dimensional analytic manifold which means that the elements are labeled by a set of continuous parameters with a multiplication law that depends smoothly (concepts of continuity, connectedness, and compactness apply) on the parameters. A group is said to be **compact** if all its elements are represented by points within a finite region of the manifold; otherwise it is said to be **noncompact**. A group is called **simply connected** if any closed loop in the manifold can be continuously deformed to a point. Our focus is

 $^{^{14}}$ Sophus Lie (1842–1899), Norwegian mathematician who made major contributions in the theory of continuous groups of transformations and in differential equations.

applications in quantum mechanics, and the group elements will be considered to be linear operators that are Hermitian.

Any element of a compact Lie group which can be obtained from the identity by continuous change in the parameters can be written in the form

$$\exp\left(i\sum_{k=1}^{n}a_{k}X_{k}\right).$$
(2.17)

In the above expression, the a_k are real parameters and X_k are linearly independent Hermitian operators called **generators**. While all the properties of a finite group can be obtained from its multiplication table, the commutators of its generators $[X_i, X_j]$ determine the structure of the Lie group. That is to say, the commutator $[X_i, X_j]$ must be a linear combination of the generators and is written in the form

$$[X_i, X_j] = \sum_{k=1}^{n} C_{ij}^k I_k \quad \text{where} \quad i \ge 1 \quad \text{and} \quad j \le n.$$
 (2.18)

In Eq.(2.18), the constants C_{ij}^k are called the **structure constants** since commutators of pairs of generators completely determine the structure of the Lie group. The structure constants are not unique since the generators of the Lie group are not unique. The generators of a Lie group is a **Lie algebra** since the set of all linear combinations $a_k X_k$ is an *n*-dimensional vector space V with basis vectors X_k and the above equation is a law of composition between any pair of elements of the space. A linear Lie algebra (matrix algebra) is a vector space over a field F on which a commutator is defined such that the following three properties hold for all $x, y, z \in V$.

1.
$$[x, y] \in V;$$

2.
$$[x, y] = -[y, x];$$
 and

3. [x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0.

Property 3 is known as the Jacobi¹⁵ identity. By use of the above three properties and Eq.(2.18), we find that

$$C_{ij}^{k} = -C_{ji}^{k}$$
 and $C_{ij}^{m}C_{mk}^{r} + C_{jk}^{m}C_{mi}^{r} + C_{ki}^{m}C_{mj}^{r} = 0; r = 1, 2, \dots, n.$ (2.19)

The rank of a Lie group is the minimum number of mutually commuting generators. An operator that commutes with all the generators of a Lie group is referred to as a **Casimir operator** (1931) for the Lie group. It can be shown (a theorem due to Racah, 1950) that the number of independent Casimir operators of a Lie group equals its rank.

Matrix Groups During the period 1850–1859, Cayley, Hamilton, and Sylvester introduced the concepts of matrices and matrix groups. This subsection is devoted to a discussion of the general linear group and some of its subgroups that are widely used in physics. The set of all non-singular $n \times n$ matrices over a field F with matrix multiplication as the

 $^{^{15}}$ Karl Gustav Jacob Jacobi (1804–1851), German mathematician who founded the theory of elliptic functions. He worked on determinants and studied the functional determinant now known as the Jacobian.

binary operation is a group called the **general linear group**, denoted by GL(n, F). The fields normally considered in physics are the real numbers, complex numbers, and quaternions. We will restrict this discussion to the complex numbers, and use the notation GL(n) for GL(n, C). Here, GL(n) is a $2n^2$ -parameter group. The set of all $n \times n$ matrices with determinant +1 is an important subgroup of GL(n); it is called the **special linear group**, SL(n), and is a $(2n^2 - 1)$ -parameter group.

The set of all non-singular orthogonal matrices (i.e., $A^T A = I$) is a subgroup GL(n)and is called the **orthogonal group** O(n), an n(n-1)-parameter group. In mathematical physics, the orthogonal group is viewed as the set of all orthogonal transformations in a real *n*-dimensional vector space; in this case, we have the n(n-1)/2- parameter group $O(n, \mathbb{R})$. The rotation group is a subgroup of $O(n, \mathbb{R})$. Note that the determinant of an orthogonal matrix equals ± 1 since

$$det(A^T A) = det A^T det A$$

= $(det A)^2$ since $det A^T = det A$
= 1.

Hence, the parameter space of O(n, C) consists of the two disconnected pieces: (a) +1 corresponds to proper rotations and (b) -1 corresponds to reflections. Only the proper rotations can be reached continuously from the identity, and this subgroup is called the **special orthogonal group**, $SO(n, \mathbb{R})$. The orthogonal group is a continuous, compact, disconnected Lie group.

The set of all non-singular $n \times n$ unitary matrices (i.e., $A^{\dagger}A = I$) is called the **unitary group** U(n, C). The unitary group is a continuous, connected, compact, n^2 -parameter Lie group. The elements of the 1-parameter Lie group U(1) can be generated by the transformations (phase change) $e^{im\alpha}$. In quantum mechanics, the probability that (at time t) a particle is in the volume element dxdydz is given by $\Psi^*\Psi dxdydz$. The quantity $\Psi^*\Psi$ is called the **probability density** and is associated with a measurement. A transformation of the wave function may be written as

$$\Psi' = e^{im\alpha}\Psi \quad \text{and} \quad \Psi^{*\prime} = e^{-im\alpha}\Psi^*$$

Note that

$$\Psi^{*'}\Psi' = \left(e^{-imlpha}\Psi^*\right)\left(e^{imlpha}\Psi
ight)$$

= $\Psi^*\Psi$ (invariant).

Because of the above relation, we see that U(1) is a symmetry group for any quantum mechanical system.

The set of all $n \times n$ unitary matrices with determinant equal +1 is a subgroup of U(n, C) called the **special unitary group** and is denoted by SU(n, C) or SU(n). The group SU(n) is a continuous, compact, connected, $(n^2 - 1)$ -parameter Lie group. Since

$$\det e^A = e^{\operatorname{Tr} A}$$

and $U = e^{iH}$ is unitary for H Hermitian, we find that SU(n) can be generated by $(n^2 - 1)$ traceless Hermitian matrices along with $(n^2 - 1)$ independent parameters a_i .

When practical, one may choose the $(n^2 - 1)$ generators (traceless Hermitian matrices) and add the unit matrix to obtain the n^2 generators of U(n).

Representation and Realization of Abstract Groups In mathematical physics, one prefers to work with algebraic structures (e.g., groups and fields) that can be written explicitly so that calculations can be made. A mapping onto an algebraic structure (e.g., a group) that can be explicitly written and described analytically in terms of physical quantities is called a **realization**, and a mapping onto a set of matrices is an example of a **representation** (group representation). A mapping of one algebraic structure (e.g., a group) into a similar algebraic structure is called a **homomorphism** if it preserves all combinatorial operations associated with that structure. Homomorphisms permit the comparison of different groups. For example, a homomorphism of a newly discovered group in physics and some well-known group from geometry allows much knowledge about the new group to be ascertained. A homomorphism that is one to one such that a well defined inverse exists is called an **isomorphism**. An isomorphism of an algebraic structure onto itself is referred to as an **automorphism**.

The theory of group representations may be approached from the following points of view: (a) representation by a set of non-singular matrices, due to Frobenius¹⁶ and Schur¹⁷ and (b) representation module due to Noether¹⁸. The matrix approach is widely used in mathematical physics, and we restrict our discussion to this approach. A homomorphism of a finite group G into a group of $n \times n$ non-singular matrices is a representation of G of degree n if

$$\Gamma(a)\Gamma(b) = \Gamma(ab)$$
 and $\Gamma(e) = I.$ (2.20)

In Eq. (2.20), the quantities $\Gamma(a)$, $\Gamma(b)$, and $\Gamma(ab)$ are matrices associated with elements a, b, and the product ab respectively. If this homomorphism is one to one, the representation is said to be **faithful** (or an isomorphism). The transformation,

$$\Gamma'(a) = s^{-1} \Gamma(a) s,$$

is referred to as a similarity transformation, and it leaves the representation in Eq.(2.20) unchanged since

$$\Gamma'(a)\Gamma'(b) = \left\{s^{-1}\Gamma(a)s\right\} \left\{s^{-1}\Gamma(b)s\right\}$$
$$= s^{-1}\Gamma(a)\Gamma(b)s$$
$$= \Gamma'(ab).$$

Here we see that the Γ' matrices form a representation since the Γ matrices form a representation. The infinity of such representations for various s are said to be equivalent.

¹⁶Ferdinand Georg Frobenius (1849–1917), German mathematician who combined results from the theory of algebraic equations, geometry, and number theory to obtain important results in abstract group theory. His representation theory for finite groups has important applications in quantum mechanics. Also, he is known for work in the theory of differential equations.

¹⁷Issai Schur (1875–1941) was born in Mogilyov, Belarus and is known for his work on representation theory of groups, number theory, and analysis.

¹⁸Emmy Amalie Noether (1882–1935), German mathematician who is known for her contributions to abstract algebra. She is best known in theoretical physics for Noether's theorem which proves a relation between symmetries in physics and conservation laws.

2.5 Problems

2.1 Given $A = \begin{pmatrix} 3 & 2 \\ 1 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & 4 \\ 1 & 2 \end{pmatrix}$. Find: (a) A + B, (b)B - A, (c) AB, and (d) BA.

2.2 Does AB = AC imply that B = C? Illustrate by means of an example.

2.3 Show that $AB \neq BA$ for general A and B.

2.4 For the Pauli¹⁹ spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

show that (a) $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = I$, (b) $[\sigma_1, \sigma_2] = 2i\sigma_3$ (cyclic), and (c) $\{\sigma_j, \sigma_k\} = 2\delta_{jk}$. The curly brackets mean **anticommutator**; for example, $\{A, B\} = AB + BA$. In general, the algebra generated by a set of quantities satisfying the relations $\{\alpha_{\mu}, \alpha_{\nu}\} = 2\delta_{\mu\nu}$ is called a **Clifford**²⁰ **Algebra**.

2.5 By use of a specific example, show that

$$\frac{d(AB)}{dx} = \frac{dA}{dx}B + A\frac{dB}{dx}$$

where A = A(x) and B = B(x) are two matrices. 2.6 Write the two equations indicated by

$$i\hbar\frac{d}{dt}\left(\begin{array}{c}a(t)\\b(t)\end{array}\right) = \left(\begin{array}{cc}\omega_0 & \omega_1\cos\omega t\\\omega_1\cos\omega t & -\omega_0\end{array}\right)\left(\begin{array}{c}a(t)\\b(t)\end{array}\right).$$

2.7 The rank of a matrix equals the order of the largest nonvanishing determinant contained within the matrix. Find the rank of each of the following matrices:

(a)
$$\begin{pmatrix} 1 & 2 & -1 \\ 4 & 1 & 5 \\ 3 & -1 & 6 \end{pmatrix}$$
, (b) $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$,
(c) $\begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}$, and (d) $\begin{pmatrix} 2 & 4 \\ -4 & -8 \\ 1 & 2 \end{pmatrix}$.

2.8 Where it exists, calculate the trace of the matrices in Problem 2.7.

¹⁹Wolfgang Pauli (1900–1958), Austrian physicist who is known for his work in quantum theory and particle physics. He is best known for the Pauli exclusion principle. He was awarded the Nobel Prize in physics in 1945.

²⁰William Kingdon Clifford (1845–1879), English mathematician who studied non-Euclidean geometry by arguing that energy and matter are simply different types of curvature of space. He introduced a generalization of Grassmann's exterior algebra, now known as Clifford algebra.

2.9 Find the transpose of the following matrices:

(a)
$$\begin{pmatrix} 2\\4\\6 \end{pmatrix}$$
, (b) $\begin{pmatrix} 3 & 4 & -2 \end{pmatrix}$, and (c) $\begin{pmatrix} 3 & 2 & 1\\2 & 0 & -6\\1 & -6 & 1 \end{pmatrix}$.

2.10 Of the following matrices, determine which are symmetric and which are antisymmetric:

(a)
$$\begin{pmatrix} 1 & 2 & 5 \\ 2 & 2 & -1 \\ 5 & -1 & 3 \end{pmatrix}$$
, (b) $\begin{pmatrix} 2 & 3 \\ 3 & 4 \\ 0 & 0 \end{pmatrix}$,
(c) $\begin{pmatrix} 2 & -1 & -2 \\ 1 & 2 & -1 \\ 2 & 1 & 2 \end{pmatrix}$, and (d) $\begin{pmatrix} 2 & 1 \\ 2 & 4 \end{pmatrix}$.

2.11 Find the inverse of the following matrix:

$$A = \left(\begin{array}{cc} 3 & 2\\ 1 & 6 \end{array}\right).$$

2.12 Find the Hermitian conjugate of the following matrix:

$$A = \begin{pmatrix} i & 2 & 3+i \\ -2 & 2i & 0 \\ -3+i & 0 & -i \end{pmatrix}.$$

- 2.13 Prove that: (a) $\operatorname{Tr}(AB) = \operatorname{Tr}(BA)$ and (b) $\operatorname{Tr}(A+B) = \operatorname{Tr}A + \operatorname{Tr}B$.
- 2.14 Prove the following: (a) $(AB)^T = B^T A^T$ and (b) $(AB)^{\dagger} = B^{\dagger} A^{\dagger}$.

2.15 Prove that (a) $A + A^{\dagger}$, (b) $i(A - A^{\dagger})$, and (c) AA^{\dagger} are all Hermitian for arbitrary A. 2.16 If A and B are two Hermitian matrices, prove that AB is Hermitian only if A and B commute.

2.17 If A is a Hermitian matrix, show that e^{iA} is unitary.

2.18 Given $U = e^{iH}$. (a) Show that U is unitary if H is Hermitian. (b) Show that H is Hermitian if U is unitary.

- 2.19 Show that $\det A^T = \det A$.
- 2.20 Show that $\det e^A = e^{\operatorname{Tr} A}$.

2.21 Prove that the eigenvalues of a Hermitian matrix (Hermitian operator) are all real. 2.22 By use of the determinant method, solve the following systems of linear equations:

(a)
$$\begin{array}{c} a_{11}x_1 + a_{12}x_2 = k_1 \\ a_{21}x_1 + a_{22}x_2 = k_2 \end{array}$$
 (b) $\begin{array}{c} x + 3y = 4 \\ 2x - 2y = 6 \end{array}$

(c)
$$\begin{array}{c} x - 4y = 2\\ 2x - y = 1 \end{array}$$
 (d) $\begin{array}{c} x + 5y + 3z = 1\\ 3x + y + 2z = 1\\ x + 2y + z = 0 \end{array}$

2.23 By use of the matrix method, solve the systems of equations in Problem 2.22.2.24 Find the eigenvalues of the following matrices:

(a)
$$\begin{pmatrix} 4 & -2 \\ 1 & 1 \end{pmatrix}$$
, (b) $\begin{pmatrix} 1 & 2 \\ -8 & 11 \end{pmatrix}$, (c) $\begin{pmatrix} 1 & 0 \\ 2 & -1 \end{pmatrix}$, and
(d) $\begin{pmatrix} 13 & -3 & 5 \\ 0 & 4 & 0 \\ -15 & 9 & -7 \end{pmatrix}$.

2.25 Verify the Cayley-Hamilton theorem for

$$\left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right).$$

2.26 By use of the Cayley-Hamilton theorem, compute the inverse of

$$\left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right).$$

2.27 Solve $X' = R_2 X$ for x and y where R_2 is the 2×2 rotation matrix.



2.28 By use of the matrix method, find (a) R_3 , (b) $|R_3|$, and (c) the required transformation equations for the indicated inversion in Fig. 2.7.



Figure 2.8

2.29 By use of the matrix method, find (a) R_3 , (b) $|R_3|$, and (c) the required transformation equations for the indicated reflection in Fig. 2.8.

2.30 Show that the function $T: V \mapsto V$ defined by $T(v) = \lambda v$ is a linear operator. 2.31 Given u = (-3, 1) and v = (2, 3). Calculate (a) $\langle u, v \rangle$ and (b) ||u||. 2.32 Given

$$u = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad \text{and} \quad v = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

Calculate $\langle u, v \rangle$.

2.33 If AA = A, then matrix A is said to be **idempotent**. Calculate the determinant of a general idempotent matrix.

2.34 If A^n equals the zero matrix for some n, then A is said to be **nilpotent**. Prove that a nilpotent matrix is singular.

2.35 Show that $\sigma_j/2$ are Hermitian for j = 1, 2, 3. The σ_j are the three Pauli spin matrices.

2.36 For the quaternion group, show that the eight matrices, q_j for j = 1, 2, ..., 8, define the group with matrix multiplication as the group operation.

2.37 Write down the multiplication table for the third order group with elements given by $\{a,b,e\}$.

2.38 Write down the multiplication table for the fifth order group with elements given by $\{a, b, c, d, e\}$.

2.39 If matrix A is similar to matrix B, show that matrix B is similar to matrix A.

2.40 Assume that the elements of a group are distinct and prove that elements in each row and in each column of the multiplication table must be distinct (e.g., appear once in each row and in each column.)

2.41 Show that the following six matrices form a group.

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad B = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix};$$

$$C = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}; \ D = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}; \ F = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}.$$

2.42 If

$$T(\theta) = \left(\begin{array}{cc} \cos\theta & -\sin\theta\\ \sin\theta & \cos\theta \end{array}\right),$$

show that $T(\theta_1)T(\theta_2) = T(\theta_2)T(\theta_1) = T(\theta_1 + \theta_2).$

Chapter 3

Functions of a Complex Variable

3.1 Introduction

The imaginary number, $i = \sqrt{-1}$, was introduced into mathematics during the latter part of the sixteenth century. Imaginary numbers are needed since certain equations, for example $x^2 + 1 = 0$, have no solutions that involve only real numbers. In mathematical physics, one writes the solution of the equation of motion for the linear harmonic oscillator, $\ddot{x} + \omega^2 x = 0$, in the form $x(t) = A \exp(i\omega t)$. In modern optics, index of refraction is written in complex (containing real and imaginary parts) form, and the wave function in quantum mechanics is often a complex variable will be explained below. Complex variables and functions of a complex variable are used throughout physics; this chapter is devoted to certain features of complex variable theory that are most useful in physical applications.

3.2 Complex Variables and Their Representations

A complex variable may be written in the general form

$$z = x + iy = re^{i\theta}. (3.1)$$

In Eq.(3.1),

- 1. x and y are the respective real and imaginary parts of z and are written as $x = \operatorname{Re} z$ and $y = \operatorname{Im} z$;
- 2. θ is the **argument** (**phase**) of z and is written as $\theta = \arg z = \theta_p + 2\pi n$ for $n = 0, 1, 2, \ldots$; θ_p is the **principal argument** of z and varies from 0 to 2π ;
- 3. $e^{i\theta} = \cos\theta + i\sin\theta$ (Euler's¹ formula); and
- 4. r = |z| is the absolute value (magnitude, modulus, Mod z) of z where $r = \sqrt{x^2 + y^2} = \sqrt{(\text{Re } z)^2 + (\text{Im } z)^2}$.

¹Leonhard Euler (1707–1783), Swiss mathematician who is known for his contributions in analytic geometry and trigonometry, calculus, and number theory.

The complex conjugate of z is denoted as z^* (For convenience, \bar{z} is sometimes used to denote complex conjugate.) and is obtain by changing the sign of the imaginary part (or imaginary terms) of z, $z^* = x - iy$. In connection with the complex conjugate, we have

- 1. $zz^* = (x + iy)(x iy) = |z|^2$;
- 2. $(z_1 + z_2)^* = z_1^* + z_2^*$; and

3.
$$(z_1/z_2)^* = z_1^*/z_2^*$$
.

It is useful to note for physical purposes that z^*z is a real quantity. Complex variables are subject to the same algebraic laws as real variables; they are

- 1. Associative law of addition: $z_1 + (z_2 + z_3) = (z_1 + z_2) + z_3;$
- 2. Commutative law of multiplication: $z_1 z_2 = z_2 z_1$;
- 3. Associative law of multiplication: $z_1(z_2z_3) = (z_1z_2)z_3$; and
- 4. Distributive law: $z_1(z_2 + z_3) = z_1 z_2 + z_1 z_3$.

The algebraic operations for two complex variables are the same as for real variables and are as follows.

1. Addition (subtraction):

$$z_1 + z_2 = (x_1 + iy_1) + (x_2 + iy_2)$$
$$= (x_1 + x_2) + i(y_1 + y_2).$$

2. Multiplication:

$$z_1 z_2 = (x_1 + iy_1)(x_2 + iy_2) = (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x_2 y_1).$$

3. Division $(z_2 \neq 0)$: To facilitate the separation into real and imaginary parts, note the technique of multiplying the numerator and denominator by the complex conjugate of the denominator.

$$\frac{z_1}{z_2} = \frac{x_1 + iy_1}{x_2 + iy_2} = \frac{x_1 + iy_1}{x_2 + iy_2} \cdot \frac{x_2 - iy_2}{x_2 - iy_2} = \frac{x_1x_2 + y_1y_2}{x_2^2 + y_2^2} + i\left\{\frac{x_2y_1 - x_1y_2}{x_2^2 + y_2^2}\right\}.$$

A plane is required for the geometric representation of a complex variable; this plane is called the **complex plane** or z-**plane**. In the z-plane, the representation of a complex variable is done by labeling the x-axis as the real axis and labeling the y-axis as the imaginary axis; such a rectangular diagram used to represent a point in the z-plane is sometimes referred to as the **Argand**² **diagram** and is illustrated in Fig. 3.1.

 $^{^{2}}$ Jean Robert Argand (1768–1822), Swiss accountant and amateur mathematician who is known for his geometrical interpretation of the complex number.



Figure 3.1

Example 32 Given z = (1+i)/(2-3i). (a) Put z in the standard form, x + iy. Find (b) Re z, (c) Im z, (d) Mod z, and (e) arg z. (f) Locate z on an Argand diagram.

Solution : On multiplying the numerator and denominator of z by the complex conjugate of the denominator of z, we obtain

Part A:

$$z = \frac{1+i}{2-3i} \cdot \frac{2+3i}{2+3i} = -\frac{1}{13} + i\frac{5}{13}$$
 (standard form).

Part B:

$$\operatorname{Re} z = -\frac{1}{13}.$$

Part C:

$$\operatorname{Im} z = \frac{5}{13}.$$

Part D:

Mod
$$z = \sqrt{(\operatorname{Re} z)^2 + (\operatorname{Im} z)^2} = \frac{1}{13}\sqrt{26} = r$$

Part E:

$$x = r \cos \theta = -\frac{1}{13}$$
 and $y = r \sin \theta = \frac{5}{13}$
arg $z = \theta = \tan^{-1}\left(\frac{y}{x}\right) = \tan^{-1}(-5).$

Part F: The Argand diagram representation of z is given in Fig. 3.2.



Figure 3.2

Example 33 Show that (a) $|z_1z_2| = |z_1| |z_2|$, (b) arg $(z_1z_2) = \arg z_1 + \arg z_2$, and (c) arg $(z_1/z_2) = \arg z_1 - \arg z_2$.

Solution:

Part A: By use of $|z| = \sqrt{x^2 + y^2}$, we find that

$$|z_1| |z_2| = \sqrt{x_1^2 + y_1^2} \sqrt{x_2^2 + y_2^2} = \sqrt{(x_1^2 + y_1^2)(x_2^2 + y_2^2)} = |z_1 z_2|$$

Part B: By use of $z = x = iy = re^{i\theta}$, we find that

$$\arg(z_1 z_2) = \arg\left\{\left(r_1 e^{i\theta_1}\right)\left(r_2 e^{i\theta_2}\right)\right\} = \arg(r_1 r_2 e^{i(\theta_1 + \theta_2)}) = \arg z_1 + \arg z_2.$$

Part C: Since $z = x + iy = re^{i\theta}$, we may write

$$\arg\left(\frac{z_1}{z_2}\right) = \frac{r_1 e^{i\theta_1}}{r_2 e^{i\theta_2}} = \frac{r_1}{r_2} e^{i(\theta_1 - \theta_2)} = \arg z_1 - \arg z_2.$$

3.3 The de Moivre Theorem

On raising Eq.(3.1) to the *n*th power, one obtains

$$z^{n} = r^{n} (\cos \theta + i \sin \theta)^{n} = r^{n} e^{in\theta}; \quad z \neq 0.$$
(3.2)

Equation (3.2) is known as the **de Moivre³ theorem** and is valid for positive, negative, and fractional n; it is often written as

$$(\cos\theta + i\sin\theta)^n = \cos(n\theta) + i\sin(n\theta). \tag{3.3}$$

 $^{^{3}}$ Abraham de Moivre (1667–1754), French mathematician who is known for his work in analytic and probability theory. He is best known for the trigonometric formula, now known as de Moivre's theorem. He was a friend of Newton.

The de Moivre theorem may be used to obtain certain relations involving sines and cosines of multiple angles. On considering de Moivre's theorem for n = 2 and equating corresponding real and imaginary parts, the following well-known relations are obtained: $\cos 2\theta = \cos^2 \theta - \sin^2 \theta$ and $\sin 2\theta = 2\cos\theta \sin \theta$. For n > 2, the binomial expansion

$$(1+x)^n = \sum_{k=1}^{\infty} \frac{n!}{k!(n-k)!} x^n$$
 where $n! = n(n-1)(n-2)...$ (factorial)

may be used to expand the left-hand side of de Moivre's theorem, Eq. (3.3). By use of de Moivre's theorem, the *n*th root of z may be written as

$$z^{1/n} = r^{1/n} \left\{ \cos\left(\frac{\theta_p + 2\pi k}{n}\right) + i\sin\left(\frac{\theta_p + 2\pi k}{n}\right) \right\}.$$
(3.4)

In Eq.(3.4), k = 0, 1, 2, ..., n-1, the quantity $r^{1/n}$ represents the positive *n*th root of r, and $0 \le \theta_p < 2\pi$.

Example 34 By use of de Moivre's theorem, find the square root of *i*.

Solution: The square root of *i* is obtained when r = 1 (since $r \cos \theta = 0$ and $r \sin \theta = 1$), $\theta_p = \pi/2$, and n = 2 are substituted in Eq.(3.4); for k = 0 and 1 respectively, we obtain

$$i^{1/2} = \cos\left(\frac{\pi}{4}\right) + i\sin\left(\frac{\pi}{4}\right) = \frac{1+i}{\sqrt{2}}$$
 where $k = 0$

and

$$i^{1/2} = \cos\left(\frac{3\pi}{4}\right) + i\sin\left(\frac{3\pi}{4}\right) = -\frac{1+i}{\sqrt{2}}$$
 where $k = 1$.

The above two roots may be checked for correctness. The Argand diagram representation of these roots is given in Fig. 3.3. The procedure used to calculate the square root of i can be applied to calculate the *n*th root of any quantity z ($z \neq 0$).

3.4 Analytic Functions of a Complex Variable

A function, f(z), of a complex variable is itself a complex quantity and may be written in terms of real and imaginary parts in the following manner:

$$f(z) = u(x, y) + iv(x, y).$$
 (3.5)

The representations of z and f(z) in the complex plane are respectively called z-plane and w-plane diagrams. The number w = f(z) is the value of f(z) at z. A single-valued function f(z) is said to be **analytic** (regular, holomorphic) at z_0 if it has a unique derivative at z_0 and at every point in the neighborhood of z_0 . If a function fails to be analytic at some point z_0 but is analytic at points in the neighborhood of z_0 , then z_0 is said to be a singular point (singularity) of f(z). In this connection, note that the function 1/z is analytic everywhere except at z = 0 (singular point).



Figure 3.3

By analogy with real variables, the derivative of a function of a complex variable is defined as

$$f'(z) = \lim_{\Delta x \to 0} \left[\frac{f(z + \Delta z) - f(z)}{\Delta z} \right] = \lim_{\Delta x \to 0} \left[\frac{\Delta u + i\Delta v}{\Delta x + i\Delta y} \right].$$

Equation (3.5), where $\Delta f = \Delta u + i\Delta v$ and $\Delta z = \Delta x + i\Delta y$, was used to obtain the above equation. In the above equation, there is an infinite number of ways of obtaining $\Delta z \rightarrow 0$ in the z-plane, and the result is independent of the choice. For convenience, we select the simple scheme illustrated in Fig. 3.4.



Figure 3.4

Case 1 $\Delta x = 0$ and $i\Delta y \to 0$.

$$f_1'(z) = \lim_{i\Delta y \to 0} \left[\frac{\Delta u + i\Delta v}{i\Delta y} \right] = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}$$

The partial derivatives are used in the above equation since u and v are functions of both x and y.

Case 2 $i\Delta y = 0$ and $\Delta x \to 0$.

$$f_2'(z) = \lim_{\Delta x \to 0} \left[\frac{\Delta u + i \Delta v}{\Delta x} \right] = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}.$$

If f(z) is analytic in the region Γ (see Fig. 3.4), it is required to have a unique derivative at every point in the region; therefore, we require that $f'_1(z) = f'_2(z)$. As a result of this requirement, we obtain the following relations:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}$$
 and $\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$. (3.6)

To obtain the relations in Eq.(3.6), we equated corresponding real and imaginary parts of the equations for $f'_1(z)$ and $f'_2(z)$. The relations in Eq.(3.6) are the well-known **Cauchy-Riemann⁴ relations**; they constitute the necessary conditions for a unique derivative of f(z) at each point within the region Γ , analytic f(z).

On differentiating the equations in Eq.(3.6) with respect to x and y respectively, we obtain

$$rac{\partial^2 u}{\partial x^2} = rac{\partial^2 v}{\partial x \partial y} \quad ext{and} \quad rac{\partial^2 u}{\partial y^2} = -rac{\partial^2 v}{\partial y \partial x}.$$

If u and v possess continuous partial derivatives to second order (smooth functions), the above equations lead to

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0; \quad \text{similarly, we obtain} \quad \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = 0. \tag{3.7}$$

The equations in Eq.(3.7) are two-dimensional Laplace equations, and functions u and v (called **harmonic** or **conjugate functions**) are, therefore, solutions of the two-dimensional Laplace equations. The theory of analytic functions is extremely useful in solving problems that involve the two-dimensional Laplace equation such as problems in electrostatics and fluid mechanics. Also, note that the function f(z) satisfies the two-dimensional Laplace equation.

Example 35 (a) Show that $v(x,y) = 3x^2y - y^3$ is a harmonic function. (b) Find the conjugate function, u(x,y). (c) Find the analytic function f(z) = u(x,y) + iv(x,y).

Solution : Part A: If

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = 0,$$

⁴Georg Friedrich Bernhard Riemann (1826–1866), German mathematician whose ideas concerning the geometry of space had a profound effect on the development of modern theoretical physics. He clarified the notion of an integral by defining what is now known as the Riemann integral. His Ph.D. thesis was supervised by Gauss at Göttingen.

then v is said to be a harmonic function. Note that

$$\frac{\partial v}{\partial x} = 6xy \qquad \qquad \frac{\partial^2 v}{\partial x^2} = 6y \\ \frac{\partial v}{\partial y} = 3x^2 - 3y^2 \qquad \frac{\partial^2 v}{\partial y^2} = -6y$$

Adding the above two second derivative terms shows that v is a harmonic function. Part B: Note that

$$rac{\partial v}{\partial y}=3x^2-3y^2=rac{\partial u}{\partial x} \quad ext{and} \quad rac{\partial v}{\partial x}=6xy=-rac{\partial u}{\partial y}.$$

Integrating the two above equations with respect to x and y respectively, we obtain

$$u(x,y) = x^3 - 3xy^2 + g_1(y)$$
 and $u(x,y) = -3xy^2 + g_2(x)$

or

$$x^3 - 3xy^2 + g_1(y) = -3xy^2 + g_2(x).$$

In the above equation, we must have $g_1(y) = 0$ and $g_2(x) = x^3$. The required conjugate function is therefore given by

$$u(x,y) = x^3 - 3xy^2.$$

Part C: The corresponding analytic function is given by

$$f(z) = x^3 - 3xy^2 + i(3x^2y - y^3) = z^3.$$

Note that f(z) satisfies the two-dimensional Laplace equation,

$$\frac{\partial^2 f(z)}{\partial x^2} + \frac{\partial^2 f(z)}{\partial y^2} = 0.$$

3.5 Contour Integrals

The integral (in the Riemannian sense) of a function of a complex variable f(z) is defined in a manner that is analogous to the case of real variable theory and may be written as

$$\int_{C} f(z)dz \equiv \lim_{\substack{n \to \infty \\ |z_{j} - z_{j-1}| \to 0}} \left\{ \sum_{j=1}^{n} f(\xi_{j})(z_{j} - z_{j-1}) \right\} = \int_{z_{a}}^{z_{b}} f(z)dz.$$
(3.8)

In Eq.(3.8), the path (or contour) of integration C is divided into n segments by points z_j , and ξ_j is a point between z_j and z_{j-1} (see Fig. 3.5). In complex variable theory, the integral in Eq.(3.8) is referred to as the contour integral of f(z) along the path C from z_a to z_b . The integral around a closed path is denoted as $\oint f(z)dz$. The sign convention for contour integrals is as follows: When the path of integration is traversed such that the region of interest is on the left, the integral is considered to be positive.



Regions in the complex plane are classified as either simply connected or multiply connected. **Simply connected regions** are regions without holes and possess the following three equivalent properties: (a) every closed path within the region contains only points that belong to the region, (b) every closed path within the region can be shrunk to a point (e.g., the region can be continuously deformed to a point), and (c) every scissors cut starting at an arbitrary point on the boundary and finishing at another point on the boundary separates the region into two unconnected pieces. Regions that are not simply connected are said to be **multiply connected**.

Three extremely important relations involving integrals of functions of a complex variable are (a) the Cauchy integral theorem, (b) the Cauchy integral formula, and (c) differentiation inside the sign of integration; these integral relations will now be discussed.

The Cauchy Integral Theorem If f(z) is analytic throughout a simply connected region Γ and C is a closed path within Γ , then

$$\oint_C f(z)dz = 0. \tag{3.9}$$

The curl theorem (in two dimensions) due to Stokes and the Cauchy-Riemann conditions can be used to prove this theorem (see Problem 3.13). We, however, apply the following simple idea from topology to develop a proof of this theorem. Consider two paths Γ_1 and Γ_2 between points *a* and *b* in region Γ (see Fig. 3.6). Path Γ_1 may be deformed continuously into path Γ_2 since the region is simply connected and f(z) is analytic throughout the region, and we may write

$$\int_{\Gamma_1} f(z)dz = \int_{\Gamma_2} f(z)dz.$$

If the direction along path Γ_1 is reversed, the value of the integral along Γ_1 becomes



Figure 3.6

negative, and we obtain proof of the Cauchy integral theorem

$$-\int_{\Gamma_1} f(z)dz = \int_{\Gamma_2} f(z)dz$$
 or $\oint_C f(z)dz = 0.$

The Cauchy integral theorem applies to special cases that are important in physics where the value of the integral of a function depends only on the end points and is independent of the path taken between the end points. The inverse of this theorem is known as Morera's theorem.

The Cauchy Integral Formula This formula is another important and extremely useful relation concerning the integral of a function of a complex variable; it may be written as

$$\oint_C \frac{f(z)dz}{z - z_0} = 2\pi i f(z_0).$$
(3.10)



Figure 3.7

In Eq.(3.10), point z_0 is within C, and f(z) is assumed to be analytic within C; the integrand, $f(z)/(z-z_0)$, is clearly not analytic at $z = z_0$. Figure 3.7 is used to derive the

Cauchy integral formula in Eq.(3.10). Note that Fig. 3.7(a) is equivalent to Fig. 3.7(b) as r approaches zero. Also, note that $f(z)/(z-z_0)$ is analytic in the region between C and C'. Counterclockwise integration around C is positive by convention, and clockwise integration around C' is negative; hence, we may apply Cauchy's integral theorem and obtain

$$\oint_C \frac{f(z)dz}{z-z_0} - \oint_{C'} \frac{f(z)dz}{z-z_0} = 0.$$

Around path C', we set $z - z_0 = re^{i\theta}$; hence $dz = ire^{i\theta}d\theta$. As r approaches zero, the above equation reduces to

$$\oint_C \frac{f(z)dz}{z-z_0} = \int_0^{2\pi} \frac{f(z_0 + re^{i\theta})ire^{i\theta}d\theta}{re^{i\theta}}$$
$$= i \int_0^{2\pi} f(z_0 + re^{i\theta})d\theta$$
$$= 2\pi i f(z_0). \tag{3.10'}$$

The above equation establishes the Cauchy integral formula. The first two important integral relation may be summary as

$$\frac{1}{2\pi i} \oint_C \frac{f(z)dz}{z-z_0} = \begin{cases} f(z_0) & \text{for } z_0 \text{ inside } C\\ 0 & \text{for } z_0 \text{ outside } C \end{cases}$$

Differentiation Inside the Sign of Integration The derivative of f(z) with respect to z is defined by

$$f'(z) = \lim_{\Delta z \to 0} \left\{ \frac{f(z + \Delta z) - f(z)}{\Delta z} \right\}.$$

On applying Cauchy's integral formula to the two functions on the right-hand side of the above equation, we obtain

$$\begin{aligned} f'(z) &= \lim_{\Delta z \to 0} \left\{ \frac{1}{\Delta z} \left[f(z + \Delta z) - f(z) \right] \right\} \\ &= \lim_{\Delta z \to 0} \left\{ \frac{1}{2\pi i \Delta z} \left[\oint_C \frac{f(\xi) d\xi}{\xi - z - \Delta z} - \oint_C \frac{f(\xi) d\xi}{\xi - z} \right] \right\} \\ &= \frac{1}{2\pi i} \oint_C \frac{f(\xi) d\xi}{(\xi - z)^2}. \end{aligned}$$

The above equation results from combining the integrands of the previous two integrals and finding the limit as Δz goes to zero. For the *n*-th derivative of f(z) with respect to z, we have

$$f^{(n)}(z_0) \equiv f^{(n)}(z) \mid_{z=z_0} = \frac{n!}{2\pi i} \oint_C \frac{f(\xi)d\xi}{(\xi - z_0)^{(n+1)}}.$$
(3.11)

Equation (3.11) is valid when $f(\xi)$ is analytic within C, z_0 is within C and the integrand is not analytic at $z = z_0$. Equation (3.11) will be used below in developing the Taylor expansion for f(z).

3.6 The Taylor Series and Zeros of f(z)

In this Section, we develop the Taylor⁵ series for the expansion of a function of a complex variable and explain the classification of the zeros of f(z) by use the Taylor expansion.

3.6.1 The Taylor Series

If f(z) is analytic in some region Γ and C is a circle within Γ with center at z_0 , then f(z) can be expanded in a **Taylor series** in the form

$$f(z) = \sum_{n=0}^{\infty} \frac{(z-z_0)^n}{n!} f^{(n)}(z_0) = \sum_{n=0}^{\infty} a_n (z-z_0)^n.$$
(3.12)

The series in Eq.(3.12) converges absolutely and uniformly for $|z - z_0| < R$ where R is the radius of convergence.



Figure 3.8

Proof: From the Cauchy integral formula, we note that (see Fig. 3.8)

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(\xi)d\xi}{\xi - z}$$
(3.13)

where $|z - z_0| < R$ and $R = |\xi - z_0|$. To prove that the Taylor expansion holds, a series expansion for $1/(\xi - z)$ will be developed. For convenience, we set

$$K_T = \frac{z - z_0}{\xi - z_0}.$$

 $^{{}^{5}}$ Brook Taylor (1685–1731), English mathematician who added to mathematics a new branch known as the calculus of finite differences, invented integration by parts, and discovered the formula known as the Taylor expansion.

Subtracting unity from both sides of the above equation yields

$$1 - K_T = 1 - \frac{z - z_0}{\xi - z_0} = \frac{\xi - z}{\xi - z_0}.$$

Inverting both sides of the above equation, we obtain

$$\frac{1}{1-K_T} = \frac{\xi - z_0}{\xi - z} = \sum_{n=0}^{\infty} K_T^n; \quad |K_T| < 1.$$

The above equation results from noting that the left-hand side is just the sum of a geometric series (see the Appendix at the end of this chapter). The required expansion for $1/(\xi - z)$ is obtained by dividing the above equation by $\xi - z_0$; the result is

$$\frac{1}{\xi - z} = \frac{1}{\xi - z_0} \sum_{n=0}^{\infty} \left(\frac{z - z_0}{\xi - z_0} \right)^n = \sum_{n=0}^{\infty} \frac{(z - z_0)^n}{(\xi - z_0)^{n+1}}.$$
(3.14)

Substituting Eq.(3.14) into Eq.(3.13), we obtain

$$\frac{1}{2\pi i} \oint_C \frac{f(\xi)d\xi}{\xi - z} = \sum_{n=0}^{\infty} \left\{ \oint_C \frac{f(\xi)(z - z_0)^n d\xi}{(\xi - z_0)^{n+1}} \right\}$$
$$= \sum_{n=0}^{\infty} \left\{ (z - z_0)^n \left(\frac{1}{2\pi i} \oint_C \frac{f(\xi)d\xi}{(\xi - z_0)^{n+1}} \right) \right\}$$
$$= \sum_{n=0}^{\infty} \frac{(z - z_0)^n}{n!} f^{(n)}(z_0)$$

or

$$f(z) = \sum_{n=0}^{\infty} \frac{(z-z_0)^n}{n!} f^{(n)}(z_0) = \sum_{n=0}^{\infty} a_n (z-z_0)^n$$
(3.12')

where $a_n = f^{(n)}(z_0)/n!$. Equation (3.12') is the required Taylor series. When $z_0 = 0$, the Taylor series becomes the Maclaurin⁶ series.

Example 36 Expand 1/(1-z) in a Taylor series about $z_0 = i$ and find the radius of convergence.

Solution : The Taylor expansion of f(z) is obtained and applied in a manner similar to that in real variable theory. We have

$$f(z) = (1-z)^{-1}; \quad f'(z) = (1-z)^{-2};$$

$$f''(z) = 2(1-z)^{-3}; \quad f^{(3)}(z) = 3 \cdot 2(1-z)^{-4}.$$

The general term is

$$f^{(n)}(z) = n!(1-z)^{-(n+1)}.$$

⁶Colin Maclaurin (1698–1746), Scottish mathematician who worked in algebra, geometry, and calculus. He is best known for using a special case of the Taylor series, now known as the Maclaurin series.

The required expansion is therefore

$$f(z) = \sum_{n=0}^{\infty} \frac{(z-z_0)^n}{n!} f^{(n)}(z_0) = \sum_{n=0}^{\infty} \frac{(z-i)^n}{(1-i)^{n+1}}.$$

The radius of convergence of the above series where $a_n = 1/(1-i)^{n+1}$ is

$$R \equiv \lim_{n \to \infty} \left| \frac{a_n}{a_{n+1}} \right| = |1 - i| = \sqrt{2}.$$

3.6.2 Zeros of f(z)

Classification of the zeros of f(z) is made by use of Taylor's expansion of f(z) as follows:

- 1. If f(z) = 0 at $z = z_0$, the point z_0 is said to be a zero of f(z).
- 2. If $a_0 = a_1 = \cdots = a_{m-1} = 0$ but $a_m \neq 0$, then the Taylor expansion becomes

$$f(z) = a_m(z-z_0)^m + a_{m+1}(z-z_0)^{m+1} + \dots = \sum_{n=m}^{\infty} a_n(z-z_0)^n.$$

In this case, f(z) is said to have a zero of order m at $z = z_0$. A zero of order unity (m = 1) is called a simple zero. In this connection (m = 1), note that

$$f(z) = f(z_0) + (z - z_0)f'(z_0) + \frac{(z - z_0)^2}{2!}f^{(2)}(z_0) + \cdots$$

The conditions

$$f(z_0) = 0$$
 and $f'(z_0) \neq 0$ (3.15)

indicate the existence of a simple zero for f(z) at $z = z_0$.

3.7 The Laurent Expansion

The Laurent⁷ expansion of f(z) has no real variable counterpart and is key in discussions of singularities and the calculus of residues. If f(z) is analytic in the interior and on the boundary of the circular ring between two circles C_1 and C_2 (see Fig. 3.9.), it may be represented as a **Laurent expansion** which has the form

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \sum_{n'=1}^{\infty} \frac{b_{n'}}{(z - z_0)^{n'}}.$$
(3.16)

The a_n and $b_{n'}$ coefficients in Eq.(3.16) are respectively given by

$$a_n = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{(\xi - z_0)^{n+1}} \qquad (n = 0, 1, \dots)$$



and

$$b_{n'} = \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{(\xi - z_0)^{-n'+1}} \qquad (n' = 1, 2, \dots).$$

Proof: In Fig. 3.9, make a scissors cut from C_1 to C_2 as shown in Fig. 3.10. On applying the Cauchy integral formula in Fig. 3.10, we find that

$$f(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{\xi - z} - \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{\xi - z} = f_A(z) + f_P(z).$$
(3.17)

The functions $f_A(z)$ and $f_P(z)$ are given respectively by

$$f_A(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{\xi - z} \quad \text{and} \quad f_P(z) = \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{z - \xi}.$$
 (3.18)

Consider $f_A(z)$ where ξ is on C_1 and z is inside the region between C_1 and C_2 .

 $^{^{7}}$ Matthieu Paul Hermann Laurent (1841–1908) was born in Luxembourg and is known for his work in complex variable theory.

Using the expansion for $1/(\xi - z)$ developed in Eq.(3.14), we may write

$$f_A(z) = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{\xi - z} = \sum_{n=0}^{\infty} a_n (z - z_0)^n.$$

The a_n coefficients in the above equation are given by

$$a_n = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{(\xi - z_0)^{n+1}}$$
 and $|z - z_0| < |\xi - z_0|$.

Note that the a_n cannot be represented by $f^{(n)}(z)/n!$ since $f_A(z)$ is not analytic at $z = z_0$ as in the case of the Taylor expansion.



Now consider the integral over C_2 , f_P , where it is assumed that ξ is now on C_2 and z is inside the ring (see Fig. 3.11). We need the appropriate expansion for $1/(z - \xi)$; it is obtained by use of a method similar to that used in the Taylor series case. Here we set

$$K_L = \frac{\xi - z_0}{z - z_0}.$$

Subtracting unity from both sides of the above equation and inverting the resulting equation, we obtain

$$\frac{1}{1-K_L} = \frac{z-z_0}{z-\xi} = \sum_{n=0}^{\infty} K_L^n \quad \text{where} \quad |K_L| < 1.$$

Dividing the above equation by $z - z_0$ yields

$$\frac{1}{z-\xi} = \sum_{n=0}^{\infty} \frac{(\xi-z_0)^n}{(z-z_0)^{n+1}} \quad \text{where} \quad |\xi-z_0| < |z-z_0| \quad \text{since} \quad |K_L| < 1.$$

On substituting the above equation into $f_P(z)$ in Eq.(3.18), we obtain

$$f_P(z) = \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{z-\xi}$$

= $\sum_{n=0}^{\infty} \left\{ \frac{1}{(z-z_0)^{n+1}} \frac{1}{2\pi i} \oint_{C_2} f(\xi)(\xi-z_0)^n d\xi \right\}$
= $\sum_{n'=1}^{\infty} \frac{1}{(z-z_0)^{n'}} \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{(\xi-z_0)^{-n'+1}}$
= $\sum_{n'=1}^{\infty} \frac{b_{n'}}{(z-z_0)^{n'}}$ where $b_{n'} = \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi)d\xi}{(\xi-z_0)^{-n'+1}}$.

Hence the Laurent expansion in Eq.(3.16) is established when expressions for $f_A(z)$ and $f_P(z)$ are substituted into Eq.(3.17).

The Laurent expansion consists of two series. The first series in Eq.(3.16) is called the analytic part, $f_A(z)$, of the expansion, and it converges everywhere inside C_1 . The second series, $f_P(z)$, is referred to as the principal part, and it converges everywhere outside C_2 . If f(z) is analytic within C_2 , the principal part equals zero, and the Laurent expansion reduces to the Taylor expansion since $a_n = f^{(n)}(z_0)/n!$ in that case. In addition to Eq.(3.16), the Laurent expansion can be written in the following useful forms: Form 2:

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \sum_{n=1}^{\infty} \frac{a_{-n}}{(z - z_0)^n}$$
(3.19a)

where

$$a_n = \frac{1}{2\pi i} \oint_{C_1} \frac{f(\xi)d\xi}{(\xi - z_0)^{n+1}} \qquad (n = 0, 1, \dots)$$
(3.19b)

and

$$a_{-n} = \frac{1}{2\pi i} \oint_{C_2} \frac{f(\xi) d\xi}{(\xi - z_0)^{-n+1}} \qquad (n = 1, 2, ...)$$
(3.19c)

Form 3:

$$f(z) = \sum_{n = -\infty}^{\infty} A_n (z - z_0)^n$$
 (3.20*a*)

where

$$A_n = \frac{1}{2\pi i} \oint_C \frac{f(\xi)d\xi}{(\xi - z_0)^{n+1}} \qquad (n = 0, \pm 1, \pm 2, \dots).$$
(3.20b)

In Form 3, C is any circle between C_1 and C_2 .

Example 37 By the direct evaluation of A_n , find the Laurent expansion for

$$f(z) = \frac{1}{z(z-1)}$$
 about $z_0 = 0$.

Solution : Here we have

$$f(z) = \sum_{n = -\infty}^{\infty} A_n (z - z_0)^n = \sum_{n = -\infty}^{\infty} A_n z^n$$

where

$$A_{n} = \frac{1}{2\pi i} \oint_{C} \frac{f(\xi)d\xi}{(\xi - z_{0})^{n+1}}$$

= $\frac{1}{2\pi i} \oint_{C} \frac{f(\xi)d\xi}{\xi^{n+1}}$
= $\frac{1}{2\pi i} \oint_{C} \frac{d\xi}{\xi^{n+1}\xi(\xi - 1)}$
= $-\frac{1}{2\pi i} \oint_{C} \frac{d\xi}{\xi^{n+2}(1 - \xi)}$
= $-\frac{1}{2\pi i} \oint_{C} \left\{ \frac{1}{\xi^{n+2}} \sum_{k=0}^{\infty} \xi^{k} \right\} d\xi \quad (|\xi| < 1)$

The A_n coefficient therefore becomes

$$A_n = -\frac{1}{2\pi i} \sum_{k=0}^{\infty} \oint_C \frac{d\xi}{\xi^{n-k+2}} = -\frac{1}{2\pi i} \sum_{k=0}^{\infty} 2\pi i \delta_{n-k+2,1}$$
$$= \begin{cases} -1 & \text{for } n \ge -1\\ 0 & \text{for } n < -1. \end{cases}$$

The required expansion becomes

$$f(z) = \sum_{n=-\infty}^{\infty} A_n z^n = \sum_{n=-1}^{\infty} A_n z^n = -\sum_{n=-1}^{\infty} z^n.$$

The problem of developing the Laurent expansion for a function by evaluating the A_n coefficient (or a_n and a_{-n}) is, except for simple functions, tedious. It is sometimes advantageous to use a procedure similar to that illustrated in the following two Examples to obtain the required Laurent expansion for a function.

Example 38 Find the Laurent expansion for f(z) = 1/z(z-1) by use of a geometric series.

Solution:

$$f(z) = \frac{1}{z(z-1)} = -\frac{1}{z} \left(\frac{1}{1-z} \right) = -\frac{1}{z} \sum_{n=0}^{\infty} z^n = -\sum_{n=-1}^{\infty} z^n \quad (|z| < 1).$$

The above result is the same as that obtained in the previous Example.
Example 39 Find the Laurent expansion for f(z) = 1/z(z-2) in the regions (a) 0 < |z| < 2 and (b) $2 < |z| < \infty$.

Solution :

Part A: For the region 0 < |z| < 2, f(z) = 1/z(z-2) may be written as

$$f(z) = -\frac{1}{2}\frac{1}{z}\left(\frac{1}{1-z/2}\right) = -\frac{1}{2}\frac{1}{z}\sum_{n=0}^{\infty} \left(\frac{z}{2}\right)^n \quad \left(\left|\frac{z}{2}\right| < 1; \quad |z| < 2\right)$$
$$= -\frac{1}{2z}\left(1 + \frac{z}{2} + \frac{z^2}{2^2} + \frac{z^3}{2^3} + \cdots\right) = -\frac{1}{2z} - \frac{1}{2^2} - \frac{z}{2^3} - \frac{z^2}{2^4} \cdots$$

Part B: In the region $2 < |z| < \infty$, f(z) = 1/z(z-2) may be written as

$$f(z) = \frac{1}{z^2(1-2/z)} = \frac{1}{z^2} \sum_{n=0}^{\infty} \left(\frac{2}{z}\right)^n \quad \left(\left|\frac{2}{z}\right| < 1; \quad |z| > 2\right)$$
$$= \frac{1}{z^2} \left(1 + \frac{2}{z} + \frac{2^2}{z^2} + \cdots\right) = \frac{1}{z^2} + \frac{2}{z^3} + \frac{2^2}{z^4} + \cdots$$

The quantity a_{-1} is called the **residue** of f(z) at $z = z_0$ and may be obtained from Eq.(3.19c); it is given by

$$a_{-1} = \frac{1}{2\pi i} \oint_C f(z) dz.$$
 (3.21)

Note that $2\pi i a_{-1}$ is the value of the above integral. When the residue can be determined directly, an indirect method of evaluating definite integrals may be developed. We will exploit this observation and develop indirect methods of evaluating certain classes of definite integrals. First, the classification of isolated singularities and calculations of corresponding residues are considered in the next Chapter.

3.8 Problems

3.1 Show that $z + z^*$ is real, whereas $z - z^*$ is imaginary. 3.2 Find the real and imaginary parts of:

(a)
$$z^2$$
; (b) $\frac{1}{z}$; (c) $\frac{z-1}{z+1}$; (d) $\frac{1}{z^2}$.

- 3.2 Show that $|\cos \theta + i \sin \theta| = 1$.
- 3.3 Show that $|z| = |z^*|$.
- 3.4 Find the real part, modulus, and argument of:

(a)
$$\frac{1+z}{1-z}$$
; (b) $1+i\sqrt{3}$; (c) $\frac{1+i}{1-i}$; (d) $\left(\frac{3}{i-\sqrt{3}}\right)^2$.

3.5 If z + 1/z is real, prove that either Im z = 0 or |z| = 1. 3.6 Write the following in polar form:

(a)
$$z - 2i$$
; (b) $z = -2 + 2i$.

3.7 Find and graph all the roots of:

(a)
$$z^3 - 1 = 0$$
; (b) $(i)^{1/3}$; (c) $\sqrt{-1}$; (d) $\sqrt{3+4i}$.

3.8 In polar coordinates, show that the Cauchy-Riemann conditions become

$$\frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial v}{\partial \theta} \quad \text{and} \quad \frac{1}{r} \frac{\partial u}{\partial \theta} = -\frac{\partial v}{\partial r}.$$

3.9 Show that the following are analytic functions of z:

(a)
$$e^{z}$$
; (b) e^{iz} ; (c) e^{-iz} .

3.10 If $f(z) = u(x, y) + iv(x, y) = z^2 + 3z + 4$, find u and v. 3.11 Show that the following functions are harmonic and find the corresponding conjugate function:

(a)
$$u = x^3 - 3xy^2 + 3x - 3y$$
 (b) $v = 2xy + 3y$
(c) $u = x^3 - 3xy^2$ (c) $u = e^x \cos y$.

3.12 Find A and B so that $x^2 + Axy + By^2$ is a harmonic function.

3.13 By use of the curl theorem in two dimensions, prove the Cauchy integral theorem. 3.14 Suppose the position of a particle, moving in a plane, is represented by $z = re^{i\theta}$. (a) From the expression of the complex velocity of the particle, identify the radial and tangential components. (b) From the expression for the complex acceleration, identify the tangential, centripetal, radial, and Coriolis components.

3.15 Show that the sum, s, of n terms of a geometric series is given by

$$s = \frac{a(1-r^n)}{1-r}$$

where a is the first term and r is the common ratio. 3.16 Find the radius of convergence of the power series

$$\sum_{r=0}^{\infty} \frac{z^r}{r!}.$$

3.17 Find the radius of convergence of

$$\sum_{n=0}^{\infty} z^n.$$

3.18 Find the radius of convergence of

$$\sum_{n=0}^{\infty} n! z^n.$$

3.19 Show that

$$\sum_{n=0}^{\infty} c_n z^n$$

and its derivative have the same radius of convergence.

3.20 Develop the Taylor expansion and find the radius of convergence for: (a) $\ln z$ about $z_0 = 1$; (b) $\ln (1 + z)$ about $z_0 = 0$; and (c) 1/(1 - z) about $z_0 = -i$. 3.21 Develop the Laurent expansion for:

(a)
$$\frac{1}{z(1-z)^2}$$
 about $z_0 = 0, 1$; (b) $\frac{e^z}{(z-2)^3}$ about $z_0 = 3$
(c) $\frac{1}{(z-1)(z-2)}$.

Hint for part (c): Use the method of partial fractions and develop the expansion in the region |z| < 1.

3.22 Evaluate (select a convenient path) the following:

(a)
$$\int_{(0,0)}^{(1,1)} z^* dz$$
; (b) $\oint \frac{dz}{z}$; (c) $\oint \frac{dz}{z^2}$

3.23(a) Show that

$$\int_{z_0}^z dz = \frac{z^{n+1} - z_0^{n+1}}{n+1}$$

for all n except n = -1. (b) Discuss the case for n = -1. 3.24 Show that

$$\frac{1}{2\pi i}\oint_C z^{m-n-1}dz = \delta_{m,n}.$$

3.9 Appendix: Series

3.9.1 Introduction

In this appendix, we summarize the essentials of infinite series without detailed proofs since proofs may be found in standard treatments of infinite series.

Infinite sequences and series are important in mathematical physics. Let $w_1, w_2, \ldots, w_n, \ldots$ be a sequence of numbers (real or complex). If

$$s = \lim_{k \to \infty} s^k = \lim_{k \to \infty} \sum_{n=1}^{k} w_n,$$

then the series $\sum_{n=1}^{\infty} w_n$ is said to be **convergent**. The number s is called the **sum** (or **value**) of the series and is given by

$$s = a + ib$$
 where $a = \sum_{n=1}^{\infty} u_n$ and $b = \sum_{n=1}^{\infty} v_n$ for $w_n = u_n + iv_n$.

If the series

$$\sum_{n=1}^{\infty} |w_n| = |w_1| + |w_2| + \cdots$$

is convergent, then $\sum_{n=1}^{\infty} w_n$ is said to be **absolutely convergent**. If $\sum_{n=1}^{\infty} w_n$ is convergent but $\sum_{n=1}^{\infty} |w_n|$ diverges, then $\sum_{n=1}^{\infty} w_n$ is said to be **conditionally convergent**.

3.9.2 Simple Convergence Tests

Comparison Test: If $\sum_{n} a_n$ is a convergent series and $u_n \leq a_n$ for all n, then $\sum_{n} u_n$ is a convergent series.

If $\sum_n b_n$ is a divergent series and $v_n \ge b_n$ for all n, then $\sum_n v_n$ is also a divergent series.

Ratio Test: Consider the series $\sum_{n} a_n$. If

$$\lim_{n \to \infty} \left(\frac{a_{n+1}}{a_n} \right) \begin{cases} < 1, \text{ then the series converges absolutely.} \\ > 1, \text{ then the series diverges.} \\ = 1, \text{ then the test is indeterminate.} \end{cases}$$

Limit Test: If

$$\lim_{n \to \infty} a_n \neq 0, \quad \text{then} \quad \sum_n a_n \quad \text{is divergent.}$$

Cauchy Root Test: Let

$$\alpha = \lim_{n \to \infty} \left| a_n \right|^{1/n}.$$

If

 $\alpha \left\{ \begin{array}{ll} <1, \ \ {\rm then \ the \ series \ converges}.\\ >1, \ \ {\rm then \ the \ series \ diverges}. \end{array} \right.$

The Gauss Test: If

$$\left|\frac{a_{n+1}}{a_n}\right| = 1 - \frac{h}{n} + \frac{B_n}{n^q}$$
 where $q > 1$ and

the sequence $\{B_n\}$ is bounded, then the series converges for n > 1.

3.9.3 Some Important Series in Mathematical Physics

Geometric Series The sequence

$$s_n = 1 + z + z^2 + \dots + z^{n-1}$$

is called a **geometric sequence**. On multiplying this sequence by z and subtracting the resulting sequence zs_n from s_n , we obtain

$$(1-z)s_n = 1 - z^n$$
 or $s_n = \frac{1-z^n}{1-z}$ $(z \neq 1).)$

The corresponding infinite geometric series converges, for |z| < 1, to

τ

$$\lim_{n \to \infty} s_n = \sum_{n=0}^{\infty} z^n = \frac{1}{1-z} \quad (|z| < 1).$$

The region |z| < 1 is called the **circle of convergence** of the infinite geometric series.

Series of Functions Consider

$$s_n(z) = U_1(z) + U_2(z) + \dots + U_n(z)$$

and

$$f(z) = \lim_{n \to \infty} s_n(z) = \sum_{n=1}^{\infty} U_n(z).$$

 \mathbf{If}

$$|f(z) - s_n(z)| < \epsilon$$
 (for all $n \ge N$)

where N is independent of z in the region $a \leq |z| \leq b$ and ϵ is an arbitrarily small quantity greater than zero, then the series $s_n(z)$ is said to be **uniformly convergent** in the closed region $a \leq |z| \leq b$.

If the individual terms, $U_n(z)$, of a uniformly convergent series are continuous, the series may be integrated term by term, and the resultant series will always be convergent. Thus

$$\int_a^b f(z)dz = \int_a^b \sum_{n=1}^\infty U_n(z)dz = \sum_{n=1}^\infty \int_a^b U_n(z)dz$$

The derivative of f(z),

$$\frac{df(z)}{dz} = \frac{d}{dz} \sum_{n=1}^{\infty} U_n(z),$$

equals

$$\sum_{n=1}^{\infty} \frac{dU_n}{dz}$$

only if

$$U_n(z)$$
 and $rac{dU_n}{dz}$

are continuous in the region and

$$\sum_{n=1}^{\infty}rac{dU_n}{dz}$$

is uniformly convergent in the region.

The Taylor Series Two equivalent forms for the Taylor expansion of a function f(x) about x = a may be written as follows:

Form 1:

$$f(x) = \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!} f^{(n)}(a) \text{ where } f^{(n)}(a) = \left. \frac{d^n f(x)}{dx^n} \right|_{x=a}$$

and

Form 2:

$$f(x+a) = \sum_{n=0}^{\infty} \frac{x^n}{n!} f^{(n)}(a).$$

The Taylor expansion of a function f(x, y) may be written in the following forms: Form 1:

$$f(x,y) = f(a,b) + (x-a)f_x(a,b) + (y-b)f_y(a,b) + \frac{1}{2!} \left[(x-a)^2 f_{xx}(a,b) + 2(x-a)(y-b)f_{xy}(a,b) + (y-b)^2 f_{yy} \right] + \cdots$$

and

Form 2:

$$f(x + a, y + b) = f(a, b) + xf_x(a, b) + yf_y(a, b) + \frac{1}{2!} \left[x^2 f_{xx}(a, b) + 2xy f_{xy}(a, b) + y^2 f_{yy}(a, b) \right] + \cdots$$

Chapter 4

Calculus of Residues

4.1 Isolated Singular Points

Points at which the function f(z) is not analytic are called **singular points** (also called **singularities**). If f(z) is analytic throughout the neighborhood of a point z_0 , $|z - z_0| < \epsilon$, but is not analytic at z_0 , then the point z_0 is called an **isolated singularity** of f(z). That is to say, the singularity at z_0 is isolated if a circle, containing no other singularities, can be drawn with z_0 as its center. By use of this definition, we see that z = 0 for f(z) = 1/z is an isolated singular point. The function $f(z) = 1/\sin(1/z)$ has an isolated singularity when $z = 1/(n\pi)$ for n = 1, 2, The origin where z = 0, however, is not an isolated singular point since every neighborhood contains other singular points (an infinite number) as a result of $z = 1/(n\pi)$. In other words, the singularities from $z = 1/(n\pi)$ for $n \to \infty$ are arbitrarily close to the origin (z = 0).

The Laurent expansion of f(z) with an isolated singularity at z_0 is given by

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \sum_{n'=1}^{\infty} \frac{b_{n'}}{(z - z_0)^{n'}}.$$
 (3.16')

As mentioned in derivation of the Laurent expansion, the above expansion converges for $r_2 < |z - z_0| < r_1$ where r_1 is the radius of C_1 and r_2 is the radius of C_2 in Fig. 3.9. A singular point, z_0 , of the analytic part of the Laurent expansion is called a **removable** singularity since $f_A(z)$ may be redefined as follows so that $f_A(z)$ becomes analytic at $z = z_0$:

$$a_0 = \lim_{z \to z_0} f_A(z).$$

The importance of singularities of this type is not great in mathematical physics. Singularities of $f_P(z)$, however, are of immense importance in the mathematical analysis of physical problems.

If $b_m \neq 0$ but $b_{m+1} = b_{m+2} = \cdots 0$ in the principal part of the Laurent expansion of f(z), then $f_P(z)$ becomes (see Eq.3.16' above)

$$f_P(z) = \frac{b_1}{z - z_0} + \dots + \frac{b_m}{(z - z_0)^m}$$
$$= \sum_{n'=1}^m \frac{b_{n'}}{(z - z_0)^{n'}}.$$

Analytic Methods in Physics. Charlie Harper Copyright © 1999 WILEY-VCH Verlag Berlin GmbH, Berlin ISBN: 3-527-40216-0 In the above equation, f(z) is said to have a **pole of order** m at $z = z_0$. When m = 1, the singularity at $z = z_0$ is called a simple pole.

Example 40 Find the pole and its order for

$$f(z) = \frac{\sin z}{z^4}.$$

Solution :

$$f(z) = \frac{\sin z}{z^4}$$

= $\frac{z - z^3/3! + z^5/5! - z^7/7! + \cdots}{z^4}$
= $\frac{1}{z^3} - \frac{1}{3!} \frac{1}{z} + \frac{z}{5!} - \frac{z^3}{7!} + \cdots$

In this example, we see that f(z) has a 3rd-order pole at z = 0.

The function f(z) is said to have an essential singularity (pole of infinite order) at $z = z_0$ if there exists no m such that $b_s = 0$ for all s > m. That is to say, $f_P(z)$ contains an infinite number of terms when $z = z_0$ is an essential singularity. The peculiar behavior of the function f(z) in the neighborhood of an essential singularity is revealed by a theorem due to Picard¹, often called the Weierstrass²-Casorati³ theorem. This theorem states that the function f(z) oscillates so rapidly in the neighborhood of an essential singularity that it comes arbitrarily close to any possible complex number. In symbolic form, we write

$$|f(z) - g| < \epsilon \quad \text{(for } |z - z_0| < \delta\text{)}$$

where ϵ and δ are arbitrary positive numbers and g is an arbitrary complex number. We restrict our discussion of analytic functions to this limited information concerning the behavior of functions in the vicinity of an essential singularity.

Example 41 Classify the singularity of the function

$$f(z) = z \exp \frac{1}{z}.$$

Solution :

$$f(z) = z \sum_{n=0}^{\infty} \frac{(1/z)^n}{n!}$$

= $z \left(1 + \frac{1}{z} + \frac{1}{2!z^2} + \cdots \right)$
= $z + 1 + \frac{1}{2!z} + \frac{1}{3!z^2} + \cdots$

There is an essential singularity at z = 0.

¹Charles Émile Picard (1856–1941), French mathematician whose study of the integrals attached to algebraic surfaces and related topological questions constituted an important part of algebraic geometry.

 $^{^{2}}$ Karl Theodor Wilhelm Weierstrass (1815–1897), German mathematician who is best known for his construction of the theory of complex functions by use of power series.

³Felic Casorati (1835–1890), Italian mathematician who worked in complex variable theory and is best known for the Weierstrass-Casorati theorem.

A fourth kind of singularity, **branch point**, which results from the consideration of multivalued functions (fractional powers in the Laurent expansion) will be treated in the Section 4.8 on multi-valued functions.

4.2 Evaluation of Residues

4.2.1 *m*-th-Order Pole

The Laurent expansion of f(z), Eq.(3.19), for the case of a pole of order m becomes

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \frac{a_{-1}}{z - z_0} + \dots + \frac{a_{-m}}{(z - z_0)^m}.$$
(4.1)

The residue of f(z) at $z = z_0$, Eq.(3.21), is given by

$$a_{-1} = \frac{1}{2\pi i} \oint_C f(z) dz.$$
 (4.2)

In the above equation, C encloses z_0 . Except for the numerical factor $2\pi i$, the residue of f(z) is the value the integral of f(z) over C. In those cases where the residue a_{-1} can be determined directly (without carrying out the integration), we would have a method of evaluating the definite integral of over C indirectly. We now develop important expressions for evaluating a_{-1} directly.

On multiplying Eq.(4.1) by $(z - z_0)^m$, we obtain

$$\phi(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^{m+n} + \sum_{n=1}^{m} a_{-n} (z - z_0)^{m-n}$$

= $a_0 (z - z_0)^m + a_1 (z - z_0)^{m+1} + \cdots$
+ $a_{-1} (z - z_0)^{m-1} + a_{-2} (z - z_0)^{m-2} + \cdots + a_{-m}.$ (4.3)

The function $\phi(z)$ on the right-hand side of Eq.(4.3) is given by

$$\phi(z) = (z - z_0)^m f(z).$$

For minimum m, we require that $\phi(z_0)$ be analytic and not equal zero. Since $\phi(z)$ is analytic at $z = z_0$, Eq.(4.3) may be thought of as the Taylor expansion of $\phi(z)$ about $z = z_0$. The coefficient a_{-1} in this expansion must be the coefficient of the $(z - z_0)^{m-1}$ term. Thus, the general equation for calculating a residue is given by

$$a_{-1} = \frac{1}{(m-1)!} \left. \frac{d^{m-1}\phi(z)}{dz^{m-1}} \right|_{z \to z_0}.$$
(4.4)

4.2.2 Simple Pole

For a simple pole (m = 1) at $z = z_0$, the residue, Eq.(4.4), of f(z) reduces to

$$a_{-1} = \lim_{z \to z_0} (z - z_0) f(z).$$

In this connection, suppose the function f(z) can be represented by

$$f(z) = \frac{g(z)}{h(z)}$$

where g(z) and h(z) are analytic functions. If $g(z_0) \neq 0$, $h(z_0) = 0$, but $h'(z_0) \neq 0$, then h(z) has a simple zero at $z = z_0$, and f(z) has a simple pole at $z = z_0$. The residue of f(z) at $z = z_0$ is given by

$$a_{-1} = \lim_{z \to z_0} \left[\frac{g(z)(z - z_0)}{h(z)} \right] = \lim_{z \to z_0} g(z) \lim_{z \to z_0} \left[\frac{z - z_0}{h(z) - h(z_0)} \right] = \frac{g(z_0)}{h'(z_0)}.$$

The above expression for the residue when m = 1 is extremely useful. The procedure for evaluating the residue of a function f(z) at $z = z_0$ may be summarized as follows.

1. The general expression for a_{-1} is

$$a_{-1} = \frac{1}{(m-1)!} \left. \frac{d^{m-1}\phi(z)}{dz^{m-1}} \right|_{z \to z_0}$$

where $\phi(z) = (z - z_0)^m f(z)$ and $\phi(z_0)$ is analytic and not equal zero. The value of m is required before the general expression for a_{-1} can be used to evaluate the residue. The above conditions on $\phi(z)$ as z approaches z_0 may be used to determine the minimum value for m for a certain class of functions.

2. For a simple pole (m = 1), we have

$$a_{-1} = \lim_{z \to z_0} (z - z_0) f(z).$$

3. If f(z) = g(z)/h(z) (where g(z) and h(z) are analytic functions, $g(z_0) \neq 0$, $h(z_0) = 0$, but $h'(z_0) \neq 0$), then the residue is

$$a_{-1} = \frac{g(z_0)}{h'(z_0)}$$

4. If f(z) is such that its residue at $z = z_0$ cannot be obtained by use of the above procedures, then one must rewrite the function by (a) expanding the transcendental functions that may appear in f(z), (b) developing a geometric series for the function, or (c) developing the full Laurent expansion for the function. The classification and location of the singularities and the value of the residue can always be obtained from the full Laurent expansion for the function.

Example 42 Classify the singularities and calculate the residue for

$$f(z) = \frac{1}{z^2 - 1}.$$

Solution : We may rewrite the function as follows:

$$f(z) = \frac{1}{z^2 - 1} = \frac{1}{(z - 1)(z + 1)}.$$

There are poles at z = +1 and z = -1. To find m, we write

$$\phi(z)|_{z_0 \to +1} = (z-1)^m f(z) = (z-1)^m \cdot \frac{1}{(z-1)(z+1)} = \frac{1}{z+1}.$$

Hence z = +1 is a simple pole (m = 1) since $\phi(z)$ is analytic at z = +1 and $\phi(+1) \neq 0$. Similarly, we find that z = -1 is a simple pole. The residues at the two poles are given by

$$a_{-1} = \lim_{z \to +1} (z-1) \cdot \frac{1}{(z-1)(z+1)} = \frac{1}{2}$$

and

$$a_{-1} = \lim_{z \to -1} (z+1) \cdot \frac{1}{(z-1)(z+1)} = -\frac{1}{2}$$

Example 43 Classify the singularities and calculate the residue for

$$f(z) = \frac{1}{(z^2 + a^2)^2}$$
 (where $a > 0$).

Solution : We may rewrite the function in the following form:

$$f(z) = \frac{1}{(z^2 + a^2)^2} = \frac{1}{(z + ia)^2(z - ia)^2}.$$

There are poles at z = ia and z = -ia. To find m, we write

$$\phi(z)|_{z \to z_0} = (z - ia)^m \cdot \frac{1}{(z + ia)^2 (z - ia)^2} = \frac{1}{(z + ia)^2}.$$

Hence z = ia is a second-order pole since $m = 2, \phi(z)$ is analytic at z = ia, and $\phi(ia) \neq 0$. Similarly, we find that z = -ia is a second-order pole. The two residues are

$$|a_{-1}|_{z \to ia} = \left. \frac{d\phi(z)}{dz} \right|_{z \to ia} = -\left. \frac{2}{(z+ia)^3} \right|_{z \to ia} = \frac{1}{4ia^3}$$

and

$$a_{-1}|_{z \to -ia} = -\frac{1}{4ia^3}.$$

Example 44 Classify the singularities and calculate the residue for

$$f(z) = rac{z^{-k}}{z+1}$$
 (where $0 < k < 1$).

Solution : Note that there is a pole at z = -1 and a branch point at z = 0. To find m, we write

$$\phi(z)|_{z \to z_0} = (z+1)^m \cdot \frac{1}{z^k(z+1)} = \frac{1}{z^k}.$$

Hence z = -1 is a simple pole since $m = 1, \phi(-1)$ is analytic, and $\phi(-1) \neq 0$. The residue is

$$a_{-1} = \lim_{z \to -1} \left[(z+1) \cdot \frac{1}{z^k (z+1)} \right] = e^{-ik\pi}.$$

Example 45 Classify the singularities and calculate the residue for

$$f(z) = \frac{A(z)}{\sin z}$$

where A(z) is analytic and contains no zeros.

Solution: Let $h(z) = \sin z$. Since $h(\pm k\pi) = 0$ but $h'(\pm k\pi) \neq 0$, the zeros of h(z) at $z = \pm k\pi$ are simple zeros; hence, the poles of the function f(z) at $z = \pm k\pi$ are simple poles. The residue is

$$a_{-1} = \frac{A(z)}{h'(z)}\Big|_{z \to \pm k\pi} = \frac{A(z)}{\cos z}\Big|_{z \to \pm k\pi} = \frac{A(\pm i\pi)}{\cos k\pi} = \frac{A(\pm k\pi)}{(-1)^k} \quad (k = 0, 1, 2, \dots)$$

Example 46 Classify the singularities and calculate the residue for

$$f(z) = \frac{\sin z}{z^4}.$$

Solution : Since there is a zero in the numerator of f(z) for z = 0, it is not clear from the use of the general expression for a_{-1} where (and to what order) the poles are located. To resolve the problem, we expand sinz and obtain

$$f(z) = \frac{1}{z^4} \left(z - \frac{z^3}{3!} + \frac{z^5}{5!} - \frac{z^7}{7!} + \cdots \right)$$
$$= \frac{1}{z^3} - \frac{1}{3!z} + \frac{z}{5!} - \frac{z^3}{7!} + \cdots .$$

The above equation is the Laurent expansion for f(z) about $z_0 = 0$. From this expansion, we observe that z = 0 is a third-order pole with residue given by

$$a_{-1} = -\frac{1}{3}.$$

Example 47 Determine the residue for the function in Example 40.

$$f(z) = z \exp \frac{1}{z}.$$

Solution : By use of the expansion in Example 40, we note that the residue of f(z) equals 1/2.

4.3 The Cauchy Residue Theorem

The Cauchy Residue Theorem If the function f(z) is analytic within and on a closed region Γ (except at a finite number of isolated singular points within Γ), then

$$\oint_{\Gamma} f(z)dz = 2\pi i \sum_{j=1}^{n} \text{Res(enclosed residues)}$$
$$= 2\pi i \sum_{j=1}^{n} a_{-1z_j}$$
(4.5)

where $z_j (j = 1, 2, ..., n)$ are the enclosed singular points and a_{-1z_j} are the corresponding residues.



Proof: Applying Cauchy's integral theorem in Fig. 4.1, we obtain

$$\oint_{\Gamma} f(z)dz - \oint_{C_1} f(z)dz - \cdots - \oint_{C_j} f(z)dz = 0.$$

The value of the circular integral around an isolated singular point (see Eq.(4.1)) is $2\pi i a_{-1}$. Hence the above equation becomes

$$\oint_{\Gamma} f(z)dz = 2\pi i \left(a_{-1z_1} + a_{-1z_2} + \dots + a_{-1z_n} \right)$$
$$= 2\pi i \sum_{j=1}^{n} a_{-1z_j}.$$

Thus, Cauchy's residue theorem is established. We will use this theorem below to evaluate certain classes of definite integrals.

4.4 The Cauchy Principal Value

Thus far, we have considered contours that enclose and/or exclude singularities. Now, we consider the case where the path of integration passes through a singularity of the integrand. In a strict sense, this integral does not exits, and we must choose a path that circumvents the singularity. Since many physical problems involve the evaluation of integrals in which an isolated simple pole is on the contour of integration, it is useful to consider the details of dealing with this situation. We deform the contour to include or exclude the simple pole with a semicircular of infinitesimal radius as shown in Fig. 4.2.



Figure 4.2:

Counterclockwise and clockwise integrations over the dashed semicircles yield $\pi i a_{-1}$ and $-\pi i a_{-1}$, respectively. On using the residue theorem in Fig. 4.2(a) and noting that the simple pole is now enclosed, we obtain

$$\oint_{\Gamma} f(z)dz + \pi i a_{-1} = 2\pi i a_{-1} \quad \text{or} \quad \oint_{\Gamma} f(z)dz = \pi i a_{-1}.$$

Using the residue theorem in Fig. 4.2(b) and noting that the simple pole is not enclosed, we obtain

$$\oint_{\Gamma} f(z)dz - \pi i a_{-1} = 0 \quad \text{or} \quad \oint_{\Gamma} f(z)dz = \pi i a_{-1}.$$

The net result for Fig. 4.2(a) or Fig. 4.2(b) is that a simple pole on the contour counts one-half of what it would if it were within the contour, the **Cauchy principal value**.

For the case of a simple pole on the real axis, it is useful to express the result in terms of the Cauchy principal value of an integral. The integral of a function f(x) which has a simple pole at $x = x_0$ for x_0 within the closed interval [a, b] may be written as

$$\int_{a}^{b} f(x)dx = \lim_{\epsilon \to 0} \left[\int_{a}^{x_{0}-\epsilon} f(x)dx + \int_{x_{0}+\epsilon}^{b} f(x)dx \right]$$
$$\equiv P \int_{a}^{b} f(x)dx.$$
(4.6)

In the above equation, P denotes the Cauchy principal value of the integral, and it means carry out the indicated limiting process. Note that

$$P\int_{-\infty}^{\infty}f(x)dx$$

may exist even if

$$\lim_{a \to \infty} \int_{-a}^{0} f(x) dx + \lim_{a \to \infty} \int_{0}^{a} f(x) dx$$

does not exist. For example,

$$\lim_{a \to \infty} \int_{-a}^{a} x dx = \lim_{a \to \infty} \left(\frac{a^2}{2} - \frac{a^2}{2} \right) = 0$$

but

$$\lim_{a\to\infty}\int_0^a xdx\to\infty.$$

We will return to the concept of Cauchy principal value of an integral in Section 4.6 on dispersion relations.

4.5 Evaluation of Definite Integrals

This Section is devoted to the evaluation of certain classes of definite integrals by use of the Cauchy residue theorem.

4.5.1 Integrals of the Form $\int_0^{2\pi} f(\sin\theta,\cos\theta)d\theta$

Consider the real integral

$$I_1 = \int_0^{2\pi} f(\sin\theta, \cos\theta) d\theta \tag{4.7}$$

where $f(\sin \theta, \cos \theta)$ is a rational function (which contains no isolated singularities other than poles) of $\sin \theta$ and/or $\cos \theta$. Let $z = e^{i\theta}$ (unit circle) where $d\theta = -idz/z$. For this case,

$$\sin \theta = \frac{e^{i\theta} - e^{-i\theta}}{2i} = \frac{z^2 - 1}{2iz}$$

and

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2} = \frac{z^2 + 1}{2z}.$$

In terms of z, Eq.(4.7) becomes

$$I_1 = -i \oint_{\substack{\text{unit}\\\text{circle}}} f\left(\frac{z^2 - 1}{2iz}, \frac{z^2 + 1}{2z}\right) \frac{dz}{z}.$$
(4.8)

The contour is a unit circle in the above equation. Applying the residue theorem in the above equation, the value of the integral in Eq.(4.8) becomes

$$I_1 = (-i)(2\pi i) \sum_{j=1}^n a_{-1z_j} = 2\pi \sum_{j=1}^n a_{-1z_j}.$$

Example 48 By use of the residue theorem, evaluate

$$I = \int_0^{2\pi} \frac{d\theta}{5 + 4\cos\theta}$$

Solution : Using Eq.(4.8), we obtain

$$I = -i \oint_{\substack{\text{unit}\\\text{circle}}} \frac{dz}{z \left\{ 5 + 4\left(\left(z^2 + 1 \right) / 2z \right) \right\}} = -i \oint_{\substack{\text{unit}\\\text{circle}}} \frac{dz}{(2z+1)(z+2)}.$$

There are singularities at z = -1/2 and z = -2. The singularity at z = -2 is outside the unit circle. At z = -1/2, there is a simple pole inside the unit circle since

$$\phi(z) = \left(z + \frac{1}{2}\right) \cdot \frac{1}{(2z+1)(z+2)}$$
$$= \frac{1}{2(z+2)} \quad \text{(for } m = 1\text{)}$$

and $\phi(-1/2)$ is analytic and is not equal zero. The residue of the enclosed singularity is

$$a_{-1}|_{z=-1/2} = \lim_{z \to -1/2} \phi(z) = \frac{1}{3}.$$

By use of the residue theorem, the value of the integral is

$$I = (-i)(2\pi i)\left(\frac{1}{3}\right) = \frac{2\pi}{3}$$

4.5.2 Integrals of the Form $\int_{-\infty}^{\infty} f(x) dx$

Consider definite integrals of the form

$$I_2 = \int_{-\infty}^{\infty} f(x) dx.$$
(4.9)

If f(z) (a) is analytic in the upper half-plane except for a finite number of poles and (b) has only simple poles on the real axis, and if (c) $zf(z) \to 0$ for all values of z as $|z| \to 0$ for $0 \le \arg z \le \pi$ where $z = \operatorname{Re}^{i\theta}$, then

$$I = \lim_{R \to \infty} \int_{-R}^{R} f(x) dx + \lim_{R \to \infty} \int_{0}^{\pi} f(\operatorname{Re}^{i\theta}) i \operatorname{Re}^{i\theta} d\theta$$
$$= \pi i \sum_{k=1}^{m} a_{-1x_{k}} + 2\pi i \sum_{j=1}^{n} a_{-z_{j}}.$$
(4.10)

The contour of integration in Eq.(4.10) is the real axis and the semicircle in the upper half-plane (see Fig. 4.3). The first term on the right-hand side of Eq.(4.10) results from simple poles on the real axis, and the second term results from enclosed singularities in the upper half-plane.



Figure 4.3:

Note that $|z|^2 = zz^* = R^2$; also, note that $f(\operatorname{Re}^{i\theta})i\operatorname{Re}^{i\theta} = if(z)z \to 0$ for $R = |z| \to \infty$ by use of condition (c) above. That is to say,

$$\lim_{R\to\infty}\int_0^{\pi} f(\operatorname{Re}^{i\theta})i\operatorname{Re}^{i\theta}d\theta\to 0.$$

Now, Eq. (4.10) reduces to Eq.(4.9), and the value of the integral becomes

$$I_2 = \int_{-\infty}^{\infty} f(x) dx = 2\pi i \sum_{j=1}^{n} a_{-1z_j} + \pi i \sum_{k=1}^{m} a_{-1x_k}.$$
(4.11)

Example 49 Using the residue theorem, evaluate

$$I = \int_{-\infty}^{\infty} \frac{dx}{1 + x^2}$$

Solution : By use of Eq.(4.11), we may write

$$I = \lim_{R \to \infty} \int_{-R}^{R} \frac{dx}{1+x^2} = \oint_{\substack{\text{semi} \\ \text{circle}}} \frac{dz}{1+z^2} = \oint_{\substack{\text{semi} \\ \text{circle}}} \frac{dz}{(z-i)(z+i)}.$$

Here there are singularities at z = -i and z = i. Note that z = -i is not within the semicircle in the upper-half plane. There is a simple pole at z = i since

$$\phi(z) = \frac{z-i}{(z-i)(z+i)}$$

where $\phi(i)$ is analytic and is not equal zero. The corresponding residue is

$$a_{-1} = \frac{1}{z+i}\Big|_{z=i} = \frac{1}{2i}.$$

Hence the required value of the integral is

$$I = \int_{-\infty}^{\infty} \frac{dx}{1 + x^2} = (2\pi i) \left(\frac{1}{2i}\right) = \pi.$$

4.5.3 A Digression on Jordan's Lemma

Let Γ be a semicircle of radius R in the upper half-plane, and let f(z) be a function satisfying the following conditions:

- 1. f(z) is analytic in the upper half-plane except for a finite number of enclosed isolated singularities and/or simple poles on the real axis and
- 2. $f(z) \to 0$ uniformly as $|z| \to \infty$ such that $|f(z)| \to 0$ for $|z| = R \to \infty$ where $|f(z)| \le M(R)$ and $0 \le \arg z \le \pi$.

In equation form, Jordan's⁴ lemma is

$$J = \lim_{R \to \infty} \int_{\Gamma} f(z) e^{imz} dz \to 0 \quad \text{(for } m > 0\text{)}.$$
(4.12)

Proof: For $z = \operatorname{Re}^{i\theta}$, we have

$$\left|e^{imz}\right| = \left|e^{imR(\cos\theta + i\sin\theta)}\right| = e^{-mR\sin\theta}$$

We may therefore write

$$\begin{split} |J| &= \left| \int_{\Gamma} f(z) e^{imz} dz \right| \\ &= \left| \int_{0}^{\pi} f(\operatorname{Re}^{i\theta)e^{imR(\cos\theta + i\sin\theta)}} i \operatorname{Re}^{i\theta} d\theta \right| \\ &\leq M(R) R \int_{0}^{\pi} e^{-mR\sin\theta} d\theta. \end{split}$$

In the range $0 \le \theta \le \pi/2$, we have $2\theta/\pi \le \sin \theta \le 0$ (see Problem 4.7) and may write

$$\int_0^{\pi} e^{-mR\sin\theta} d\theta = 2 \int_0^{\pi/2} e^{-mR\sin\theta} d\theta.$$

The above equation is valid since $\sin\theta$ is symmetric about $\theta = \pi/2$. We may therefore write the equation for |J| in the form

$$|J| \le 2M(R)R \int_0^{\pi/2} e^{-2m\theta/\pi} d\theta$$
$$= \frac{M(R)\pi}{m} (1 - e^{-mR}).$$

Hence, $|J| \to 0$ as $R \to \infty$ since $M(R) \to 0$ as $R \to \infty$, and the lemma is established.

 $^{^{4}}$ Marie Ennemond Camille Jordan (1838–1922), French mathematician who was highly regarded by his contemporaries for his work in algebra and group theory. Sophus Lie and Felix Klein were two of his students.

4.5.4 Integrals of the Form $\int_{-\infty}^{\infty} f(x)e^{imx}dx$

Consider integrals of the following (Fourier transform form) form such that the Jordan's lemma is valid

$$I_3 = \int_{-\infty}^{\infty} f(x)e^{imx}dx.$$
(4.13)

By use of Fig. 4.3, we obtain for this case

$$I = \int_{-\infty}^{\infty} f(x)e^{imx}dx + \lim_{R \to \infty} J = \pi i \sum_{k=1}^{p} a_{-1xk} + 2\pi i \sum_{j=1}^{n} a_{-1z_j}.$$

Applying Jordan's lemma to the above equation, we obtain

$$I_3 = \int_{-\infty}^{\infty} f(x)e^{imx}dx = 2\pi i \sum_{j=1}^n a_{-1z_j} + \pi i \sum_{k=1}^p a_{-1x_k}.$$
(4.14)

In Eq.(4.14), singularities in the upper half-plane leads to the first term, and simple poles on the real axis give rise to the second term. Equation (4.14) may be put in the following useful form:

$$\int_{-\infty}^{\infty} f(x)e^{imx}dx = 2\pi i \sum \operatorname{Res}\left\{f(z)e^{imz}\right\}.$$

On equating the real and imaginary parts on both sides of the above equation, we obtain

$$\int_{-\infty}^{\infty} f(x) \cos mx dx = -2\pi \sum \operatorname{ImRes} \left\{ f(z) e^{imz} \right\} -\pi \sum \operatorname{ImRes} \left\{ f(z) e^{imz} \right\}$$
(4.15)

and

$$\int_{-\infty}^{\infty} f(x) \sin mx dx = 2\pi \sum \operatorname{ReRes} \left\{ f(z) e^{imz} \right\} + \pi \sum \operatorname{ReRes} \left\{ f(z) e^{imz} \right\}.$$
(4.16)

The first sum in Eqs.(4.15 and 4.16) is over the enclosed poles, and the second sum is over simple poles on the x-axis.

Example 50 By use of the residue theorem, evaluate

$$I = \int_{-\infty}^{\infty} \frac{\sin x dx}{x}$$

Solution : On using Eq.(4.16), we write

$$I = \int_{-\infty}^{\infty} \frac{e^{iz}}{z} dz = 2\pi \sum \operatorname{Re} \operatorname{Res} \left\{ \frac{e^{iz}}{z} \right\} + \pi \sum \operatorname{Re} \operatorname{Res} \left\{ \frac{e^{iz}}{z} \right\}.$$

In the above equation, the first sum is over the enclosed poles and the second sum is over simple poles on the x-axis. There is a simple pole on the path at z = 0. The corresponding residue is

$$a_{-1}|_{z=0} = \lim_{z \to 0} (z-0)f(z) = \frac{ze^{iz}}{z}\Big|_{z=0} = 1.$$

The value of the integral is

$$I = \int_{-\infty}^{\infty} \frac{\sin x}{x} dx = \pi \sum \operatorname{Re} \operatorname{Re} \left\{ \frac{e^{iz}}{z} \right\} = \pi$$

4.6 Dispersion Relations

Dispersion relations (also known as spectral representations, Kronig-Kramers relations, and Hilbert transforms) result from the analytic properties of the complex representation of physical quantities and use of the Cauchy residue theorem. Originally, Kronig (1926) and Kramers (1927) were concerned with the dispersion of light and the relation between the real (i.e., dispersive) and imaginary (i.e., absorptive) parts of the index of refraction at different frequencies. The basic idea of dispersion relations is applied in areas of physics ranging from electronic design to quantum field theory. Here, general forms for dispersion relations will be presented. For physical quantity $\chi(\omega)$ which approaches zero as ω approaches infinity and is analytic in the upper-half plane (see Fig. 4.4), consider the evaluation of the integral

$$\oint_C \frac{\chi(\omega)d\omega}{\omega - \omega_0} \tag{4.17}$$

around the contour shown in Fig. 4.4. Equation (4.17) becomes

$$\begin{split} 0 &= \int_{-Q}^{\omega_0 - \delta} \frac{\chi(\omega) d\omega}{\omega - \omega_0} + \int_{\omega_0 + \delta}^{Q} \frac{\chi(\omega) d\omega}{\omega - \omega_0} \\ &+ \int_{\pi}^{0} \frac{\chi(\omega_0 + \delta e^{i\theta}) i \delta e^{i\theta} d\theta}{\delta e^{i\theta}} + \int_{0}^{\pi} \frac{\chi(Q e^{i\theta}) i Q e^{i\theta} d\theta}{Q e^{i\theta} - \omega_0}. \end{split}$$

Note that

$$\lim_{\delta \to 0} i \int_{\pi}^{0} \chi(\omega_0 + \delta e^{i\theta}) d\theta = -\pi i \chi(\omega_0).$$

Since χ represents a physical quantity, we require $\chi(\infty) \to 0$. Hence

$$\lim_{Q \to \infty} \int_0^{\pi} \frac{\chi(Qe^{i\theta})iQe^{i\theta}d\theta}{Qe^{i\theta} - \omega_0} \to 0.$$



For Eq. (4.17), we therefore obtain

$$\pi i \chi(\omega_0) = \lim_{\substack{Q \to \infty \\ \delta \to 0}} \left\{ \int_{-Q}^{\omega_0 - \delta} \frac{\chi(\omega) d\omega}{\omega - \omega_0} + \int_{\omega_0 + \delta}^{Q} \frac{\chi(\omega) d\omega}{\omega - \omega_0} \right\}$$
$$= \lim_{\substack{Q \to \infty \\ Q \to \infty}} \left\{ \int_{-Q}^{\omega_0} \frac{\chi(\omega) d\omega}{\omega - \omega_0} + \int_{\omega_0}^{Q} \frac{\chi(\omega) d\omega}{\omega - \omega_0} \right\}$$
$$= \lim_{\substack{Q \to \infty \\ -\infty}} \int_{-Q}^{\infty} \frac{\chi(\omega) d\omega}{\omega - \omega_0}.$$
(4.18)

The P in front of the last integral in Eq.(4.18) means the Cauchy principal value of the integral. Equation (4.18) may be rewritten as

$$-\chi(\omega_0) = \frac{i}{\pi} P \int_{-\infty}^{\infty} \frac{\chi(\omega) d\omega}{\omega - \omega_0}.$$
(4.19)

On substituting

$$\chi(\omega_0) = U(\omega_0) + iV(\omega_0)$$
 and $\chi(\omega) = U(\omega) + iV(\omega)$

into Eq.(4.19), we obtain

$$U(\omega_0) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{V(\omega) d\omega}{\omega - \omega_0}$$
(4.20)

and

$$V(\omega_0) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{U(\omega)d\omega}{\omega - \omega_0}.$$
(4.21)

Equations (4.20 and 4.21) express one part of an analytic function in terms of an integral involving the other part. In mathematics, the functions U and V are referred to as the **Hilbert transforms** of one another. In physics, these equations are usually written as

$$\operatorname{Re}\chi(\omega_0) = \frac{1}{\pi}P \int_{-\infty}^{\infty} \frac{\operatorname{Im}\chi(\omega)d\omega}{\omega - \omega_0}$$
(4.22)

and

$$\operatorname{Im} \chi(\omega_0) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\operatorname{Re} \chi(\omega) d\omega}{\omega - \omega_0}.$$
(4.23)

Equations (4.22 and 4.23) are called dispersion relations. In electronics, one has

$$Z(\omega) = R(\omega) + i\chi(\omega).$$

In the above equation, Z is impedance, R is resistance, and χ is reactance. Dispersion relations may be used to express resistance in terms of reactance. Dispersion relations for light (complex index of refraction $\eta = \eta_c + ia\alpha$) yield relations between dispersive power and absorption. In addition, a large number of definite integrals may be evaluated by use of the dispersion relations. Dispersion relations applied to $f(z) = \cos x + i \sin x$ lead to values of integrals with integrands of forms $(\sin x)/x$ and $(\cos x)/x$ for limits of integration from minus infinity to plus infinity.

4.7 Conformal Transformations

An analytic function f(z) = u(x, y) + iv(x, y) for z = x + iy is completely characterized by two pairs of variables (x, y) and (u, v). Hence, a four-dimensional space is needed to plot the real values x, y, u, and v. The mathematical subject of quaternions was developed by Hamilton and Frobenius to treat such systems. Limited applications of quaternions in quantum mechanics and in certain other areas of physics have been made in recent years, but it is not a widely discussed subject in mathematical physics.

Riemann developed a widely used mode of visualizing the relation w = f(z) which uses two separate complex planes, z-plane for (x, y) and w-plane for the corresponding (u, v). By use of the two-plane picture, the equation w = f(z) defines the transformation (relation, correspondence, or mapping) between the two planes. That is to say, w = f(z) may be viewed as the mapping a set of points (locus, figure) in the z-plane into the corresponding figure in the w-plane. For physical problems, the basic idea involves (a) transforming the geometry of a complicated problem in the z-plane into a simpler geometry in the w-plane, (b) solving the problem with the simpler geometry, and (c) inverting the transformations to obtain the desired solution in the z-plane. The most important class of transformations used in solving physical problems are those that preserve the angle between two straight lines (conformal transformations). The angle preserving property of conformal transformations will be illustrated as follows:

1. Assume two lines intersect at z = a in the z-plane and at w = f(a) in the w-plane with elements of length along two lines given, respectively, by

$$dz_1 = |dz_1| \exp(i\theta_1)$$
 and $dz_2 = |dz_2| \exp(i\theta_2)$.

2. The corresponding respective elements of length in the w-plane are

$$dw_1 = |dz_1| |f'(z)| \exp i(\phi + \theta_1)$$
 and $dw_2 = |dz_2| |f'(z)| \exp i(\phi + \theta_2)$

since

$$dw = dz |f'(z)| \exp(i\phi).$$

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3. Note that the direction of the corresponding lines in the *w*-plane is rotated by ϕ , but the angle between the lines in the *z*-plane $(\theta_2 - \theta_1)$ equals the angle between the lines in the *w*-plane $[(\phi + \theta_2) - (\phi + \theta_1)]$.

Now, we show the above analytically. On differentiating w with respect to z, we obtain

$$\lim_{\Delta z \to 0} \left(\frac{\Delta w}{\Delta z} \right) = \frac{dw}{dz} = f'(z) = a e^{i\alpha}$$
(4.24)

where

$$a = |f'(z)| \neq \begin{cases} \infty \\ 0. \end{cases}$$

Note that

$$\arg\left\{\lim_{\Delta z \to 0} \left(\frac{\Delta w}{\Delta z}\right)\right\} = \arg f'(z) = \lim_{\Delta z \to 0} \left\{\arg\left(\frac{\Delta w}{\Delta z}\right)\right\}$$
$$\lim_{\Delta z \to 0} (\arg \Delta w) - \lim_{\Delta z \to 0} (\arg \Delta z).$$

We may therefore write

$$\alpha = \phi_w - \phi_z$$

since

$$\arg f'(z) = \alpha = \lim_{\Delta z \to 0} (\arg \Delta w) - \lim_{\Delta z \to 0} (\arg \Delta z).$$

Thus, any line oriented at θ_z in the z-plane is rotated through α in the w-plane (see Fig. 4.5).



Figure 4.5

The angle between two lines ℓ_1 and ℓ_2 gives rise to

$$\phi_2 - \phi_1 = \theta_2 - \theta_1$$

Hence the angle is preserved under an analytic transformation; this is referred to as a conformal transformation (mapping). On taking the modulus of both sides of Eq.(4.24), we obtain

$$|dw| = \left|ae^{i\alpha}dz\right| = a\left|dz\right|.$$

The above equation shows that an infinitesimal arc of Γ_w is *a* times the corresponding arc Γ_z (magnification).

Example 51 Translation Consider the transformation $w = z + z_0$. In terms of x and y, we have

$$w = (x + iy) + (x_0 + iy_0) = (x + x_0) + i(y + y_0)$$

or (see Fig. 4.6)

$$u = x + x_0$$
 and $v = y + y_0$.



Figure 4.6

Example 52 Rotation Consider the transformation $w = z_0 z$ where $z = re^{i\theta}, z_0 = r_0 e^{i\theta}$, and $w = \rho e^{i\phi}$. Here we may write

$$w = \rho e^{i\phi} = r_0 r e^{i(\theta + \phi)}.$$

Note that $\phi = \theta + \theta_0$ where θ_0 is the angle of rotation and r_0 is the corresponding modification of r ($\rho = r_0 r$).

Example 53 Inversion Consider the transformation w = 1/z, where $z = re^{i\theta}$ and $w = \rho e^{i\phi}$. The quantity w becomes

$$w = \rho e^{i\phi} = \frac{1}{\rho} e^{-i\theta}.$$

In this case, we have $\rho = 1/r$ and $\phi = -\theta$.

Now we develop a scheme for transforming a locus (set of points) in the z-plane into the corresponding locus in the w-plane by inversion. Note that

$$w = u + iv = \frac{1}{z} = \frac{1}{x + iy} = \frac{x - iy}{x^2 + y^2}$$

In this case, we have

$$u = \frac{x}{x^2 + y^2}; \qquad x = \frac{u}{u^2 + v^2}; v = -\frac{y}{x^2 + y^2}; \quad y = -\frac{v}{u^2 + v^2}$$

Example 54 By use of inversion, transform the equation of a circle centered at the origin in the z-plane, $x^2 + y^2 = r^2$, into the corresponding locus in the w-plane.

Solution: : In this example, we obtain

$$\frac{u^2}{(u^2+v^2)^2} + \frac{v^2}{(u^2+v^2)^2} = r^2 \quad \text{or} \quad u^2+v^2 = r^2(u^2+v^2)^2 = \rho^2$$

since $u + iv = \rho e^{i\phi}$, $\rho^2 = u^2 + v^2$, and $\rho = 1/r$. The equation, $u^2 + v^2 = \rho^2$, is that of a circle in the *w*-plane centered at the origin with radius ρ . It is interesting to note that the interior points of the *z*-plane circle are exterior points of the *w*-plane circle.

Example 55 By use of inversion, transform the horizontal line y = c into the corresponding locus in the w-plane.

Solution : Here we have

$$y = c = -\frac{v}{u^2 + v^2}.$$

Simplifying the above equation, we obtain

$$cu^{2} + cv^{2} + v = 0$$
 or $(u - 0)^{2} + \left(v + \frac{1}{2c}\right)^{2} = \left(\frac{1}{2c}\right)^{2}$.

The last equation is that of a circle centered at (0, -1/2c) with radius 1/2c in the w-plane (see Fig. 4.7).



4.8 Multi-valued Functions

In addition to the above transformations, the following transformation is useful in physical applications: $w = z^2$ which yields $w = \rho \exp(i\phi) = r^2 \exp(i2\theta)$ or $\rho = r^2$ and $\phi = 2\theta$ with transformation equations given by $u = x^2 - y^2$ and v = 2xy. Here one finds that a circle with radius r_0 is mapped into a corresponding circle with radius $R = r_0^2$, and θ_0 is

mapped into $2\theta_0$. In potential theory, the two-dimensional Laplace equation is to be solved with appropriate boundary conditions. Note that the transformation $w = z^2$ maps the right angle in the z-plane into a straight line in the w-plane (see Fig. 4.8) where boundary conditions may be applied more conveniently.

In connection with the transformation $w = z^2$ (and other multi-valued functions), note that the transformation is conformal except at w = 0, and it, separately, maps the upper- and lower-half planes of the z-plane into the whole w-plane (Points z and -z are mapped into the same points in the w-plane.). The inverse transformation $z = \sqrt{w}$ cannot be unique. By use of the de Moivre theorem, the quantity z may be written as

$$z = \sqrt{\rho} \exp\left(i\frac{\phi}{2}\right) = \sqrt{\rho} \exp\left(i\frac{\phi_p}{2} + i\pi k\right), \quad k = 0, 1, \dots, n-1.$$
(4.25)

Note that z has many values for each w; if $0 \le \phi < 2\pi$, then z has only one value for each w, and this value for z is called a **branch** of z. In this case, there are two branches (k = 0, principal branch, and k = 1, second branch). In general, the collection of all branches is referred to as a multi-valued function.



Figure 4.8

Note that the two values of k in Eq.(4.25) yield opposite signs for z. In describing values of a unit circle about the origin in the z-plane for k = 0, it is found that (a) z = 1 for $\phi_p = 0$ and (b) z = -1 when $\phi_p = 2\pi$. When k = 1, the values become the opposite (a) z = -1 when $\phi_p = 0$ and (b) z = 1 when $\phi_p = 2\pi$. One may avoid these double values by assuming a cut (called a **branch cut**), which may not be crossed, exists from 0 to ∞ along the *u*-axis in the *w*-plane. A point which cannot be encircled without crossing a branch cut is called a **branch point**. In this case, the origin w = 0 is a branch point. Riemann introduced the scheme of two cut planes (sheets, surfaces) joined edge to edge at the cut as a way to combine both branches and to eliminate the cut. For example, a lower sheet contains the set of values for k equals zero and an upper sheet contains the values for k equals unity (see Fig. 4.9).

The function \sqrt{w} is analytic over the whole Riemann surface (two sheets) except at the branch point, w equals zero. In summary, it is found that the *w*-plane is mapped into two sheets (Riemann surfaces). The concept of Riemann surfaces has broad application in physics.



Figure 4.9

Example 56 The value of the following integral is important in many physics problems. Show that

$$\int_0^\infty \frac{x^{a-1} dx}{1+x} = \frac{\pi}{\sin a\pi} \quad 0 < a < 1.$$

Solution : Consider the following integral

$$I = \oint_C \frac{z^{a-1}dz}{1+z}.$$



Figure 4.10

Note that the integrand of I is single-valued since the contour (see Fig. 4.10) does not include the branch point of z^{a-1} , and there is a simple pole at z = -1 within the contour. By use of the residue theorem, the value of I is

$$I = \oint_C \frac{z^{a-1}dz}{1+z} = \int_{\Gamma} + \int_{\gamma} + \int_{C_+} + \int_{C_-} = 2\pi i \sum \text{Res.}$$

Path Γ : Around the circle $\Gamma(r \to \infty)$, we have (a) $z = e^{i\theta}$, (b) $dz = rie^{i\theta}d\theta$, and (c) $z^{a-1} = r^{a-1}e^{i(a-1)\theta}$. The integral around Γ reduces to

$$\begin{split} \int_{\Gamma} \frac{z^{a-1}dz}{1+z} &= \lim_{r \to \infty} \int_{\Gamma} \frac{r^{a-1}e^{i(a-1)\theta}rie^{i\theta}d\theta}{1+re^{i\theta}} = \lim_{r \to \infty} i \int_{\Gamma} \frac{r^{a}e^{ia\theta}d\theta}{1+re^{i\theta}}\\ &\to \lim_{r \to \infty} i \int_{\Gamma} \frac{r^{a}e^{i(a-1)\theta}d\theta}{r} \to 0. \end{split}$$

Path γ : Similarly, around the circle γ $(r \rightarrow 0)$, we have

$$\int_{\gamma} \frac{z^{a-1}dz}{1+z} = \lim_{r \to \infty} i \int_{\gamma} \frac{r^a e^{ia\theta} d\theta}{1+r e^{i\theta}} \to 0.$$

Path C_+ : Along the upper cut where $\theta = 0$, we have (a) $z = re^{i\theta} = r$, (b) dz = dr, and (c) $z^{a-1} = r^{a-1}$. The value of the integral becomes

$$\int_{C_+} \frac{z^{a-1} dz}{1+z} = \int_0^\infty \frac{r^{a-1} dr}{1+r}.$$

Path C_- : Along the lower cut where $\theta = 2\pi$, we have (a) $z = re^{2\pi i} = r$, (b) dz = dr, and (c) $z^{a-1} = r^{a-1}e^{i2\pi(a-1)} = r^{a-1}e^{2\pi ai}$. The value of the integral reduces to

$$\int_{C_{-}} \frac{z^{a-1}dz}{1+z} = \int_{\infty}^{0} \frac{r^{a-1}e^{2\pi a i}dr}{1+r}$$

The value of the integral I now becomes

$$I = \oint_C \frac{z^{a-1}dz}{1+z} = (1 - e^{2\pi a i}) \int_0^\infty \frac{r^{a-1}dr}{1+r} = 2\pi i \sum \text{Res.}$$

The residue at $z = -1 = e^{i\pi}$ is obtained as follows

$$\phi(z)\big|_{z \to z_0} = (z - z_0) \cdot \frac{z^{a-1}}{1+z}\bigg|_{z \to z_0} = (1+z) \cdot \frac{z^{a-1}}{1+z}\bigg|_{z \to z_0} = -e^{\pi a z_0}$$

On substituting the value for the enclosed residue into the equation for I, we obtain

$$(1 - e^{2\pi ai}) \int_0^\infty \frac{r^{a-1}dr}{1+r} = 2\pi i (-e^{\pi ai}).$$

The above equation leads to

$$\int_0^\infty \frac{x^{a-1}dx}{1+x} = -\frac{2\pi i e^{\pi a i}}{1-e^{2\pi a i}} = \pi \frac{2i}{e^{ia\pi} - e^{-ia\pi}} = \frac{\pi}{\sin \pi a}.$$

The above result will be used in the development of beta functions in Chapter 9 and in the development of the solution of the Abel problem in Chapter 11.

4.9 Problems

4.1 Locate and classify the singular points of the following functions and evaluate the residues:

(a)
$$\frac{e^{1/z}}{z^2}$$
 (b) $\frac{1}{(z^2-1)^2}$ (c) $\frac{\sin z}{z^2}$
(d) $\frac{e^z}{z}$ (e) $\frac{\sin z}{(z-1)^3}$ (f) $\frac{\cos(\sin z)}{\sin z}$

4.2 Evaluate the residues of the following functions:

(a)
$$\frac{z^2 - 1}{z^2 + 1}$$
 (b) $\frac{e^z}{(z - 2)^3}$ (c) $\frac{1}{z^2 + 4z + 1}$
(d) $\frac{1}{(z - 1)^3}$ (e) $\frac{e^{iz}}{z^2 - a^2}$ (f) $\frac{1}{\cos z}$.

4.3 By use of the residue theorem, evaluate the following:

(a)
$$\int_{0}^{2\pi} \frac{d\theta}{5 - 4\cos\theta}$$
 (b) $\int_{0}^{2\pi} \frac{d\theta}{a + b\cos\theta}$ for $|a| > |b|$
(c) $\int_{0}^{2\pi} \frac{d\theta}{3 - 2\cos + \sin\theta}$.

4.4 By use of the residue theorem, evaluate the following:

(a)
$$\int_{|z|=2} \frac{\cos z dz}{z^3}$$
 (b) $\int_{|z|=2} \frac{dz}{1-z^2}$ (c) $\int_{|z|=1} \frac{dz}{z+2}$

4.5 Show that:

(a)
$$\int_{0}^{2\pi} \frac{d\theta}{a + \cos \theta} = \frac{\pi}{\sqrt{a^2 + 1}}$$
 (a > 1) (b) $P \int_{-\infty}^{\infty} \frac{e^{ix} dx}{x} = \pi i$

(c)
$$\int_0^\infty \frac{\sin mx dx}{x} = \frac{\pi}{2}$$
 for $m > 0$. Discuss the cases $m < 0$ and $m = 0$.

4.6 Of the following functions, determine the ones that satisfy the conditions of Jordan's lemma:

(a)
$$\frac{1}{z^2+1}$$
 (b) $\sin z$ (c) e^z (d) $\frac{e^{iz}}{z^2+z+1}$.

4.7 Jordan's Inequality: Show that

$$rac{2 heta}{\pi} \leq \sin heta \leq 0 \quad ext{where} \quad 0 \leq heta \leq rac{\pi}{2}.$$

Hint: Use the fact that the mean ordinate

$$\frac{1}{\theta} \int_0^\theta \cos x dx$$

of the graph $y = \cos x$ over the range $0 \le x \le \theta$ decreases steadily since $\cos \theta$ decreases steadily as θ increases from 0 to $\pi/2$. 4.8 Evaluate

$$P\int_{-1}^{2}\frac{dx}{x^{3}}.$$

4.9 Show that $U(\omega_0) = \cos(k\omega_0)$ and $V(\omega_0) = \sin(k\omega_0)$ are a Hilbert transform pair for k > 0.

4.10 For $\chi(\omega_0) = \chi(-\omega_0)$: (a) Show that $U(\omega_0) = U(-\omega_0)$ and $V(\omega_0) = -V(-\omega_0)$; these are referred to as **crossing relations** in collision theory. (b) Develop the corresponding equations for the Hilbert transform pair which involve integrations over the positive *x*-axis only.



Figure 4.11

4.11 (a) Refer to Fig. 4.11, and determine R_w if w = z + (1-2i). (b) Draw the appropriate w-plane diagram.

4.12 Show that $w = z^2$ is conformal except at z = 0. Discuss the case for z = 0. 4.13 For $w = z^2$: (a) show that $u(x, y) = x^2 - y^2$ and (b) sketch the z-plane and w-plane areas bounded by u = 1, v = 2, and u = 4, v = 8.

Chapter 5

Fourier Series

5.1 Introduction

The theory of the representation of a function of a real variable by means of series of sines and cosines is an indispensable technique in mathematical physics; Fourier analysis is such a theory. We begin the discussion of the Fourier series with a statement of Fourier's theorem. In 1807, Fourier stated without proof and used, in developing a solution of the heat conduction equation, the following theorem.

Fourier's Theorem: Any single-valued function f(x) defined on the closed interval $[-\pi,\pi]$ may be represented over this interval by the trigonometric series

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos nx + b_n \sin nx \right]$$
(5.1)

provided the expansion coefficients, a_n and b_n are determined by use of the Euler's formulas,

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx dx \qquad (n = 0, 1, 2, ...)$$
(5.2)

and

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx dx \qquad (n = 1, 2, 3, \dots).$$
 (5.3)

For historical reasons, it is important to note that d'Alembert, Euler, D. Bernoulli, and Lagrange¹ had previously made fruitful use of the trigonometric series in solving the mechanical wave equation for a vibrating string. However, the trigonometric series associated with a function f(x) by means of Euler's formulas is known as a Fourier series.

Fourier investigated many special cases of the above theorem, but he was unable to develop a mathematical proof of it (In fact, the theorem is not valid as stated.). The first step toward a mathematical proof was made by Dirichlet^2 in 1829; he proved the following theorem.

 $^{^{1}}$ Joseph-Louis Lagrange (1736–1813) was born in Turin, Sardinia-Piedmont (now Italy). He is known for his work in number theory and analytical and celestial mechanics.

 $^{^{2}}$ Johann Peter Gustav Lejeune Dirichlet (1805–1859), German mathematician who is best known for his papers on conditions for the convergence of the Fourier series. In 1855, he replaced Gauss at the University of Göttingen and was himself replaced by Riemann two years later.

Dirichlet's Theorem: If f(x) (a) is defined and bounded in the interval $[-\pi, \pi]$, (b) has at most a finite number of maxima and minima and has only a finite number of discontinuities in this interval, and (c) if f(x) is defined by the periodic condition $f(x+2\pi) = f(x)$ for values of x outside of this interval, then

$$s_p = \frac{a_0}{2} + \sum_{n=1}^{p} \left[a_n \cos nx + b_n \sin nx \right]$$
(5.4)

converges to f(x) as $p \to \infty$ at values of x for which f(x) is continuous, and it converges to [f(x+0) + f(x-0)]/2 at points of discontinuity.

Quantities f(x+0) and f(x-0) refer to the limits from the right and left, respectively. It is assumed that the coefficients in Eq.(5.4) are given by Euler's formulas. A function f(x) is said to be **bounded** if the inequality $[f(x)] \leq M$ holds for some constant M for all values of x. The conditions imposed on f(x) by Dirichlet's theorem are called the **Dirichlet conditions**. From a rigorous mathematical point of view, the Dirichlet conditions are sufficient but not necessary. They, however, are satisfied by most functions representing the solutions of physical problems, and we will work within the constraints of Dirichlet's theorem. Although a rigorous proof of Dirichlet's theorem is beyond the scope of this book, we discuss the convergence properties of the Fourier series.

5.2 The Fourier Cosine and Sine Series

If f(x) is an even function (that is to say, f(x) = f(-x)) in Eqs.(5.2 and 5.3), then we obtain the Fourier cosine series which has the form

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx$$
 (f(x) is even) (5.5)

Equation (5.5) results from the fact that $b_n = 0$ for even f(x). Similarly, $a_n = 0$ for odd f(x) (that is to say, f(x) = -f(-x)), and we obtain the Fourier sine series which has the form

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx \qquad (f(x) \text{ is odd}).$$
(5.6)

The expansion coefficients in the Fourier cosine and sine series, a_n and b_n , are given by the Euler formulas in Eqs. (5.2 and 5.3).

5.3 Change of Interval

Thus far, the expansion interval as been restricted to $[-\pi,\pi]$. To solve many physical problems, it is necessary to develop a Fourier series that will be valid over a wider interval. Consider developing the Fourier series expansion for the interval $[-\ell,\ell]$; let

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \phi x + b_n \sin \phi x \right].$$
 (5.7)

The object here is to determine ϕ such that $f(x) = f(x + 2\ell)$. In this case, $\phi = n\pi/\ell$; hence, we obtain

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{\ell} + b_n \sin \frac{n\pi x}{\ell} \right].$$
(5.8)

The expansion in Eq.(5.8) is valid if f(x) satisfies the Dirichlet conditions in the interval $[-\ell, \ell]$. The corresponding Euler coefficients are

$$a_n = \frac{1}{\ell} \int_{-\ell}^{\ell} f(x) \cos \frac{n\pi x}{\ell} dx \qquad (n = 0, 1, 2, ...)$$
(5.9)

and

$$b_n = \frac{1}{\ell} \int_{-\ell}^{\ell} f(x) \sin \frac{n\pi x}{\ell} dx \qquad (n = 1, 2, 3, \dots).$$
 (5.10)

5.4 Complex Form of the Fourier Series

By expressing $\cos(n\pi x/\ell)$ and $\sin(n\pi x/\ell)$ in exponential form, the complex form of the Fourier series is obtained; we may write

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{\ell} + b_n \sin \frac{n\pi x}{\ell} \right]$$

= $\frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \left[\frac{e^{in\pi x/\ell} + e^{-in\pi x/\ell}}{2} \right] + \sum_{n=1}^{\infty} b_n \left[\frac{e^{in\pi x/\ell} - e^{-in\pi x/\ell}}{2i} \right].$

The expansion for f(x) therefore reduces to

- -

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/\ell} \quad \text{for} \quad [-\ell, \ell]$$
(5.11)

where

$$c_0 = \frac{a_0}{2};$$
 $c_n = \frac{a_n - ib_n}{2};$ $c_{-n} = \frac{a_n + ib_n}{2}.$

Equation (5.11) is the complex form of the Fourier series. On multiplying both sides of Eq.(5.11) by $\exp(-im\pi x/\ell)$ and integrating with respect to x, we obtain

$$\int_{-\ell}^{\ell} f(x)e^{-im\pi x/\ell} dx = \sum_{n=-\infty}^{\infty} c_n \int_{-\ell}^{\ell} e^{i\pi x(n-m)/\ell} dx$$
$$= \sum_{n=-\infty}^{\infty} c_n 2\ell \delta_{mn} = 2\ell c_m.$$

The coefficients in Eq.(5.11) are therefore given by

$$c_n = \frac{1}{2\ell} \int_{-\ell}^{\ell} f(x) e^{-in\pi x/\ell} dx.$$
 (5.12)

Before investigating other mathematical properties of the Fourier series, we consider several examples so that a working knowledge of the Fourier series can be achieved. In these examples, it is assumed that (a) the developed Fourier expansions converge uniformly to the original functions and (b) there is a steady increase in the accuracy of the developed expansion as the number of terms included is increased. A proof of this convergence is given below.

Example 57 Expand $f_1(x) = x^2$ for $-\pi \le x \le \pi$ in a Fourier series.



Figure 5.1

Solution: The graphical representation of $f_1(x)$ in $[-\pi,\pi]$ and its periodic extension outside of $[-\pi,\pi]$ and shown in Fig. 5.1. The expansion coefficients are given by

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f_1(x) dx = \frac{1}{\pi} \int_{-\pi}^{\pi} x^2 dx = \frac{2}{3} \pi^2;$$

$$\begin{aligned} a_{n>0} &= \frac{1}{\pi} \int_{-\pi}^{\pi} f_1(x) \cos x dx = \frac{2}{\pi} \int_{0}^{\pi} x^2 \cos nx dx \quad \text{(by symmetry)} \\ &= \frac{2}{\pi n^2} \left[2\pi n (-1)^n \right] = (-1)^n \frac{4}{n^2}; \quad \text{and} \end{aligned}$$

$$b_{n>0} = \frac{1}{\pi} \int_{-\pi}^{\pi} f_1(x) \sin nx dx$$
$$= \frac{1}{\pi} \int_{-\pi}^{\pi} x^2 \sin nx dx = 0 \qquad \text{(by symmetry)}.$$

The required Fourier expansion is

$$f_1(x) = x^2 = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$
$$= \frac{\pi^2}{3} + 4 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos nx.$$

Example 58 Sawtooth Wave Expand $f_2(x) = x$ for $-\pi \le x \le \pi$ in a Fourier series.



Figure 5.2

Solution: The graphical representation of $f_2(x)$ in $[-\pi,\pi]$ and its periodic extension outside of $[-\pi,\pi]$ are shown in Fig. 5.2. The expansion coefficients are given by

$$a_{0} = \frac{1}{\pi} \int_{-\pi}^{\pi} f_{2}(x) dx = \frac{1}{\pi} \int_{-\pi}^{\pi} x dx = 0,$$

$$a_{n>0} = \frac{1}{\pi} \int_{-\pi}^{\pi} f_{2}(x) \cos nx dx = \frac{1}{\pi} \int_{-\pi}^{\pi} x \cos nx dx = 0,$$

$$b_{n>0} = \frac{1}{\pi} \int_{-\pi}^{\pi} f_{2}(x) \sin nx dx = \frac{1}{\pi} \int_{-\pi}^{\pi} x \sin nx dx$$

$$= -\frac{2}{n} \cos nx = \frac{2}{n} (-1)^{n+1}.$$

The required Fourier expansion is

$$f_2(x) = x = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$
$$= 2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin nx.$$

Example 59 Square Wave Expand the following function in a Fourier series:

$$f_3(x) = \begin{cases} 0 & for \quad -\pi \le x < 0 \\ h & for \quad 0 = x \le \pi. \end{cases}$$

Solution : The graphical representation of $f_3(x)$ in $[-\pi,\pi]$ and its periodic extension outside of $[-\pi,\pi]$ are shown in Fig. 5.3. The expansion coefficients are

$$a_0 = \frac{1}{\pi} \int_{-\pi}^0 f_3(x) dx + \frac{1}{\pi} \int_0^{\pi} f_3(x) dx = \frac{1}{\pi} \int_0^{\pi} h dx = h,$$

$$a_{n>0} = \frac{1}{\pi} \int_{-\pi}^{0} f_3(x) \cos nx dx + \frac{1}{\pi} \int_{0}^{\pi} f_3(x) \cos nx dx$$
$$= \frac{h}{\pi} \int_{0}^{\pi} \cos nx dx = 0, \text{ and}$$

$$b_{n>0} = \frac{1}{\pi} \int_{-\pi}^{0} f_3(x) \sin nx \, dx + \frac{1}{\pi} \int_{0}^{\pi} f_3(x) \sin nx \, dx = \frac{h}{\pi} \int_{0}^{\pi} \sin nx \, dx$$
$$= \frac{h}{\pi} \left[-\frac{\cos nx}{n} \right] \Big|_{x=0}^{x=\pi} = \begin{cases} 0 & \text{for } n \text{ even} \\ 2h/n\pi & \text{for } n \text{ odd.} \end{cases}$$



Figure 5.3

The required Fourier expansion is

$$f_3(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$
$$= \frac{h}{2} + \frac{2h}{\pi} \sum_{\substack{n=1 \\ \text{odd}}}^{\infty} \frac{\sin nx}{n}.$$

Example 60 Full-Wave Rectifier Expand the following function in a Fourier series.

$$f_4(x) = \begin{cases} -\sin x & \text{for } -\pi \le x < 0\\ \sin x & \text{for } 0 = x < \pi. \end{cases}$$


Figure 5.4

Solution : The graphical representation of $f_4(x)$ in $[-\pi,\pi]$ and the periodic extension outside of $[-\pi,\pi]$ are shown in Fig. 5.4. The expansions coefficients are

$$\begin{aligned} a_0 &= \frac{1}{\pi} \int_{-\pi}^0 f_4(x) dx + \frac{1}{\pi} \int_0^{\pi} f_4(x) dx = \frac{1}{\pi} \int_{-\pi}^0 \sin x dx + \frac{1}{\pi} \int_0^{\pi} \sin x dx \\ &= \frac{2}{\pi} \int_0^{\pi} \sin x dx = \frac{4}{\pi}, \\ a_{n>0} &= \frac{1}{\pi} \int_0^0 -\sin x \cos nx dx + \frac{1}{\pi} \int_0^{\pi} \sin x \cos nx dx \end{aligned}$$

$$= \frac{2}{\pi} \int_{0}^{\pi} \sin x \cos nx dx = \begin{cases} \pi \int_{0}^{\pi} \sin x \cos nx dx = \begin{cases} -4/\pi (n^{2} - 1) & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd,} \end{cases}$$

and

$$b_{n>0} = \frac{2}{\pi} \int_0^\pi \sin x \sin nx dx = 0.$$

The required Fourier expansion is

$$f_4(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$
$$= \frac{2}{\pi} - \frac{4}{\pi} \sum_{\substack{n=0\\ \text{even}}}^{\infty} \frac{\cos nx}{n^2 - 1}.$$

5.5 Generalized Fourier Series and the Dirac Delta Function

If the set of functions $\{\psi_n(x)\}\$ is the orthonormal basis for a vector space and F(x) is an arbitrary function on then (see page 72)

$$F(x) = \sum_{n=-\infty}^{\infty} c_n \psi_n.$$
(5.13)

The c_n in Eq.(5.13) are called expansion coefficients. For this set of functions, we have

$$\int_{-\infty}^{\infty} \psi_{n'}^*(x)\psi_n(x)dx = \delta_{n'n}.$$
(5.14)

The orthonormality property for this set of functions is expressed in Eq.(5.14) and will now be used to develop an expression for c_n in Eq.(5.13). On multiplying Eq.(5.13) by $\psi_{n'}^*(x)$ and integrating over the range of x, we obtain

$$\int_{-\infty}^{\infty} \psi_{n'}^{*}(x)F(x)dx = \sum_{n=-\infty}^{\infty} c_n \int_{-\infty}^{\infty} \psi_{n'}^{*}(x)\psi_n(x)dx$$
$$= \sum_{n=-\infty}^{\infty} c_n \delta_{nn'} = c_{n'}.$$
(5.15)

Substituting c_n from Eq.(5.15) into Eq.(5.13), we find that

$$F(x) = \sum_{n = -\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{n'}^{*}(x') F(x') \psi_{n}(x) dx'.$$
(5.16)

The expansion in Eq.(5.16) is referred to as a generalized Fourier series. Interchanging the sum with the integral in Eq.(5.15), we may write

$$F(x) = \int_{-\infty}^{\infty} F(x') \left[\sum_{n=-\infty}^{\infty} \psi_{n'}^{*}(x')\psi_{n}(x) \right] dx'$$
$$\int_{-\infty}^{\infty} F(x')\delta(x-x')dx'$$

where

$$\delta(x - x') = \sum_{n = -\infty}^{\infty} \psi_{n'}^{*}(x')\psi_{n}(x).$$
(5.17)

The above quantity $\delta(x - x')$ is the one-dimensional **Dirac delta function**, and its most important property is expressed by Eq.(5.17). The following are the various notations for the Dirac δ -function used in the literature: $\delta(x - x'), \delta(x)$, and $\delta(x, x')$. In terms of the x variable, the Dirac δ -function is defined such that

$$\int_{-\infty}^{\infty} \delta(x - x') dx' = 1 \quad \text{and} \quad \delta(x - x') = \begin{cases} 0 & \text{for } x - x' \neq 0\\ \infty & \text{for } x - x' = 0. \end{cases}$$
(5.18)

The properties of the Dirac δ -function listed in Eq.(5.18) make it clear that the Dirac δ -function is not a function in a rigorous mathematical sense since the integral (if it exists) of a function that is zero everywhere except at one point must vanish.

We will develop some other useful relations involving the Dirac δ -function since its concept is extremely useful in analyzing physical properties of certain systems. Consider the following set of orthonormal functions:

$$\psi_n(x) = \frac{1}{\sqrt{2\ell}} e^{in\pi x/\ell}.$$
(5.19)

5.6. SUMMATION OF THE FOURIER SERIES

On substituting Eq.(5.19) into Eq.(5.17), we obtain

$$\delta(x - x') = \frac{1}{2\ell} \sum_{n = -\infty}^{\infty} e^{in\pi(x - x')/\ell} = \frac{1}{2\pi} \sum_{\substack{n = -\infty \\ = k\ell/\pi}}^{\infty} \Delta k e^{ik(x - x')}.$$
 (5.20)

Note that the dimension of the Dirac δ -function is inverse length. Quantities in the above equation are given by $k = \pi n/\ell$ and $1/2\ell = \Delta k/2\pi$ since $\Delta n = 1$. Here k has the dimension of inverse length and is called **wave vector** (more precisely, it is the magnitude of the x-component k_x of the wave vector). If $\ell \to \infty$ ($\Delta k \to 0$) in Eq.(5.20), the sum changes into an integral, and we may write

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x - x')} dk.$$
 (5.21)

The above expression for the Dirac δ -function may be written as

$$\delta(x - x') = \frac{1}{2\pi} \lim_{\ell \to \infty} \int_{-\ell}^{\ell} e^{ik(x - x')} dk$$

=
$$\lim_{\ell \to \infty} \frac{\sin\left[\ell (x - x')\right]}{\pi (x - x')}.$$
 (5.22)

Equations (5.21 and 5.22) are two widely used representations for the Dirac δ -function. In three dimensions, we write

$$\delta(\mathbf{r}) = \delta(x)\delta(y)\delta(z) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{r}} d^3k.$$
(5.23)

In the above equation, we have

$$\delta(\mathbf{r}) = 0 \quad (\text{for } \mathbf{r} \neq \mathbf{0}) \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(\mathbf{r}) d^3 r = 1.$$
 (5.24)

5.6 Summation of the Fourier Series

Thus far, it has been necessary to accept, without proof, the fact that the Fourier series of a function does indeed converge to the function in question. In this section, it is shown that

$$\lim_{p \to \infty} s_p(x) \to \frac{1}{2} \left[f(x+0) + f(x-0) \right];$$

that is to say, Dirichlet's theorem in Eq.(5.4) is valid. Consider the partial sum of a Fourier series

$$s_p(x) = \frac{a_0}{2} + \sum_{n=1}^p [a_n \cos nx + b_n \sin nx]$$

= $\frac{1}{2\pi} \int_0^{2\pi} f(t) dt$
+ $\frac{1}{\pi} \sum_{n=1}^p \left[\cos nx \int_0^{2\pi} f(t) \cos nt dt + \sin nx \int_0^{2\pi} f(t) \sin nt dt \right].$

The above equation reduces to

$$s_p(x) = \frac{1}{\pi} \int_0^{2\pi} \left[\frac{1}{2} + \sum_{n=1}^p \cos n(x-t) \right] f(t) dt.$$
 (5.25)

It can be shown (see Problem 5.15) that

$$\frac{1}{2} + \sum_{n=1}^{p} \cos nx = \frac{\sin(p+1/2)x}{2\sin x/2}.$$
(5.26)

On substituting Eq.(5.26) into Eq.(5.25), we obtain the **Dirichlet integral**

$$s_{p}(x) = \frac{1}{2\pi} \int_{0}^{2\pi} \frac{\sin\left[(p+1/2)(x-t)\right]f(t)}{\sin\left[(x-t)/2\right]} dt$$
$$= \frac{1}{2\pi} \int_{-\pi+x}^{\pi+x} \frac{\sin\left[(p+1/2)(x-t)\right]f(t)}{\sin\left[(x-t)/2\right]} dt.$$
(5.27)

The last step in Eq.(5.27) is valid since the integrand is periodic in the indicated interval. Now we make the following change of variable:

$$\theta = -\frac{x-t}{2}.\tag{5.28}$$

On substituting Eq. (5.28) into Eq. (5.27), we find that

$$s_p(x) = rac{1}{\pi} \int_{-\pi/2}^{\pi/2} rac{\sin\left[(2p+1) heta
ight]f(x+2 heta)}{\sin heta} d heta.$$

The path of integration in the above equation will now be bisected so that

$$s_p(x) = \frac{1}{\pi} \int_0^{\pi/2} \frac{\sin\left[(2p+1)\theta\right] f(x+2\theta)}{\sin\theta} d\theta$$
$$+ \frac{1}{\pi} \int_0^{\pi/2} \frac{\sin\left[(2p+1)\theta\right] f(x-2\theta)}{\sin\theta} d\theta.$$

The above equation reduces to

$$s_p(x) = \frac{1}{\pi} \int_0^{\pi/2} \frac{\sin\left[(2p+1)\theta\right]}{\sin\theta} \left[f(x+2\theta) + f(x-2\theta)\right] d\theta$$

The limit of $s_p(x)$ as $p \to \infty$ is given by

$$\lim_{p \to \infty} s_p(x) = \lim_{p \to \infty} \int_0^{\pi/2} \frac{\sin\left[(2p+1)\theta\right]}{\pi \sin\theta} \left[f(x+2\theta) + f(x-2\theta) \right] d\theta$$
$$\approx \int_0^{\pi/2} \delta(\theta) \left[f(x+2\theta) + f(x-2\theta) \right] d\theta.$$

Since $\delta(\theta)$ is an even function, the above equation may be written as

$$\lim_{p \to \infty} s_p(x) = \frac{1}{2} \int_{-\infty}^{\infty} \delta(\theta) \left[f(x+2\theta) + f(x-2\theta) \right] d\theta$$
$$= \frac{1}{2} \left[f(x+0) + f(x-0) \right].$$

In the above equation, f(x+0) and f(x-0) represent the limits from the right and left of the point x, respectively. If f(x) is continuous at the point x, then

$$\lim_{p \to \infty} s_p(x) \to f(x).$$

5.7 The Gibbs Phenomenon

The partial sums of the Fourier series of a function, f(x), approach f(x) uniformly in every interval that does not contain a discontinuity of f(x). In the immediate vicinity of a jump discontinuity, the convergence of the Fourier series is not uniform since $f(x) \rightarrow$ [f(x+0) + f(x-0)]/2. Here the partial sums move progressively closer to the function as the number of terms is increased, but the approximating curves (partial sums) overshoot, by about 18% the function at the jump discontinuity. This behavior is known as the **Gibbs phenomenon** (1899), although the behavior had apparently been investigated earlier by Wilbraham (1848) and Du Bois-Reymond (1873).

In 1906, Bôcher³ greatly extended Gibbs's results by considering the following specific series.

$$f(x) = \frac{\pi - x}{2} \quad (0 < x < 2\pi).$$

The Fourier expansion of the above function is

$$s(x) = \sum_{n=1}^{\infty} \frac{\sin nx}{n}$$

The partial sum of the above expansion is given by

$$s_p(x) = \sum_{n=1}^p \frac{\sin nx}{n} = \sin x + \frac{1}{2} \sin 2x + \dots + \frac{1}{p} \sin px$$

= $\int_0^\pi [\cos u + \cos 2u + \dots \cos pu] du$
= $\int_0^\pi \left(\sum_{n=1}^p \cos nu\right) du = \frac{1}{2} \int_0^\pi \frac{\sin [(p+1/2)u]}{\sin(u/2)} du - \frac{x}{2}.$

The last line in the above equation results from the fact that

$$\sum_{n=1}^{p} \cos nx = \frac{\sin \left[(p+1/2)x \right]}{2\sin(x/2)} - \frac{x}{2}.$$

³Maxime Bôcher (1867–1918), USA mathematician who was awarded the doctorate from the University of Göttingen. He is known for his papers on differential equations, series, and algebra. His paper on the Fourier series presented the first satisfactory treatment of the Gibbs phenomenon.

The remainder, $R_p(x)$, is

$$R_p(x) = \sum_{n=p+1}^{\infty} \frac{\sin nx}{n} = f(x) - s_p(x)$$
$$= \frac{\pi - x}{2} - s_p(x) = \frac{\pi}{2} - \frac{1}{2} \int_0^x \frac{\sin \left[(p - 1/2)u\right]}{\sin(u/2)} du.$$
(5.29)

The above remainder may be written as

$$R_p(x) = \frac{\pi}{2} - \int_0^{(p+1/2)x} \frac{\sin u}{\sin u} du + \rho_p(x)$$

where

$$\rho_p(x) = \int_0^{\pi} \left[\frac{\sin(u/2) - u/2}{u \sin(u/2)} \right] \sin\left[(p + 1/2)u \right] du$$

On differentiating $R_p(x)$ in Eq.(5.29) with respect to x, we find that $R_p(x)$ has maxima or minima at

$$x_k = \frac{2\pi k}{2p+1}$$
 $(k = 0, 1, 2, ...).$

The value of $R_p(x)$ at x_k is

$$R_p(x) = \frac{\pi}{2} - \int_0^{k\pi} \frac{\sin u}{\sin u} du + \rho_p(\frac{2\pi k}{2p+1}).$$

As $p \to \infty$ for fixed $k, \rho_p \to 0$. Hence the remainder, the deviation of the approximation from $(\pi - x)/2$ at x_k which approaches the point of the discontinuity at x = 0 (end point), tends to the limit

$$\lim_{p \to \infty} R_p(x) \to \frac{\pi}{2} - \int_0^{k\pi} \frac{\sin u}{\sin u} du.$$

For k = 1, we find that

$$\lim_{p \to \infty} R_p(x_1) \to \frac{\pi}{2} - \int_0^{\kappa \pi} \frac{\sin u}{\sin u} du = \frac{\pi}{2} - \frac{\pi}{2} (1.179) = -0.281$$

ł. –

Hence the Fourier expansion, as indicated by the negative sign in the above equation, overshoots the curve for f(x) by about 18% at x = 0, a jump discontinuity.

5.8 Summary of Some Properties of Fourier Series

- 1. The Fourier series can be used to represent discontinuous functions where all orders of derivatives need not exist. (This is not true for the Taylor expansion.)
- 2. The Fourier series is useful in expanding periodic functions since outside of the interval in question there exists a periodic extension of the function.

- 3. The Fourier expansion of an oscillating function gives all modes of oscillation (fundamental and all overtones). This kind of representation is extremely useful in mathematical physics.
- 4. Since limit of $s_p(x) \to [f(x+0) + f(x-0)]/2$ as $p \to \infty$, the Fourier series will not be uniformly convergent at all points if it represents a discontinuous function. In the vicinity of a discontinuity, the Fourier representation overshoots the function (Gibbs phenomenon).
- 5. Term-by-term integration of a convergent Fourier series is always valid, and it may be valid ever if the series is not convergent. However, term-by-term differentiation of a Fourier series must be investigated for the series in question; it is not valid in most cases.

5.9 Problems

5.1 Classify the following functions as even, odd, or neither:

(a)
$$x \sin x$$
 (b) e^x (c) $x^3 \cos nx$
(d) $|x|$ (e) $xg(x^2)$ (f) $\ln [(1+x)/(1-x)]$

5.2 Show that the period of each term in the trigonometric series is 2π . 5.3 If f(x) is periodic with period T, show that for arbitrary a and b we have

$$\int_{a}^{a+T} f(x)dx = \int_{b}^{b+T} f(x)dx$$

5.4 By use of the orthoganality property of sines and cosines,

$$\int_{-\pi}^{\pi} \sin mx \sin nx dx = \pi \delta_{mn}$$
$$\int_{-\pi}^{\pi} \cos mx \cos nx dx = \pi \delta_{mn}$$
$$\int_{-\pi}^{\pi} \sin mx \cos nx dx = 0 \quad \text{for all} \quad n, m >$$

derive the required expressions for the coefficients (Euler's formulas) in the trigonometric series.

0,

5.5 Suppose the function f(x) is represented by a finite Fourier series,

$$\frac{a_0}{2} + \sum_{n=1}^p \left[a_n \cos nx + b_n \sin nx \right].$$

A measure of the accuracy of this series representation is given by

$$\Delta_p = \int_0^{2\pi} \left[f(x) - \frac{a_0}{2} - \sum_{n=1}^p (a_n \cos nx + b_n \sin nx) \right]^2 dx.$$

By minimizing $\Delta_p (\partial \Delta_p / \partial a_n = 0)$ and $\partial \Delta_p / \partial b_n = 0$, solve for a_n and b_n . 5.6 Solve the Example for $f_2(x) = x$ by use of the complex form of the Fourier series. 5.7 Develop the Fourier sine expansion for f(x) = x in the half-interval $[0, \ell]$. 5.8 Develop the Fourier expansion for f(x) = |x| for the interval $[-\ell, \ell]$. 5.9 From the result in the Example for $f_1(x) = x^2$, show that

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2}$$

Note that

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2} \quad \text{where} \quad \zeta(k) = \sum_{n=1}^{\infty} \frac{1}{n^k}$$

is called the Riemann zeta function.

5.10 Develop the Fourier expansion for

$$f(\omega t) = \begin{cases} 0 & \text{for } -\pi \le \omega t < 0\\ \sin \omega t & \text{for } 0 = \omega t \le \pi \end{cases}$$

5.11 A triangular wave may be represented by

$$f(x) = \begin{cases} x & \text{for } 0 \le x \le \pi \\ -x & \text{for } -\pi \le x \le 0. \end{cases}$$

Develop the Fourier expansion for f(x).

5.12 Find the Fourier series expansion for f(x) if

$$f(x) = \begin{cases} \pi & \text{for } -\pi \le x < \pi/2 \\ 0 & \text{for } \pi/2 = x \le \pi. \end{cases}$$

5.13 Assuming that the Fourier expansion of f(x) is uniformly convergent, show that

$$\frac{1}{\pi} \int_{-\pi}^{\pi} |f(x)|^2 \, dx = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n^2 + b_n^2) \qquad \text{(Parseval's relation)}.$$

5.14 Show that the term-by-term integration of a convergent Fourier series results in a Fourier series that converges more rapidly than the original Fourier series. 5.15 Show that

$$\frac{1}{2} + \sum_{n=1}^{p} \cos nx = \frac{\sin(p+1/2)x}{2\sin(x/2)}.$$

5.16 Show that $f_2(x)$ in the Example is convergent and that f'(x) is not convergent. 5.17 Show that the following relations involving the Dirac delta function are valid:

(a)
$$\delta(x) = \delta(-x)$$
 (b) $x\delta(x) = 0$ (c) $\delta'(x) = -\delta'(-x)$
(d) $x\delta'(x) = -\delta(x)$ (e) $\delta(ax) = \delta(x)/a$ for $a > 0$

Hint: Multiply by an arbitrary function f(x) and integrate from $-\infty$ to ∞ .

Chapter 6

Fourier Transforms

6.1 Introduction

In mathematical physics, integrals of the form

$$F(\alpha) = \int_{a}^{b} f(x) K(\alpha, x) dx$$
(6.1)

often occur. The function $F(\alpha)$ is said to be the **integral transform** of f(x) by the **kernel** $K(\alpha, x)$. Kernels associated with Fourier, Laplace, Fourier-Bessel (Hankel), and Mellin transforms are respectively given by

$$F(\alpha) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{i\alpha x} dx \quad \text{(Fourier transform)}; \tag{6.2}$$

$$F(\alpha) = \int_0^\infty f(x)e^{-\alpha x} dx \qquad \text{(Laplace transform)}; \tag{6.3}$$

$$F(\alpha) = \int_0^\infty f(x) x J_n(\alpha x) dx \quad \text{(Fourier-Bessel transform); and} \quad (6.4)$$

$$F(\alpha) = \int_0^\infty f(x)e^{\alpha - 1}dx \qquad \text{(Mellin transform)}.$$
 (6.5)

The Fourier and Laplace transforms are the most often used in mathematical physics. The procedure for solving problems by use of the transform method is the same for all transforms, and we focus on the Fourier transform.

The form of the complex Fourier series is

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/\ell} \quad \text{for} \quad [-\ell, \ell]$$
(6.6a)

where

$$c_n = \frac{1}{2\ell} \int_{-\ell}^{\ell} f(x) e^{-in\pi x/\ell} dx.$$
 (6.6b)

To make the transition $\ell \to \infty$, we introduce a new variable which is defined by

$$k=\frac{n\pi}{\ell}$$

where $(\Delta k/\pi)\ell = 1$ since $\Delta n = 1$. Hence we may write Eqs.(6.6a and 6.6b) in the following forms:

$$f(x) = \sum_{n=-\infty}^{\infty} C_{\ell} e^{ikx} \Delta k$$
 where $n = \frac{k\ell}{\pi}$

and

$$C_{\ell}(k) = rac{1}{2\pi} \int_{-\ell}^{\ell} f(x) e^{-ikx} dx \quad ext{ where } C_{\ell}(k) = rac{\ell c_n}{\pi}.$$

If we let $\ell \to \infty$, we obtain

$$C(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$
(6.7)

and

$$f(x) = \int_{-\infty}^{\infty} C(k)e^{ikx}dk.$$
(6.8)

There are several ways of defining Fourier transforms, but the differences among the various forms are not significant. To put Eqs.(6.7 and 6.8) in the modern form (the symmetric form most often used in mathematical physics), we let $F(k) = \sqrt{2\pi}C(-k)$ and obtain

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$
(6.9)

and

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{-ikx} dk.$$
 (6.10)

Equations (6.9 and 6.10) are called the Fourier transform pair. If f(x) satisfies the Dirichlet conditions and the integral

$$\int_{-\infty}^{\infty} |f(x)| \, dx$$

is finite, then F(k) exists for all k and is called the Fourier transform of f(x). The function f(x) in Eq.(6.10) is called the Fourier transform (inverse transform) of F(k). As a physical requirement, it is usually assumed that $f(x) \to 0$ as $x \to \pm \infty$. Naturally, it is required that kx be dimensionless since it is the argument of an exponential quantity. In physics, k (or k_x) is the magnitude (x-component) of the wave vector with dimension of inverse length, and x is a distance. The combination of ωt , where ω is circular frequency with dimension of inverse time and t is time, is often used.

Example 61 Obtain the Fourier transform of the Gaussian distribution function, $f(x) = Nexp(-ax^2)$ where a and N are constants.

Solution : On applying Eq.(6.9), we obtain

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{ikx} dx = \frac{N}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx - ax^2} dx$$
$$= \frac{N}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} e^{-ax^2} \cos kx dx + i \int_{-\infty}^{\infty} e^{-ax^2} \sin kx dx \right\}$$
$$= \frac{N}{\sqrt{2\pi}} e^{-k^2/4a} \quad \text{where} \quad \int_{-\infty}^{\infty} e^{-ax^2} \cos kx dx = \sqrt{\frac{\pi}{a}} e^{-k^2/4a}.$$

The above final form for F(k) results from the fact that (a) the second integral in the second equation equals zero since the integrand is an odd function in the range of integration and (b) the first integral yields the final answer. Note that both f(x) and F(k) are Gaussian distribution functions with peaks at the origin.

A Fourier transform pair equivalent to Eqs. (6.9 and 6.10), where the signs of the exponential terms are interchanged, is widely used in quantum mechanics. In terms of the wave function (solution of the Schrödinger wave equation), the Fourier transform pair have the following forms in quantum mechanics.

$$\Psi(k_x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, t) e^{-ik_x x} dx$$
 (6.11*a*)

and

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(k_x,t) e^{ik_x x} dk_x$$
(6.11b)

or

$$\Psi(p_x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,t) e^{-ip_x x/\hbar} dx$$
(6.12a)

and

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(p_x,t) e^{ip_x x/\hbar} dp_x$$
(6.12b)

The above development of the Fourier transform is purely formal. For a rigorous treatment of the subject, many books on Fourier or integral transforms and operational mathematics are highly recommended (e.g., see Tichmarsh, 1937).

6.2 Cosine and Sine Transforms

The cosine and sine transform pairs are defined, respectively, by

$$F_c(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \cos kx dx \tag{6.13a}$$

and

$$f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_c(k) \cos kx dk.$$
(6.13b)

$$F_s(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \sin kx dx \tag{6.14a}$$

and

$$f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_s(k) \sin kx dk.$$
(6.14b)

Note that the Fourier transform of f(x) in Eq.(6.9) may be written as

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{ikx}dx$$

= $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \left[\cos kx + i\sin kx\right] dx.$ (6.15)

If f(x) is an even function of x (f(x) = f(-x)), then we see from Eq.(6.15) that the cosine transform is equal to the Fourier transform. If, however, f(x) is an odd function of x (f(x) = -f(-x)), then we see from Eq.(6.15) that the sine transform is equal to the Fourier transform provided -F(k) is replaced by $F_s(k)$.

Example 62 Find the Fourier transform for the box function f(x) where

$$f(x) = \begin{cases} 1 & for -a \le x \le a \\ 0 & for & |x| > a \end{cases}$$

Solution : By use of Eq.(6.9), we obtain

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$
$$= \int_{-a}^{a} e^{ikx} dx = \sqrt{\frac{2}{\pi}} \frac{\sin ka}{k}$$

A sketch of f(x) and F(k) are given in Fig. 6.1.

Example 63 Find the cosine and sine transforms of $f(x) = e^{-ax}$.

Solution: Using Eq.(6.13a), we find that

$$F_c(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \cos kx dx$$
$$= \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-ax} \cos kx dx = \sqrt{\frac{2}{\pi}} \left(\frac{a}{k^2 + a^2}\right).$$

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The corresponding sine transform is obtained by means of Eq.(6.14a). We obtain

$$F_s(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \sin kx dx$$
$$= \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-ax} \sin kx dx = \sqrt{\frac{2}{\pi}} \left(\frac{k}{k^2 + a^2}\right)$$

The one-dimensional Fourier transform pair of a function of two independent variables are given respectively by

$$F(k,y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x,y) e^{ikx} dx$$
 (6.16*a*)

and

$$f(x,y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k,y) e^{-ikx} dk.$$
 (6.16b)

The corresponding cosine and sine transform pairs are

$$F_c(k,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x,y) \cos kx dx \tag{6.17a}$$

and

$$f(x,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_c(k,y) \cos kx dk.$$
(6.17b)

$$F_s(k,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x,y) \sin kx dx$$
(6.18a)

and

$$f(x,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty F_s(k,y) \sin kx dk.$$
(6.18b)

The above transform pair may be extended in a straight forward manner to functions of several independent variables.

The one-dimensional transform theory may be extended in a natural way to the cases of twoand three-dimensional Fourier transforms. In equation form, the two-dimensional Fourier transform pair may be written as

$$F(\alpha,\beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) e^{i(\alpha x + \beta y)} dx dy$$
(6.19a)

$$f(x,y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(\alpha,\beta) e^{-i(\alpha x + \beta y)} d\alpha d\beta.$$
(6.19b)

6.3 The Transforms of Derivatives

Fourier transforms, cosine transforms, and sine transforms can often be used to transform a differential equation (ordinary or partial) which describes a complicated physical problem into a simpler equation (algebraic or ordinary differential) that can be easily solved. The required solution of the original differential equation is then obtained by finding the inverse transform of the solution of the simpler equation (in transform space). In order to use the transform method to solve first- and second-order differential equations, the transforms of first- and second-order derivatives are needed.

We now develop the transforms of first- and second-order derivatives. The Fourier transforms of first- and second-order derivatives will be represented by $F^{(1)}(k)$ and $F^{(2)}(k)$, respectively. That is to say,

$$F^{(1)}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{df(x)}{dx} e^{ikx} dx.$$
 (6.20)

On carrying out the integration in Eq.(6.20) by parts, we obtain

$$F^{(1)}(k) = \frac{1}{\sqrt{2\pi}} \left\{ f(x)e^{ikx} \Big|_{-\infty}^{\infty} - ik \int_{-\infty}^{\infty} f(x)e^{ikx} dx \right\} = -\frac{ik}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{ikx} dx = -ikF(k).$$
(6.21)

The development leading to Eq.(6.21) made use of the assumption that $f(x) \to 0$ as $x \to \pm \infty$. Similarly, we find that

$$F^{(2)}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{d^2 f(x)}{dx^2} e^{ikx} dx = -k^2 F(k)$$
(6.22)

where $f(x) \to 0$ and $f'(x) \to 0$ as $x \to \pm \infty$. The corresponding relation for $F^{(1)}(k, y)$ is

$$F^{(1)}(k,y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial f(x,y)}{\partial x} e^{ikx} dx = -ikF(k,y)$$
(6.23)

where $f(x,y) \to 0$ as $x \to \pm \infty$. The Fourier transform for the second derivative, $F^{(2)}(k,y)$, is given by

$$F^{(2)}(k,y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial^2 f(x,y)}{\partial x^2} e^{ikx} dx = -k^2 F(k,y)$$
(6.24)

where $f(x, y) \to 0$ and $\partial f(x, y) / \partial x \to 0$ as $x \to \pm \infty$. The cosine transform of a first-order derivative is given

$$F_{c}^{(1)}(k) = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} \frac{df(x)}{dx} \cos kx dx$$

= $kF_{s}(k) - \sqrt{\frac{2}{\pi}} f(0)$ (6.25)

where $f(x) \to 0$ as $x \to \infty$. The cosine transform of a second-order derivative is

$$F_{c}^{(2)}(k) = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} \frac{d^{2}f(x)}{dx^{2}} \cos kx dx$$
$$= -k^{2}F_{c}(k) - \sqrt{\frac{2}{\pi}}f'(0)$$
(6.26)

where $f(x) \to 0$ and $f'(x) \to 0$ as $x \to \infty$. The sine transform of a first-order derivative is given by

$$F_s^{(1)}(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{df(x)}{dx} \sin kx dx = -kF_c(k)$$
(6.27)

where $f(x) \to 0$ as $x \to \infty$. The sine transform of a second-order derivative is given by

$$F_{s}^{(2)}(k) = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} \frac{d^{2}f(x)}{dx^{2}} \sin kx dx$$
$$= \sqrt{\frac{2}{\pi}} k f(0) - k^{2} F_{s}(k)$$
(6.28)

where $f(x) \to 0$ and $f'(x) \to 0$ as $x \to \infty$.

The choice of using the cosine or sine transform is dictated by the given boundary conditions at the lower limit. The use of the cosine transform to remove (transform) a first-order derivative term in a differential equation requires a knowledge of f(0) but a knowledge of f(0) is not required when the sine transform is used to remove a first-order derivative term. A knowledge of f'(0) is required to remove a second-order derivative term in a differential equation if the cosine transform is used. However, only a knowledge of f(0) is needed to successfully use a sine transform to remove a second-order derivative term in a differential equation.

The relations for $F_c^{(1)}(k, y), F_c^{(2)}(k, y), F_s^{(1)}(k, y)$, and $F_s^{(2)}(k, y)$ are

$$F_c^{(1)}(k,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\partial f(x,y)}{\partial x} \cos kx dx$$
$$= kF_s(k,y) - \sqrt{\frac{2}{\pi}} f(0,y)$$
(6.29)

for $f(x, y) \to 0$ as $x \to \infty$;

$$F_{c}^{(2)}(k,y) = \sqrt{\frac{2}{\pi}} \int_{0}^{\infty} \frac{\partial^{2} f(x,y)}{\partial x^{2}} \cos kx dx$$

= $-k^{2} F_{c}(k,y) - \sqrt{\frac{2}{\pi}} f_{x}(0,y)$ (6.30)

for $f(x,y) \to 0$ and $\partial f(x,y)/\partial x \to 0$ as $x \to \infty$.

$$F_s^{(1)}(k,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\partial f(x,y)}{\partial x} \sin kx dx = -kF_c(k,y)$$
(6.31)

for $f(x,y) \to 0$ as $x \to \infty$; and

$$F_s^{(2)}(k,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\partial^2 f(x,y)}{\partial x^2} \sin kx dx$$
$$= \sqrt{\frac{2}{\pi}} k f(0,y) - k^2 F_s(k,y)$$
(6.32)

for $f(x,y) \to 0$ and $\partial f(x,y)/\partial x \to 0$ as $x \to \infty$.

The various transforms of derivatives will be used in solving ordinary and partial differential equations in Chapters 7 and 8.

6.4 The Convolution Theorem

In linear response theory, the general equation for the one-dimensional transform, Eq.(6.1), takes the form

$$F(\alpha) = \int_{a}^{b} f(x)K(\alpha, x)dx$$

=
$$\int_{-\infty}^{\infty} K(\alpha - x)f(x)dx$$
 (6.33)

where $K(\alpha - x)$ is called the **response** of the linear system, f(x) is the **input** (signal) to the linear system, and $F(\alpha)$ is the **output** (signal). If $K(\alpha - x) = \delta(\alpha - x)$, then

$$F(\alpha) = \int_{-\infty}^{\infty} \delta(\alpha - x) f(x) dx$$

which is consistent with the properties of the Dirac delta function. In this latter case, $K(\alpha - x)$ is called the **impulse response** of the system. When Eq.(6.33) is written in the form

$$F(x) = f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x - \xi) g(\xi) d\xi,$$
(6.34)

it is called the one-dimensional **convolution integral** (faltung or folding integral) of two integrable functions f(x) and g(x). The corresponding two-dimensional form of the convolution integral is

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x - \xi; x - \beta) g(\xi, \beta) d\xi d\beta.$$

Let F(k) and G(k) be the Fourier transforms of f(x) and g(x), respectively. For these functions, the convolution integral becomes

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x-\xi)g(\xi)d\xi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\xi) \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{-ik(x-\xi)}dk \right\} d\xi$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\{ F(k)e^{-ikx} \int_{-\infty}^{\infty} g(\xi)e^{ik\xi}d\xi \right\} dk$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)G(k)e^{-ikx}dk.$$
(6.35)

In obtaining Eq.(6.35), we have tacitly assumed that the process of interchanging the order of integration is valid. The result in Eq.(6.35) is known as the **convolution theorem** for Fourier transforms. It means that the Fourier transform (inverse transform) of the product F(k)G(k), the right-hand side of Eq.(6.35), is the convolution of the original functions, f * g.

6.5 Parseval's Relation

The integral of the product of two functions f(x) and $g^*(x)$, the complex conjugate of g(x), may be written as

$$\int_{-\infty}^{\infty} f(x)g^{*}(x)dx = \int_{-\infty}^{\infty} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{-ikx}dk \right\}$$
$$\times \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G^{*}(k')e^{ik'x}dk' \right\} dx$$
$$= \int_{-\infty}^{\infty} \left\{ f(k) \left\{ \int_{-\infty}^{\infty} G^{*}(k')\delta(k'-k)dk' \right\} \right\} dk$$
$$= \int_{-\infty}^{\infty} F(k)G^{*}(k)dk.$$
(6.36)

The relation in Eq.(6.36) is known as **Parseval's**¹ relation (or **Parseval's theorem**) and is widely used in optics, electromagnetism, and quantum mechanics.

Example 64 By use of Parseval's relation, show that

$$\int_{-\infty}^{\infty} \phi^*(p_x) \phi(p_x) dp_x = 1 \qquad (momentum \ space)$$

if

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1 \qquad (coordinate space).$$

 $^{^{1}}$ Marc-Antoine Parseval des Chênes (1755–1836), French mathematician and royalist who published only five papers in mathematics and is known for the work now called Parseval's theorem (or Parseval's relation).

Solution : Parseval's relation has the form

$$\int_{-\infty}^{\infty} f(x)g^*(x)dx = \int_{-\infty}^{\infty} F(k)G^*(k)dk.$$

For this problem, we write

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p_x) e^{ip_x x/\hbar} dp_x.$$

On applying Parseval's relation to ϕ and ψ , we obtain

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = \int_{-\infty}^{\infty} \phi^*(p_x)\phi(p_x)dp_x = 1.$$

The above result follows from

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1.$$

This result is extremely useful in quantum mechanics.

6.6 Problems

6.1 Calculate the Laplace transform of $f(x) = e^{-x}$.

6.2 Calculate the Mellin transform of $f(x) = e^{-x}$.

6.3 (a) Calculate the Fourier transform (inverse transform) of

$$F(k) = \frac{N}{\sqrt{2a}} e^{-k^2/4a}$$

(b) Sketch an appropriate diagram for f(x) and F(k) for large and small a. 6.4 Calculate the cosine and sine transforms of e^{-bx} , where b is a positive integer. 6.5 Calculate the cosine transform of $f(x) = e^{-x^2/2}$.

6.6 By use of the results in second Example, show that

(a)
$$\int_0^\infty \frac{\cos kxdk}{k^2 + a^2} = \frac{\pi}{2a}e^{-ax}$$
 and (b) $\int_0^\infty \frac{k\sin kxdk}{k^2 + a^2} = \frac{\pi}{2}e^{-ax}$.

6.7 (a) Calculate the Fourier transform, $F(\omega)$, of f(t) where

$$f(t) = \begin{cases} e^{-i\omega_0 t} & \text{for } -\tau_0/2 \le t \le \tau_0/2\\ 0 & \text{for } & |t| > \tau_0/2. \end{cases}$$

(b) Sketch $f(t), F(\omega)$, and $|F(\omega)|^2$. The power spectrum is given by $|F(\omega)|^2$. 6.8 Show that the Fourier transform of

$$\psi(x) = \begin{cases} \sum_{n=-\infty}^{\infty} c_n e^{inx} & \text{for } 0 \le x \le 2\pi \\ 0 & \text{otherwise} \end{cases}$$

does not vanish outside of any finite interval.

6.9 Show that the convolution of f(x) and g(x) is commutative, f * g = g * f. 6.10 Calculate the convolution of $f(x) = g(x) = e^{-|x|}$.

6.11 Find the Fourier transform of the box function where a > 0 and

$$f(x) = \begin{cases} 1 & \text{for } |x| \le a \\ 0 & \text{for } |x| > a. \end{cases}$$

Chapter 7

Ordinary Differential Equations

7.1 Introduction

A differential equation is an equation that contains derivative(s) of a function, and it may be either an ordinary or a partial differential equation. Ordinary differential equations contain derivative(s) with respect to one independent variable, and partial differential equations contain partial derivatives with respect to two or more independent variables. It has now become somewhat standard to use the following abbreviations: differential equation (DE), ordinary differential equation (ODE), and partial differential equation (PDE).

The **order** of a differential equation is the order of the highest derivative appearing in the equation. The **degree** of a differential equation is the power of the highest derivative after fractional powers of all derivatives have been removed. If the dependent variable and all of its derivatives are to the first power without a product of the dependent variable and a derivative, the differential equation is said to be **linear**. A differential equation is classified as **nonlinear** if it is not linear.

Applications of appropriate physical laws to a large number of problems lead to differential equations. In general, a physical process is described by use of a differential equation with appropriate boundary conditions on space and/or initial conditions on time and/or by use of an integral equation. The boundary and/or initial conditions determine from the many possible mathematical solutions the one that describes the specific physical phenomenon involved.

The main purpose here concerns the development of solutions for differential equations that adequately describe physical processes under investigation. The subjects of existence and uniqueness theorems for solutions of differential equations will not be discussed in details. Software packages such as Macsyma, Maple, and Mathematica may be used to solve differential equations with computers; these software packages are extremely useful since the solutions of many differential equations (in particular, most nonlinear differential equations) cannot be obtained in terms of familiar elementary functions. In spite of the usefulness of these programs, the knowledge for finding analytic solutions of certain classes of differential equations is indispensable in mathematical physics.

An elementary introduction to the subject of ordinary differential equations, as it relates to the needs in solving physical problems, can be reduced to that of treating linear (or reducible to the linear form) first- and second-order differential equations. This chapter is devoted to the construction of solutions and physical applications of such ordinary differential equations. The solution of a differential equation is sometimes referred to as the integral of the differential equation, and its graph is called an **integral curve** (solution curve). The general solution of an *n*-th-order ordinary differential equation contains n arbitrary constants (parameters) and is called an *n*-parameter family of curves. Boundary conditions on space and/or initial conditions on time are used to evaluate the arbitrary constants in the general solution to produce a particular solution that is free of arbitrary constants.

First- and second-order linear ordinary differential equations have the following standard forms respectively:

$$\frac{dy}{dx} + p(x)y = Q(x) \quad \text{or} \quad y' + p(x)y = Q(x)$$
(7.1)

 and

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = f(x) \quad \text{or} \quad y'' + p(x)y' + q(x)y = f(x).$$
(7.2)

In Eqs.(7.1 and 7.2), the notations y' = dy/dx and $y'' = d^2y/dx^2$ have been used. When time t is the independent variable, one writes $\dot{y} = dy/dt$ and $\ddot{y} = d^2y/dt^2$. If the right-hand sides of Eqs.(7.1 and 7.2) equal zero, the differential equations are classified as **homogeneous**; otherwise, the differential equations are classified as **nonhomogeneous** (inhomogeneous).

7.2 First-Order Linear Differential Equations

The formulation (mathematical modeling) of many physics problems leads to first-order differential equations, and this section is devoted to three methods of finding the analytic solutions for such problems.

7.2.1 Separable Differential Equations

Differential equations that can be put in the form

$$g(y)dy = f(x)dx$$

are called **separable differential equations** since the left-hand side is a function of y only and the right-hand side is a function of only x. For example, the integral (general solution) of dy = f(x)dx is

$$y = \int f(x)dx + C.$$

Since the general solution of a first-order differential equation results from one integration, it will contain one arbitrary constant. Similarly, the general solution of a second-order differential equation will contain two arbitrary constants. Values of arbitrary constants are determined by use of physical boundary or initial conditions. **Example 65** In the radioactive decay of nuclei, the process is governed by the following differential equation:

$$rac{dN}{dt} = -\lambda N \quad where \quad N(t=0) = N_0.$$

The number of parent nuclei present at time t is represented by N(t), and the decay constant λ is characteristic of the particular nuclei involved. The negative sign is used to indicate that the number of nuclei decreases with time. Find N(t) subject to the indicated initial condition.

Solution : The differential equation is separable, and we write

$$\frac{dN}{N} = -\lambda dt.$$

The integral (general solution) of the above differential equation is

$$\ln N = -\lambda t + C_1 \quad \text{or} \quad N(t) = C_2 e^{-\lambda t}.$$

The value of the constant of integration is determined by use of the initial condition $N(t = 0) = N_0$ which leads to $N(0) = N_0 = C_2$. The specific (particular) solution of the problem is the following familiar relation:

$$N(t) = N_0 e^{-\lambda t}$$

A graph of N(t) versus time shows an exponentially decaying process.

7.2.2 Exact Differential Equations

The general first-order differential equation, dy/dx = f(x, y), may be written in the form

$$M(x, y)dx + N(x, y)dy = 0.$$
 (7.3)

The total (exact) differential of F(x, y) = C (where F is continuous with continuous derivatives, i.e. a smooth function) is defined as

$$dF(x,y) \equiv \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy = 0.$$

In the above equation, $\partial F/\partial x$ means change in F with respect to x while y is held constant; change in F with respect to y while x is held constant is the meaning of the partial derivative in the second term. Note that the general first-order differential equation in Eq. (7.3) is exact if

$$M(x,y)=rac{\partial F}{\partial x} \quad ext{ and } \quad N(x,y)=rac{\partial F}{\partial y}.$$

Since it is assumed that F(x, y) is a smooth function, we have

$$\frac{\partial^2 F}{\partial y \partial x} = \frac{\partial^2 F}{\partial x \partial y} \quad \text{or} \quad \frac{\partial M}{\partial y} = \frac{\partial N}{\partial x}.$$
(7.4)

The second condition indicated in Eq.(7.4) is both necessary and sufficient for Eq.(7.3) to be an exact differential equation.

Example 66 Determine whether the following differential equation is exact and find its solution if it is exact:

$$(4x^3 + 6xy + y^2)\frac{dx}{dy} = -(3x^2 + 2xy + 2).$$

Solution : The standard form of this differential equation is

$$(4x^3 + 6xy + y^2)dx + (3x^2 + 2xy + 2)dy = 0.$$

Note that

$$\frac{\partial M}{\partial y} = \frac{\partial (4x^3 + 6xy + y^2)}{\partial y} = 6x + 2y$$

and

$$\frac{\partial N}{\partial x} = \frac{\partial (3x^2 + 2xy + 2)}{\partial x} = 6x + 2y.$$

The condition in Eq.(7.4) is satisfied, and the differential equation is exact. The solution of the original differential equation, therefore, has the form F(x, y) = C where

$$M = \frac{\partial F}{\partial x} = 4x^3 + 6xy + y^2 \quad \text{or} \quad F(x, y) = x^4 + 3x^2y + xy^2 + g_1(y)$$

 and

$$N = rac{\partial F}{\partial y} = 3x^2 + 2xy + 2$$
 or $F(x,y) = 3x^2y + xy^2 + 2y + g_2(x).$

Functions $g_1(y)$ and $g_2(x)$ are arbitrary functions that arise from integrating with respect to x and y respectively. For consistency, we require that

$$g_1(y) = 2y$$
 and $g_2(x) = x^4$.

The solution of the original differential equation is

$$F(x,y) = x^4 + 3x^2y + xy^2$$

7.2.3 Solution of the General Linear Differential Equation

A good feature of first-order linear differential equations is that a formula for solving the general equation is this category can be developed; this development is outlined in the following two steps:

Step 1 Solve the corresponding homogeneous differential equation (i.e., Q = 0)

$$rac{dy_h}{dx} + p(x)y_h = 0 \quad ext{or} \quad rac{dy_h}{y_h} = -p(x)dx.$$

The above differential equation is in separable form, and its solution is

$$y_h = A \exp \int p(x) dx.$$

The factor $\exp \int p(x) dx$ is referred to as the **integrating factor**. (If a differential equation of the form in Eqs.(7.1) or (7.3) is not exact, then the result of multiplication by an integrating factor is an exact differential equation.)

Step 2 Multiply the original differential equation, Eq.(7.1), by the integrating factor; we obtain

$$[y' + p(x)y] \exp \int p(x)dx = Q(x) \exp \int p(x)dx.$$
(7.5)

Since

$$rac{d}{dx}\left[y\exp\int p(x)dx
ight]=\left[y'+p(x)y
ight]\exp\int p(x)dx,$$

Eq.(7.5) may be written as

$$\frac{d}{dx}\left[y\exp\int p(x)dx\right] = Q(x)\exp\int p(x)dx.$$

Integrating the above differential equation, we obtain

$$y \exp \int p(x) dx = \int Q(x) \left[\exp \int p(x) dx \right] dx + C.$$

Solving the above equation for y(x), we may write

$$y(x) = \exp\left(-\int p(x)dx\right) \int Q(x) \left[\exp\int p(x)dx\right] dx + C \exp\left(-\int p(x)dx\right).$$
(7.6)

Equation (7.6) is the general solution (general formula) of the general first-order linear differential equation, Eq.(7.1).

Example 67 Solve the differential equation

$$y' + x = \frac{y}{x}.$$

Solution : In standard form, the above differential equation becomes

$$y' - rac{1}{x}y = -x$$
 where $p(x)
ightarrow rac{1}{x}$ and $Q(x)
ightarrow -x.$

On applying the formula in Eq.(7.6) to the above differential equation, we obtain

$$y(x) = -\exp \int p(x)dx \int x \exp \left[-\int p(x)dx\right] dx + C \exp \int p(x)dx$$
$$= e^{\ln x} \int x e^{-\ln x} dx + C e^{\ln x} = -x^2 + Cx.$$

Example 68 Derive the expression for the current in the circuit in Fig. 7.1.



Figure 7.1:

Solution : By use of the Kirchhoff¹ loop method in circuit theory, we obtain

$$L\frac{dI}{dt} + IR = E$$
 where $I(t=0) = 0$.

The parameters in the above differential equation have their usual meaning. The standard form for the above differential equation is

$$\frac{dI}{dt} + \frac{R}{L}I = \frac{E}{L}.$$

On applying the formula in Eq.(7.6) where $p \to R/L$ and $Q \to E/L$, we obtain

$$I(t) = e^{-Rt/L} \int \frac{E}{L} e^{Rt/L} dt + C e^{-Rt/L} = \frac{E}{R} + C e^{-Rt/L}.$$

The initial condition I(t = 0) = I(0) = 0 is used to evaluate the arbitrary constant as follows.

$$I(0) = 0 = \frac{E}{R} + C \Longrightarrow C = -\frac{E}{R}$$

The required expression for the current (particular solution) is

$$I(t) = \frac{E}{R} \left(1 - e^{-Rt/L} \right).$$

A graph of the above equation give behavior of the current as a function of time. In summary,

- 1. the method in Section 7.2.1. should be used on separable differential equations;
- 2. the method in Section 7.2.1. should be used on exact differential equations; and
- 3. the formula in Eq.(7.6) yields a solution to the general first-order linear differential equation.

It is important to substitute the obtained solution into the original differential equation to check the correctness of the solution.

¹Gustav Robert Kirchhoff (1824–1887), German physicist who was born in Königsberg, Prussia. He is known for his contributions to circuit theory and to black body radiation. He was a student of Gauss.

7.3 The Bernoulli Differential Equation

The formulation of numerous physical problems leads to differential equations of the form

$$y' + p(x)y = Q(x)y^n \quad \text{where} \quad n \neq 1.$$
(7.7)

Equation (7.7) is referred to as the **Bernoulli² differential equation** and is a nonlinear differential equation. It, however, can be reduced to the linear form, and the technique used might be useful in solving other nonlinear differential equations. The method for solving Bernoulli's differential equation was discovered by Leibniz³ and involves making the following change of variable.

$$z = y^{1-n}$$

On multiplying Eq.(7.7) by $(1-n)y^{-n}$, we obtain

$$(1-n)y^{-n}y' + (1-n)y^{1-n}p(x) = (1-n)Q(x).$$

Since $z' = (1 - n)y^{-n}y'$, we may write the above differential equation in terms of the z variable as follows.

$$z' + (1-n)p(x)z = (1-n)Q(x).$$
(7.8)

Equation (7.8) is a linear differential equation whose solution may be obtain by use of the formula in Eq.(7.6); this solution is

$$z = \exp\left(-(1-n)\int p(x)dx\right)\int (1-n)Q(x)\exp\left[(1-n)\int p(x)dx\right]dx$$
$$+C\exp\left(-(1-n)\int p(x)dx\right).$$
(7.9)

The solution of the original differential equation is obtained by solving $z = y^{1-n}$ for y.

Example 69 Solve the following differential equation:

$$y^3y' + \frac{y^4}{x} = x.$$

Solution : The standard form for the above differential equation is

$$y' + \frac{1}{x}y = xy^{-3}.$$

²This differential equation is named for Jakob (also known as Jacque or James) Bernoulli (1654–1705); his brother Johann (also known as Jean or John) Bernoulli (1667–1748) is known for his work in calculus, calculus of variations, and complex numbers. Daniel Bernoulli (1700–1782), son of Johann Bernoulli, is often called the first mathematical physicist and is known for the Bernoulli principle in hydrodynamics and for other work in astronomy, mathematics, and physics. Also, other members of the Bernoulli family are known for their work in mathematics and in the physical sciences.

 $^{^{3}}$ Gottfried Wilhelm Leibniz (1646–1716), German mathematician who is known for his development of differential and integral calculus.

The above differential equation is of the Bernoulli form where $p(x) \rightarrow 1/x, n \rightarrow -3$, and $Q(x) \rightarrow x$. On applying Eq.(7.9) to the above differential equation, we obtain

$$z = \exp\left(-4\int dx/x\right)\int 4x \exp\left(dx/x\right) dx + C \exp\left(-4\int dx/x\right)$$
$$= 4e^{-4\ln x}\int xe^{4\ln x} dx + Ce^{-4\ln x} = \frac{2}{3}x^2 + \frac{C}{x^4}.$$

Since $z = y^{1-n} = y^4 = 2x^2/3 + C/x^4$, the solution of the original differential equation is

$$y(x) = \left(\frac{2}{3}x^2 + \frac{C}{x^4}\right)^{1/4}$$

Example 70 The motion of a particle in a viscous fluid with Stokes damping, αv , and Newtonian damping, βv^2 , is characterized by an equation of motion with the form

$$\dot{v} + \alpha v = -\beta v^2$$
 subject to $v(0) = v_0$.

The damping coefficients α and β are constants. Find v(t) subject to the indicated initial condition.

Solution: The indicated equation of motion is of the Bernoulli form where $n \to 2, Q(t) \to -\beta$, and $p(t) \to \alpha$, and the general solution is obtain from

$$z = \exp\left(\int \alpha dt\right) \int (-\beta) \exp\left(-\int \alpha dt\right) dt + C \exp\left(\int \alpha dt\right)$$
$$= -\frac{\beta}{\alpha} + Ce^{\alpha t} = \frac{1}{v(t)}.$$

On applying the initial condition, we find that

$$C = \frac{\alpha + \beta v_0}{\alpha v_0}$$
 and $v(t) = \frac{\alpha v_0}{(\alpha + \beta v_0)e^{\alpha t} - \beta v_0}$

A graph of the equation for v(t) characterizes the speed of the particle as a function of time. To obtain position as a function of time, replace v with \dot{x} and solve the resulting first-order differential equation for x(t).

7.4 Second-Order Linear Differential Equations

The superposition of solutions principle, stated here in the form of two theorems, will be assumed valid for second-order linear homogeneous differential equations.

Theorem 1 The set of all solutions of an nth-order ordinary linear homogeneous differential equation forms an n-dimensional vector space.

For a second-order differential equation, Theorem 1 means that

$$y = c_1 y_1 + c_2 y_2$$

is a solution of

$$y'' + p(x)y' + q(x)y = 0$$

if y_1 and y_2 are two linearly independent solutions of the above differential equation and c_1 and c_2 are two arbitrary constants.

Theorem 2 A necessary and sufficient condition that solutions y_1 and y_2 of a secondorder linear differential equation be linearly independent is that a special determinant of these solutions be different from zero. That is to say,

$$\begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} \neq 0.$$

The above determinant is called the **Wronskian**⁴ of y_1 and y_2 , denoted by $W(y_1, y_2)$; it will play an important role in connection with Green's functions.

7.4.1 Homogeneous Differential Equations with Constant Coefficients

The standard form for the general second-order homogeneous differential equation with constant coefficients p_0 and q_0 is

$$y'' + p_0 y' + q_0 y = 0. (7.10)$$

Using the linear operator D defined by $D \equiv d/dx$, we may write the above differential equation as

 $(D^2 + p_0 D + q_0) y = 0.$

The equation

$$D^2 + p_0 D + q_0 = 0 (7.11)$$

is called the auxiliary or characteristic equation. Our procedure for solving Eq.(7.10) involves treating the characteristic equation algebraically and using techniques for solving first-order linear differential equations. The roots of the characteristic equation (a quadratic equation in D), may be (a) real and unequal, (b) real and equal, or (c) a complex-conjugate pair.

Case 1 The roots of the characteristic equation are real and unequal.

Assume the roots of the characteristic equation, Eq.(7.11) are a and b. We may therefore write the original differential equation, Eq.(7.10), in the following factored form:

$$(D-a)u = 0$$
 where $u = (D-b)y$.

The above equations are first-order linear differential equations and may be solved by use of the formula in Eq.(7.6); we obtain

$$u = ce^{ax}$$
 and $y = ce^{bx} \int e^{(a-b)x} dx + c_2 e^{bx}$.

 $^{^4}$ Josef Hoëné de Wronski (1778–1853), Polish mathematician known for work that involved applying philosophy to mathematics. He developed a series expansion whose coefficients were determinants, now known as Wronskians.

In this case, the solution of Eq.(7.10) is

$$y(x) = c_1 y_1 + c_2 y_2 = c_1 e^{ax} + c_2 e^{bx}.$$

Since $a \neq b$ by hypothesis, the Wronskian of y_1 and y_2 is not equal zero; therefore, y_1 and y_2 are two linearly independent solutions of Eq.(7.10).

Example 71 Solve y'' + y' - 2y = 0.

Solution : The corresponding characteristic equation is

$$D^2 + D - 2 = 0$$
 or $(D - 1)(D + 2) = 0$ with roots equal 1 and -2.

By use of the result for Case 1, the general solution of the differential equation to be solved is

$$y(x) = c_1 e^x + c_2 e^{-2x}.$$

Case 2: The roots of the characteristic equation are real and equal. Since the roots of the characteristic equation are real and equal a = b, we may write the original differential equation in the following factored form:

$$(D-a)u = 0$$
 where $u = (D-a)y$.

On solving the above two first-order linear differential equation, we obtain

$$y(x) = c_1 y_1 + c_2 y_2 = c_1 x e^{ax} + c_2 e^{ax}.$$

Again, note that the Wronskian of y_1 and y_2 is not equal zero; hence, y_1 and y_2 are linearly independent solutions of the original differential equation for Case 2.

Example 72 Solve y'' - 2y' + y = 0.

Solution : The characteristic equation may be factored as follows.

$$(D-1)(D-1) = 0$$
 with solutions $a = b = 1$.

By use of the development for Case 2, the general solution of the differential equation to be solved is

$$y(x) = (c_1 x + c_2)e^x.$$

Case 3 The roots of the characteristic equation are a complex conjugate pair. This case is equivalent to that outlined in Case 1 if we set $b = a^*$ where a^* means the complex conjugate of a.

Example 73 Solve y'' + 9y = 0.

Solution : Here the characteristic equation is $D^2 + 9 = 0$ with roots $\pm 3i$. The general solution of the differential equation to be solved is therefore given by

$$y(x) = c_1 e^{3ix} + c_2 e^{-3ix}.$$



Example 74 The Classical Linear Harmonic Oscillator Consider the motion of a mass m attached to the end of a spring with spring constant k (see Fig. 7.2). For applied force with magnitude F and restoring force with magnitude -kx, the equation of motion of this mass when released is Hooke's⁵ law, F = -kx or $m\ddot{x} + kx = 0$.

(a) Find x(t) subject to the initial conditions $x(0) = X_0$ and $\dot{x}(0) = 0$. Condition $x(0) = X_0$ means that initially the mass is a distance X_0 from the equilibrium position; this maximum distance from the equilibrium is called the amplitude. The condition $\dot{x}(0) = 0$ means that the mass is initially at rest. (b) Find the period of the motion.

Solution : The standard form of the equation of motion is

 $\ddot{x} + \omega^2 x = 0$ where $\omega^2 = k/m$.

Part A The corresponding characteristic equation is

 $D^2 + \omega^2 = 0$ with solutions $\pm i\omega$.

The general solution of the equation of motion is therefore

$$\begin{aligned} x(t) &= c_1 e^{i\omega t} + c_2 e^{-i\omega t} \\ &= c_1 (\cos \omega t + i \sin \omega t) + c_2 (\cos \omega t - i \sin \omega t) \\ &= A \cos \omega t + B \sin \omega t. \end{aligned}$$

Applying the initial conditions $x(0) = X_0 = A$ and $\dot{x}(0) = 0 = B\omega$ or B = 0 since $\omega \neq 0$, we obtain the following solution for the original equation of motion

$$x(t) = X_0 \cos \omega t.$$

Part B The period of the motion is the time required for the mass to repeat itself (i.e.,time per cycle); it is determined as follows:

x(t) = x(t+T) where T is the period

⁵Robert Hooke (1635–1702), English scientist known for his work in optics and elasticity. His claim of priority over the inverse square law led to a bitter dispute with Newton.

or

$$X_0 \cos \omega t = X_0 \cos \omega (t+T) = X_0 (\cos \omega t \cos \omega T - \sin \omega t \sin \omega T)$$
$$\implies \omega T = 2\pi n \quad (n = 0, 1, 2, ...).$$

The period is given by

 $T = \frac{2\pi n}{\omega} = 2\pi n \sqrt{\frac{m}{k}};$ *n* is the mode of oscillation.

Example 75 Consider the motion of a particle of mass m initially at rest and subject to a restoring force of -kx and a damping force of $-a\dot{x}$. The equation of motion of this particle is

 $m\ddot{x} = -kx - a\dot{x}$ where $x(0) = X_0$ and $\dot{x}(0) = 0$.

The equation of motion in standard form is

$$\ddot{x} + 2\delta \dot{x} + \omega^2 x = 0$$
 where $\omega^2 = k/m$ and $2\delta = a/m$.

The factor of 2 in the equation of motion is used for convenience. Find the solution of the equation of motion for the following cases (a) $\delta = 0$ (no damping), (b) $\delta = \omega$ (critical damping), (c) $\delta < \omega$ (light damping), and (d) $\delta > \omega$ (heavy damping).

Solution:

Part A The equation of motion for $\delta = 0$ reduces to

$$\ddot{x} + \omega^2 x = 0$$

The solution of the above differential equation (same as in Example 74) is

 $x(t) = X_0 \cos \omega t$ for $x(0) = X_0$ and $\dot{x}(0) = 0$.

The motion in this case ($\delta = 0$; no damping) is oscillatory and periodic with constant amplitude X_0 .

Part B For $\delta = \omega \neq 0$, the solutions of the corresponding characteristic equation are real and equal, $-\delta$. The solution of the equation of motion for critical damping is

$$x(t) = (c_1 t + c_2)e^{-\delta t} = X_0(\delta t + 1)e^{-\delta t}$$
 for $x(0) = X_0$ and $\dot{x}(0) = 0$.

The motion in this case ($\delta = \omega$; critical damping) is not oscillatory and approaches equilibrium at a rapid rate.

Part C For light damping $\delta < \omega$, the solutions of the corresponding characteristic equation are $-\delta \pm i\Delta$ where $\Delta = \sqrt{\omega^2 - \delta^2}$. The solution of the equation of motion is

$$x(t) = X_0 \left(\cos \Delta t + \frac{\delta}{\Delta} \sin \Delta t \right) e^{-\delta t}$$
 for $x(0) = X_0$ and $\dot{x}(0) = 0$.

In this case, the motion is oscillatory with decreasing amplitude, $X_0 e^{-\delta t}$, and is not periodic. Part D For heavy damping $\delta > \omega$, the solutions of the characteristic equation are $-\delta \pm \Delta'$ where $\Delta' = \sqrt{\delta^2 - \omega^2}$. The solution of the equation of motion for heavy damping subject to initial conditions, $x(0) = X_0$ and $\dot{x}(0) = 0$, is

$$x(t) = \frac{(\delta + \Delta')}{2\Delta'} X_0 \exp\left[\left(-\delta + \Delta'\right)t\right] + \frac{(\Delta' - \delta)}{2\Delta'} X_0 \exp\left[-\left(\delta + \Delta'\right)t\right].$$

Here the motion is not oscillatory and approaches equilibrium at a rate less rapid than for critical damping.

7.4.2 Nonhomogeneous Differential Equations with Constant Coefficients

The standard form for second-order nonhomogeneous differential equations with constant coefficients is

$$y'' + p_0 y' + q_0 y = f(x).$$
(7.12)

The two widely used methods for solving differential equations in the above category are

- 1. successive integration and
- 2. undetermined coefficients, $y = y_h + y_p$ where y_h is the solution of the corresponding homogeneous differential equation and y_p is any solution of the nonhomogeneous differential equation. Methods of the above Section are used to find y_h and methods of undetermined coefficients, discussed below, are used to find y_p .

Method of Successive Integration

If a and b are the roots of the characteristic equation corresponding to Eq.(7.12), then Eq.(7.12) may be written as

$$(D-a)u = f(x)$$
 where $u = (D-b)y$. (7.13)

The above two first-order differential equations may be solved by use of the general formula in Eq. (7.6); for u, we obtain

$$u = e^{ax} \int f(x)e^{-ax}dx + c_1 e^{ax}$$

$$\equiv \bar{Q}(x).$$
(7.14)

On substituting u into the second differential equation in Eq.(7.13) and solving for y, we obtain

$$y(x) = e^{bx} \int \bar{Q}(x)e^{-bx}dx + c_2e^{bx}.$$
(7.15)

The expression for $\bar{Q}(x)$ is given in Eq.(7.14). While successive integration is a general method for solving second-order nonhomogeneous differential equations with constant coefficients, it is clear from the appearance of the integrals in the general solution in Eq.(7.15) that this method can be very tedious to carry out for most functions f(x).

Example 76 By use of the method of successive integration, solve

$$y'' - 2y' + y = 2\cos x.$$

Solution : The roots of the characteristic equation of the corresponding homogeneous differential equation are real and equal, +1. The equation for $\bar{Q}(x)$ reduces to

$$\bar{Q}(x) = e^{ax} \int f(x)e^{-ax}dx + c_1e^{ax}$$
$$= 2e^x \int e^{-x}\cos x dx + c_1e^x$$
$$= \sin x - \cos x + c_1e^x.$$

On substituting the above expression for $\bar{Q}(x)$ into Eq.(7.15), the general solution of the original differential equation becomes

$$y(x) = e^{bx} \int \bar{Q}(x)e^{-bx}dx + c_2e^{bx}$$

= $e^x \int e^{-x} [\sin x - \cos x + c_1e^x] dx + c_2e^x$
= $-\sin x + (c_1x + c_2)e^x$.

Method of Undetermined Coefficients Here the general solution of the second-order nonhomogeneous differential equation with constant coefficients is assumed to have the form $y = y_h + y_p$. Physical problems are often solved by use of the method of undetermined coefficients since y_p can often be obtained without difficulty. Systematic methods such as superposition of solutions principle and annihilation operators for finding y_p for any combinations of three types of nonhomogeneous terms (polynomial, exponential, and sine and/or cosine) are given in textbooks on differential equations. Below, we summarize the results for these three cases; values for constants in the assumed expression for y_p are obtained when the appropriate expression is substituted into the original nonhomogeneous differential equation.

- 1. f(x) is a polynomial of degree $n \ge 0$.
 - (a) If 0 is not a root of the characteristic equation, then assume

$$y_p = A_0 + A_1 x + \dots + A_n x^n.$$

(b) If 0 is a single root of the characteristic equation, then assume

$$y_p = x \left(A_0 + A_1 x + \dots + A_n x^n \right).$$

(c) If 0 is a double root of the characteristic equation, then assume

$$y_p = x^2 \left(A_0 + A_1 x + \dots + A_n x^n \right).$$

- 2. f(x) is of the form Ce^{kx} .
 - (a) If k is not a root of the characteristic equation, then assume $y_p = Ae^{kx}$.
 - (b) If k is a single root of the characteristic equation, then assume $y_p = Axe^{kx}$.
 - (c) If k is a double root of the characteristic equation, then assume $y_p = Ax^2 e^{kx}$.
- 3. f(x) is of the form $\sin kx, \cos kx$, or $\sin kx + \cos kx$.
 - (a) If ik is not a root of the characteristic equation, then assume

$$y_p = A\cos kx + B\sin kx.$$

(b) If ik is a single root of the characteristic equation, then assume

$$y_p = Ax\cos kx + Bx\sin kx.$$

Example 77 The equation of motion for a mass attached to the end of a vertical spring fixed at the other end is $\ddot{y} + \omega^2 y = -g$ where g is the acceleration due to gravity. Find y(t) subject to $y(0) = Y_0$ and $\dot{y}(0) = 0$.

Solution: The general solution of the homogeneous equation, $\ddot{y}+\omega^2 y=0$, is $y_h = A\cos\omega t + B\sin\omega t$ since the roots of the characteristic equation are $\pm i\omega$. The nonhomogeneous term is a constant (polynomial form), and we assume that $y_p = A_0$. On substituting y_p into the original differential equation, we obtain $A_0 = -g/\omega^2$ or $y_p = -g/\omega^2$. The general solution $(y = y_h + y_p)$ of the original differential equation is

$$y(t) = A\cos\omega t + B\sin\omega t - g/\omega^2.$$

Initial condition $y(0) = Y_0$ leads to $A = Y_0 - g/\omega^2$, and initial condition $\dot{y}(0) = 0$ yields B = 0. The particular solution, therefore, becomes

$$y(t) = \left(Y_0 + \frac{g}{\omega^2}\right)\cos\omega t - \frac{g}{\omega^2}.$$

A graph of the above equation characterizes the motion, position as a function of time, of this particle.

Example 78 By use of the method of undetermined coefficients, solve

$$y'' - 2y' + y = 2\cos x.$$

Solution : Since the roots of the characteristic equation are both 1 (double root, real and equal), the solution of the corresponding homogeneous differential equation is

$$y_h = (c_1 x + c_2) e^x.$$

The roots of the characteristic equation are not equal ik = i (k = 1, in this case; see Case 2 above, exponential form), and the assumed form for y_p is

$$y_p = A\cos kx + B\sin kx.$$

On substituting the above equation for y_p into the original differential equation, we obtain

$$-(A\cos kx + B\sin kx) + 2(A\sin kx - B\cos kx) + A\cos kx + B\sin kx = 2\cos x.$$

From the above equation, it is clear that A = 0 and B = -1; hence, $y_p = -\sin x$. The general solution $(y = y_h + y_p)$ of the original equation is therefore

$$y(x) = (c_1 x + c_2)e^x - \sin x.$$

The above result is, of course, the same as that obtained in Example 76.

7.4.3 Homogeneous Differential Equations with Variable Coefficients

The standard form for homogeneous differential equations with variable coefficients is

$$y'' + p(x)y' + q(x)y = 0 (7.16)$$

The usual procedure for solving differential equations of the form given in Eq.(7.16) is the power series method due to Frobenius and Fuchs⁶. Here we concentrate on developing a solution of Eq.(7.16) near the origin. The Frobenius-Fuchs method, however, can easily be extended to obtain solutions away from the origin.

The Frobenius-Fuchs theorem yields the following two types of information concerning the solution of Eq. (7.16): (a) form of the solution as a result of the nature of p(x) and q(x) and (b) form of the solution as indicated by the nature of the solution of the indicial equation. We will not make use of the second type of information. Information of the first kind is as follows:

1. If p(x) and q(x) are regular at x = 0, then Eq.(7.16) possesses two distinct solutions of the form

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda} \quad (a_{\lambda} \neq 0).$$

2. If p(x) and q(x) are singular at x = 0 but xp(x) and $x^2q(x)$ are regular at x = 0, then there will always be at least one solution of Eq.(7.16) of the form

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda+k} \quad (a_{\lambda} \neq 0).$$

3. If p(x) and q(x) are irregular singular points at x = 0 (i.e., xp(x) and $x^2q(x)$ are singular at x = 0), then regular solution of Eq.(7.16) may not exist. In this case, no general method for solving the equation is known.

Since many problems in physics lead to differential equations in category 2 and differential equations in category 1 are just special cases of type 2, we only focus on differential equations in category 2. We now give the details of a simple example to illustrate the power series method.

Example 79 Consider the differential equation

$$xy'' + 2y' + xy = 0.$$

By use of the power series method, obtain the (a) indicial equation and its two solutions, (b) recursion formula, and (c) general solution of the differential equation, y(x).

⁶Lazarus Immanuel Fuchs (1833-1902), German mathematician known for his work in differential equations and the theory of functions. He studied at the University of Berlin with Kummer and Weierstrass.

Solution : The standard form of this differential equation is

$$y'' + \frac{2}{x}y' + y = 0.$$

Note that $p(x) \to 2/x$ and $q(x) \to 1$; hence the differential equation is of the type 2 form, and the form the solution is

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda+k} \quad (a_{\lambda} \neq 0).$$

On substituting the above equation into the original differential equation, one obtains

$$\sum_{\lambda=0}^{\infty} a_{\lambda} \left(\lambda+k+1\right) \left(\lambda+k\right) x^{\lambda+k-2} + \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda+k} = 0.$$

The basic plan at this stage is to write the above equation using a single sum. On replacing λ with $\lambda' + 2$ in the first sum, the power of x in the first sum becomes the same as that in the second sum. The above equation now becomes

$$\sum_{\substack{\lambda=\lambda'+2=0;\\\lambda'=-2}}^{\infty} a_{\lambda'+2} \left(\lambda'+k+3\right) \left(\lambda'+k+2\right) x^{\lambda'+k} + \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda+k} = 0.$$

Since the sum is independent of the index, λ' (a dummy index) in the first sum may be replaced with λ , and we may write the above equation as

$$0 = a_0 k(k+1) x^{k-2} + a_1(k+1)(k+2) x^{k-1} + \sum_{\lambda=0}^{\infty} \{a_{\lambda+2} (\lambda+k+3) (\lambda+k+2) + a_{\lambda}\} x^{\lambda+k}.$$

Terms in the above equation are linearly independent, and we required that

 $a_0k(k+1) = 0$ (indicial equation);

$$a_1(k+1)(k+2) = 0;$$
 and

$$a_{\lambda+2}(\lambda+k+3)(\lambda+k+2)+a_{\lambda}=0$$
 (recursion formula).

The **indicial equation** results from equating the coefficient of the lowest power of the variable to zero. The **recursion** (one-after-another) **formula** is used to evaluate the coefficients for the remaining powers of the variable. In this case, the solutions of the indicial equation are k = 0 and k = -1. When k = 0, $a_1 = 0$, because (in this case) of equation between the indicial equation and the recursion formula. The coefficient a_1 is arbitrary when k = -1, and two independent solutions of the original differential equation may be obtained by use of k = -1 since a_0 is arbitrary by hypothesis. (Use of k = 0, in addition

to k = -1, will produce a redundant set of coefficients; see Problem 7.31.) The form of the solution of the original differential equation becomes

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{\lambda-1}.$$
(7.17)

Values for the coefficients in the above equation are obtained from the recursion formula using k = -1. The general expressions for even and odd expansion coefficients respectively are

$$a_{2j} = \frac{(-1)^j a_0}{(2j)!}$$
 and $a_{2j+1} = \frac{(-1)^j a_1}{(2j+1)!}$ $(j = 0, 1, 2, ...).$

The general solution of the original differential equation is obtained by substituting the above coefficients into Eq.(7.17), we obtain

$$y(x) = a_0 \sum_{j=0}^{\infty} \frac{(-1)^j x^{2j}}{(2j)!} + a_1 \sum_{j=0}^{\infty} \frac{(-1)^j x^{2j+1}}{(2j+1)!}.$$

7.4.4 Nonhomogeneous Differential Equations with Variable Coefficients

Variation of parameters and Green's functions methods are normally used to solved nonhomogeneous linear differential equations with variable coefficients that occur in mathematical physics. The standard form for these differential equations is

$$y'' + p(x)y' + q(x)y = f(x).$$
(7.18)

The method of variation of parameters due to Lagrange will now be used to solve Eq.(7.18) subject to the conditions given below. Assume the solution has the form

$$y(x) = v_1(x)y_1 + v_2(x)y_2.$$
(7.19)

In the above equation, y_1 and y_2 are two linearly independent solutions of the corresponding homogeneous differential equation; they can be determined by use of the power series method developed in the previous Section. Functions v_1 and v_2 are unknown parameters to be determined. We assume that f(x) is continuous in some region of interest $a \le x \le b$ and that

$$v_1'y_1 + v_2'y_2 = 0. (7.20)$$

Note that

$$y' = v_1 y'_1 + v_2 y'_2$$
 and $y'' = v'_1 y'_1 + v_1 y''_1 + v'_2 y'_2 + v_2 y''_2$. (7.21)

Substituting Eqs.(7.19 and 7.21) into Eq.(7.18) and using the fact that y_1 and y_2 are solutions of the homogeneous equation corresponding to Eq.(7.18), we obtain

$$v_1'y_1' + v_2'y_2' = f(x).$$
Solving the above equation and Eq.(7.20) for v'_1 and v'_2 , we obtain

$$v_1' = \frac{\begin{vmatrix} 0 & y_2 \\ f(x) & y_2' \end{vmatrix}}{\Delta} = -\frac{y_2 f(x)}{\Delta} \quad \text{where} \quad \Delta = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix}$$

and

$$v_2' = \frac{\begin{vmatrix} y_1 & 0 \\ y_1' & f(x) \end{vmatrix}}{\Delta} = \frac{y_1 f(x)}{\Delta}.$$

The quantity Δ is just the Wronskian $W(y_1, y_2)$ of y_1 and y_2 ; it is not equal zero since y_1 and y_2 are linearly independent by hypothesis. Solving the above equations for v_1 and v_2 and substituting the results into Eq.(7.19), we obtain the solution of Eq.(7.18) subject to the assumption in Eq.(7.20); the general solution of Eq.(7.18) may be written as

$$y(x) = -y_1 \int \frac{f(x)y_2 dx}{W(y_1, y_2)} + y_2 \int \frac{f(x)y_1 dx}{W(y_1, y_2)}.$$
(7.22)

Example 80 By use of the variation of parameters method, solve

$$x^{2}y'' - 2xy' + 2y = x\ln x \quad (x \neq 0).$$

Solution : The standard form for this differential equation is

$$y'' - \frac{2}{x}y' + \frac{2}{x^2}y = \frac{\ln x}{x}.$$

On comparing the above equation with Eq.(718), we find that p = -2/x, $q = 2/x^2$, and $f(x) = \ln/x$. Take $y_1 = x$ and $y_2 = x^2$ where $W(y_1, y_2) = x^2$. The general solution of the original differential equation is

$$y(x) = -x \int \frac{x^2 (\ln x/x) dx}{x^2} + x^2 \int \frac{x (\ln x/x) dx}{x^2}$$
$$= -x \int \frac{\ln x dx}{x} + x^2 \int \frac{\ln x dx}{x^2}$$
$$= -x \left[\frac{1}{2} (\ln x)^2 + \ln x + 1 \right] - c_1 x + c_2 x^2.$$

Equation (7.22) will now be put in the form of a definite integral that is useful in solving initial or boundary value problems. Let x be a point in the closed interval [a, b] such that the first term in Eq.(7.22) is replaced by a definite integral from b to x and the second term in Eq.(7.22) is replaced by a definite integral from a to x. In terms of the two indicated definite integrals, Eq.(7.22) becomes

$$y(x) = \int_{a}^{x} \frac{y_{1}(t)y_{2}(x)f(t)dt}{W(t)} + \int_{x}^{b} \frac{y_{1}(x)y_{2}(t)f(t)dt}{W(t)}$$
$$= \int_{a}^{b} G(x,t)f(t)dt.$$

The function G(x,t) in the above equation is called the **Green's function** for Eq.(7.18) subject to the appropriate boundary conditions. The Green's function is defined by

$$G(x,t) = \begin{cases} y_1(t)y_2(x)/W(t) \equiv G_1 & \text{for } a < t < x \\ y_1(x)y_2(t)/W(t) \equiv G_2 & \text{for } x < t < b. \end{cases}$$

Note that the Green's function depends only on y_1, y_2 , and the Wronskian. The quantity W(t) means $W[y_1(t), y_2(t)]$. The value of the Green's function approach is related to the fact that initial or boundary conditions are incorporated in the formulation of the problem in a natural manner. At t = a, $G_1(x, t)$ satisfies the boundary condition imposed on y(x) and $G_2(x, t)$ satisfies the boundary condition for y(x) at t = b.

Example 81 By use of the Green's function method, find the solution of

$$y'' = 6x$$
 where $y'(0) = y(1) = 0$, $y_1 = x$, and $y_2 = x - 1$.

Solution : Here the Wronskian equals 1 and the Green's functions become

$$G_1(x,t) = t(x-1)$$
 for $0 \le t \le x$
 $G_2(x,t) = x(t-1)$ for $x \le t \le 1$.

The solution of the differential equation is

$$y(x) = \int_0^1 G(x,t)(6t)dt = x^3 - x.$$

7.5 Some Numerical Methods

Numerical methods are treated in details in many textbooks on the subject, and a summary of essential features of numerical methods related to solutions of ordinary differential equations is given in this section. In general, the numerical solution of a differential equation consists of a table (or graph) of values of the dependent variable for corresponding values of the independent variable.

7.5.1 The Improved Euler Method for First-Order Differential Equations

The basic idea of Euler's method for solving first-order ordinary differential equations is to convert the differential equation (which is continuous) to a difference equation (which is discrete). The general form for a first-order ordinary differential equation will now be written as

$$\frac{dy}{dx} = f(x, y).$$

By use of the definition of a derivative, the above equation may be written as

$$\lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \left[\frac{y(x + \Delta x) - y(x)}{\Delta x} \right] = f(x, y).$$

The basic idea of the finite difference method involves writing the above equation as

$$y(x_{n+1}) = y(x_n) + f(x_n, y_n) \Delta x.$$
(7.23)

The result in Eq.(7.23) is the **Euler algorithm** for solving first-order ordinary differential equations. The notations in Eq.(7.23) have the following meanings: $x_{n+1} = x_n + \Delta x$ and $y(x_{n+1}) = y_{n+1}$. To apply Euler's method, first select the interval size Δx , then evaluate y(x) at x_0 , and after that evaluate f(x, y) at (x_0, y_0) . The result for $y(x_1)$ is

$$y(x_1) = y(x_0) + f(x_0, y_0) \Delta x.$$

A second iteration with inputs $y(x_1)$ from the above equation and $f(x_1, y_1)$ yields $y(x_2)$; the result is

$$y(x_2) = y(x_1) + f(x_1, y_1)\Delta x_1$$

The iteration is continued to yield a numerical solution of the required first-order ordinary differential equation in the region of interest. A systematic procedure for calculating the error involved during each iteration does not exist for Euler's method.

To improve the simple Euler method, the class of first-order differential equations is restricted to those whose solutions can be expanded in a Taylor series. Neglecting terms of order $(\Delta x)^3$ and smaller, one obtains

$$y(x_{n+1}) = y(x_n) + \Delta x f(x_n, y_n) + \frac{(\Delta x)^2}{2} \left[\frac{\partial f(x_n, y_n)}{\partial x} + f(x_n, y_n) \frac{\partial f(x_n, y_n)}{\partial y} \right]$$

The above equation is referred to as the **improved Euler method** and will be used to obtain solutions of first-order ordinary differential equations.

Example 82 The equation of motion for a certain particle is

$$\dot{v} + \alpha v = q; \qquad v(0) = 0.$$

For $\alpha = 0.01 \ s^{-1}$ and $g = 9.8 \ ms^{-1}$, the analytic solution of this equation of motion is

$$v(t) = rac{g}{lpha} \left(1 - e^{-lpha t}
ight).$$

Find the numerical solution of this equation of motion by use of the improved Euler method. Solution: The general form of the improved Euler method for the differential equation $\dot{v} = g - \alpha v$ is

$$v(t_{n+1}) = v(t_n) + \Delta t f(t_n, v_n) + \frac{(\Delta t)^2}{2} \left[\frac{\partial f(t_n, v_n)}{\partial t} + f(t_n, v_n) \frac{\partial f(t_n, v_n)}{\partial v} \right].$$

For arbitrary Δt in the above equation, the quantities reduce to

$$f(t_n, v_n) = g - \alpha v(t_n), \quad \frac{\partial f(t_n, v_n)}{\partial t} = 0, \text{ and } \frac{\partial f(t_n, v_n)}{\partial v} = -\alpha.$$

The essential programming statement for calculating the numerical solution of the original differential equation is

$$v(n+1) = v(n) + \left[g - \alpha v(n)\right] \left[\Delta t - \alpha \left(\Delta t\right)^2 / 2\right].$$

7.5.2 The Runge-Kutta Method for First-Order Differential Equations

There exist many methods for finding numerical solutions of first-order ordinary differential equations, and the Runge⁷-Kutta⁸ method is probably the most often used method. As with the Euler and the improved Euler methods, the essential problem is to generate a table of values for x and y for the differential equation y' = f(x, y) when y(x) at $x = x_0$ is given. The problem is to develop a method for finding y_1 at $x_0 + \Delta x$, y_2 at $x + 3\Delta x$, and successive values for y_n throughout the range of interest. For calculating successive values of $y(x_n)$ in the differential equation y' = f(x, y), the Runge-Kutta methods use a recurrence formula in the form

$$y_{i+1} = y_i + \Delta x \sum_{i=1}^n a_i k_i.$$
 (7.24)

Of the many parameters a_i and k_i in Eq.(7.24), some are chosen arbitrarily and others are obtained by use of the Taylor series involving one and two variables. The order of the Runge-Kutta approximation is indicated by the value of n in Eq.(7.24). Evaluation of the parameters in Eq.(7.24) for n > 4 in the Runge-Kutta approximation is straight forward but involves tedious algebraic manipulations. For $h = \Delta x$, the formula for the fourth-order Runge-Kutta method reduces to

$$y_{i+1} = y_i + \frac{1}{6} \left(k_1 + 2k_2 + 2k_3 + k_4 \right) + \varphi \left(h^5 \right).$$
(7.25)

In Eq.(7.25), $\varphi(h^5)$ denotes terms of order h^5 , and the k parameters are determined by use of

$$k_1 = hf(x_i, y_i); \quad k_2 = hf(x_i + h/2, y_i + k_1/2); k_3 = hf(x_i + h/2, y_i + k_2/2); \quad k_4 = hf(x_i + h, y_i + k_3).$$

Example 83 Find the numerical solution of the differential equation in the previous Example by use of the fourth-order Runge-Kutta method.

Solution : The general form of the Runge-Kutta method for the differential equation $\dot{v} = g - \alpha v$ is

$$v(n+1) = v(n) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

The parameters k reduce to

$$k_1 = h[g - \alpha v(n)]; \quad k_2 = h[g - \alpha \{v(n+h/2) + k_1/2\}];$$

$$k_3 = h[g - \alpha \{v(n+h/2) + k_2/2\}]; \quad k_4 = h[g - \{v(n+h) + k_3\}].$$

⁷Carl David Tolmé Runge (1856–1927), German mathematician known for his work in the numerical solutions of algebraic equations and for work in differential geometry.

⁸Martin Wilhelm Kutta (1867–1944), German mathematician who is best known for the Runge-Kutta method. Runge presented Kutta's method.

7.5.3 Second-Order Differential Equations

Numerical solutions of second-order differential equations are obtained by first reducing them to a system of first-order differential equations and applying the methods for solving first-order differential equations. The general second-order differential equation may be written as

$$\frac{d^2y}{dx^2} = f(x, y, y').$$
(7.26)

For z = dy/dx, Eq.(7.26) reduces to the following pair of first-order differential equations

$$\frac{dz}{dx} = f(x, y, z) \quad \text{and} \quad \frac{dy}{dx} = z = g(x, y, z).$$
(7.27)

The procedure for solving Eq.(7.26) is to solve the first equation in Eq.(7.27) with condition y'(0) and use that result as an input for the second equation in Eq.(7.27) to obtain the solution y(x) with condition y(0).

7.6 Problems

7.1 Classify (order and degree; homogeneous or nonhomogeneous; linear or nonlinear) the following differential equations:

(a)
$$(\ell + y^2) y'' + xy' + x = e^x$$
 (d) $\ddot{\theta} + g \sin \theta / \ell = 0$
(b) $y'' + (y')^2 + xy = 0$ (e) $y' + xy^2 = 0$.
(c) $y'' + (y')^{1/2} + xy = 0$

7.2 Verify that the first equation in each set is a solution of the corresponding differential equation.

(a)
$$x^{2} = 2y^{2} \ln y;$$
 $y' = xy/(x^{2} + y^{2})$
(b) $x^{2} + y = xy;$ $x^{3}y' - x^{2}y + y^{2} = 0$
(c) $y = e^{x} + e^{2x};$ $y'' - 3y' + 2y = 0$
(d) $y = x - x \ln x;$ $xy' + x - y = 0$
e) $y = x \tan(x + c);$ $xy' = x^{2} + y^{2} + y.$

7.3 Test the following differential equations for exactness and solve the exact equations:

(

(a)
$$(2x^3 - 3x^2y + y^3) dy/dx = 2x^3 - 6x^2y + 3xy^2$$

(b) $2xydy/dx + y^2 = a + 2bx$

(c)
$$x (x^2 + 2y^2) dx + y (2x^2 + y^2) dy = 0$$

(d) $mdv/dt + V dm/dt = 0$
(e) $x (y^2 + 2) dy/dx = (x + 1) (y^2 + 1)$.

7.4 Find the general solution for each of the following differential equations:

(a)
$$y' = ky$$
 (b) $y' = ax + by$ (c) $y - y' - xy^2 = 0$
(d) $y' + 2y - x - e^{-2x} = 0$ (e) $xy' + 2y = 12x$.

7.5 Find the solution of each of the following differential equations subject to the indicated condition:

(a)
$$y' = y^2$$
; $y(0) = 1$ (b) $m\dot{v} + kv = g$; $v(0) = v_0$
(c) $y' = e^y$; $y(0) = 0$ (d) $y' + y = y^2 e^{2x}$; $y(0) = 1$
(e) $e^y (y' + 1) = 1$; $y(0) = 1$.

7.6 If a rocket is projected vertically upward under gravity, the equation describing its motion is

$$m\frac{dv}{dt} + V\frac{dm}{dt} = -mg$$

where V is the speed of the exhaust gas relative to the rocket. Find v(t) for v(0) = 0and m(0) = M. (The other symbols in the equation have their usual meaning; neglect external forces.)

7.7 Assume that a spherical drop evaporates at a rate proportional to its surface area. Find an explicit expression for the radius of the drop as a function of time if r(0) = 3 mm and r(1hr) = 2 mm.

7.8 A certain radioactive material has a half-life of 2 hr. Find the time required for a given amount of this material to decay to one-tenth of its original amount.

7.9 Five percent of a radioactive substance is lost in 100 yr. How much of the original amount will be present after 250 yr?

7.10 For $\dot{v} + \alpha v = -\beta v^2$ where $v(0) = v_0$, find x(t).

7.11 (a) Write the appropriate differential equation for the circuit in Fig. 7.3. (Here I, the current, is the dependent variable, and time is the independent variable.) (b) Solve the equation in part (a) for I(0) = 0 and constant E, R, and L. (c) Now, assume $E(t) = E_0 \sin \omega t$ in part (a) and solve the resulting differential equation with constant E_0 and ω .

7.12. A metal ball having a temperature of 80° C is placed into m grams of ice water at 0° C. After ten minutes, the temperatures of the ball and water are 60° C and 20° C, respectively. Now, the ball is transferred to another m grams of ice water at 0° C. Calculate



Figure 7.3

the temperature of the ball at the end of another (a second) ten-minute interval if the only exchange of heat is between the ball and the water. (*Hint*: Use Newton's law of cooling.) 7.13 A raindrop falls from rest at a place where the air resistance is proportional to the speed, kv. (a) Derive the expression for the speed of the drop as a function of time. (b) When $t \to \infty$, the expression for the terminal speed results. Derive the expression for the terminal speed of the drop. (c) Derive the expression for the position of the drop as a function of time.

7.14 Solve the following differential equations:

(a)
$$y'' + 7y' + 12y = 0$$
 (b) $y'' + 2y' + 2y = 0$ (c) $y'' + 6y' + 9y = 0$
(d) $\frac{d}{dr} (r^2 dv/dr) = 0;$ $v(a) = v_a$ and $v(b) = v_b$
(e) $\ddot{y} + 6\dot{y} + 13y = 0;$ $y(0) = 2$ and $\dot{y}(0) = 1.$

7.15 Solve the following differential equations:

(a) y'' + y = x (b) $y'' - y' - 2y = x^3$ (c) $y'' + y' - 6y = 12e^{-x}$ (d) $y'' + 3y' + 2y = e^{-x}$ (e) $y'' + 3y' = 10\sin x$; y(0) = y'(0) = 0.

7.16 If $y_1 = x$ and $y_2 = xe^x$ are two solutions of the homogeneous differential equation associated with

$$x^{2}y'' - (x^{2} + 2x)y' + (x + 2)y = x^{3},$$

(a) show that y_1 and y_2 are linearly independent and (b) find the general solution of the differential equation.

7.17 Euler's differential equation (sometimes called Cauchy's differential equation),

$$x^{n}\frac{d^{n}y}{dx^{n}} + a_{1}x^{n-1}\frac{d^{n-1}y}{dx^{n-1}} + \dots + a_{n-1}x\frac{dy}{dx} + a_{n}y = f(x)$$

sometimes occurs in physical problems. It can be reduced to an *n*th-order linear differential equation with constant coefficients by use of a change of variable, $x = e^z$. (a) Show that

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} - y = \ln x$$

can be reduced to

$$\frac{d^2y}{dz^2} - y = z$$

(b) By first solving the reduced differential equation, find the solution of the original differential equation.

7.18 Consider the equation $y'' + \lambda^2 y = 0$. Find the eigenvalues (restricted values of λ_n) and the corresponding eigenfunctions, $y_n(x)$, of this differential equation for the conditions (a) y'(0) = 0 and $y'(\pi) = 0$ and (b) y'(0) = 0 and $y'(\pi) = 0$. 7.19 The **Riccati⁹ equation**,

$$\frac{dy}{dx} = P(x)y^2 + Q(x)y + R(x),$$

is a nonlinear differential equation that is of considerable importance in particle dynamics. By use of a change of the dependent variable y = -[1/P(x)]dz/dx, show that the Riccati differential equation becomes

$$\frac{d^2z}{dx^2} - \left(Q + \frac{1}{P}\frac{dP}{dx}\right)\frac{dz}{dx} + PRz = 0$$

which is a second-order linear differential equation. 7.20 (a) By use of $y = z \exp[-1/2 \int_{-\infty}^{\infty} p(t)dt]$, show that

$$y'' + p(x)y' + q(x)y = 0$$

transforms into

$$z'' + f(x)z = 0.$$

(b) Determine the expression for f(x). Note that **Leibniz's formula** for the derivative of an integral is useful in solving this problem,

$$\frac{d}{d\alpha} \int_{g(\alpha)}^{h(\alpha)} f(x,\alpha) dx = \int_{g(\alpha)}^{h(\alpha)} \frac{\partial f(x,\alpha)}{\partial \alpha} + f[h(\alpha),\alpha] \frac{dh(\alpha)}{d\alpha} - f[g(\alpha),\alpha] \frac{dg(\alpha)}{d\alpha}.$$

7.21 The vertical motion of a particle of mass m on a spring with spring constant k is described by the following differential equation:

$$m\ddot{y} = -ky + mg;$$
 $y(0) = y_0$ and $\dot{y}(0) = 0.$

 $^{^{9}}$ Jocopo Francesco Riccati (1676–1754), Italian mathematician who is best known for his studies of the Riccati differential equation.

Solve this differential equation for the position of the particle as a function of time. 7.22 A particle of mass m is projected vertically upward with a speed of v_0 . The particle is subject to gravity and a force of air resistance that is proportional to v. Find the expression for the maximum height reached by the particle.

7.23 The steady flow of heat in a uniform rod of length ℓ is described by the equation

$$rac{d^2T}{dx^2} - \gamma T = 0; \quad T(0) = T_1 \quad ext{and} \quad T(\ell) = T_2,$$

where γ is a constant which characterizes the material. Find the solution of this differential equation subject to the indicated boundary conditions.

7.24 If a thin wire of length ℓ is heated by an electric current, the differential equation for its temperature distribution has the form

$$\frac{d^2T}{dx^2} + b^2T = -k \quad \text{for} \quad k > 0; \quad T(0) = 0 \quad \text{and} \quad T(\ell) = 0.$$

The coefficient b characterizes the material. Discuss the solution of this differential equation for the following three cases: (a) $b^2 > 0$, (b) $b^2 = 0$, and (c) $b^2 < 0$.

 $7.25~{\rm According}$ to Kepler's 10 first law, the path of a certain planet about the sun is an ellipse

$$r = \frac{\alpha}{1 + \epsilon \cos \theta}$$

with the sun at one focus. By use of the differential equation of orbits

$$\frac{d^2 u}{d\theta^2} + u = -\frac{\mu F(1/u)}{\ell^2 u^2} \quad \text{ where } \quad u = \frac{1}{r} \quad \text{and } \quad -\frac{\partial V}{\partial r} = F(r),$$

determine the central force law F(r) for this motion.

7.26 Consider the motion of a planet such that the force law is

$$F(r) = -rac{k}{r^2} + rac{k'}{r^3}$$
 where $k' \ll k$.

By use of the differential equation for orbits (see Problem 7.25), obtain the equation for the orbit of this planet.

7.27 Consider a damped harmonic oscillator, $\ddot{x} + 2\alpha \dot{x} + \beta^2 x = F(t)/m$, with an applied force of $F_0 \sin \omega t$ and critical damping given by $\alpha = \beta$. Derive the expression for a particular solution and show that it can be put into the following form:

$$x(t) = rac{F_0 \sin{(\omega t - 2 \phi)}}{m\,(eta^2 + \omega^2)}; \qquad ext{where} \quad \phi = an^{-1}\left(rac{\omega}{eta}
ight).$$

7.28 The equation of motion for a simple pendulum is $m\ell\ddot{\theta} = -mg\sin\theta$ where ℓ is the length, m is the mass of the bob, and g is the acceleration due to gravity. (a) By use of the

¹⁰Johannes Kepler (1571–1630), German mathematician and scientist best known for his three laws of planetary motion.

small-angle approximation $[\sin \theta \approx \tan \theta \approx \theta$ (in radians)], find $\theta(t)$ and the expression for the period of the motion. (b) Show that the original equation of motion may be written as

$$rac{1}{2}rac{d(\dot{ heta}^2)}{d heta} = -n^2\sin heta \qquad ext{where} \qquad n^2 = rac{g}{\ell}.$$

(c) Show that the following integral (elliptic integral) must be evaluated to obtain the solution of the equation in part (b):

$$-\int_{\theta_0}^{\theta} \frac{d\theta}{\left(2\cos\theta - 2\cos\theta_0\right)^{1/2}} = nt \quad \text{ where } \quad \theta(0) = \theta_0 \quad \text{and } \quad \dot{\theta}(0) = 0$$

The expression for the period in this general case is

$$T = \frac{4}{\pi} \left[\frac{\pi}{2} + \frac{1}{2} \frac{\pi}{4} \sin^2 \left(\frac{\theta_0}{2} \right) + \frac{3}{8} \frac{3\pi}{16} \sin^4 \left(\frac{\theta_0}{2} \right) + \cdots \right]$$
$$\approx \frac{2\pi}{n} \left(1 + \frac{\theta_0}{16} \right).$$

7.29 In the Example involving xy'' + 2y' + xy = 0 on page 182, show that use of k = 0 (in addition to k = -1) produces a redundant set of coefficients.

7.30 By use of the generalized power series method, solve

$$xy'' + 2y' + xy = 0; \quad y(0) = 1 \quad \text{and} \quad y'(0) = 0.$$

7.31 Solve the Euler-Cauchy differential equation, $x^2y'' + 2y' = 0$, by use of the generalized power series method.

7.32 By use of the power series method, find the solution of

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = \ell(\ell+1).$$

7.33 By use of the Fourier transform method, solve the ordinary differential equation for the forced harmonic oscillator, $\ddot{x} + 2\alpha\dot{x} + \omega_0^2 x = f(t)$, subject to the initial conditions that x(t) and $\dot{x}(t)$ go to zero as t goes to plus and minus infinity.

Chapter 8

Partial Differential Equations

8.1 Introduction

Physical problems involving two or more independent variables are often described (i.e., mathematically modeled) by use of partial differential equations. **Partial differential equations** contain partial derivatives with respect to two or more independent variables. Some methods for solving partial differential equations are (a) *direct integration*; (b) *separation of variables*; (c) *Fourier and Laplace transforms*; (d) *Green's functions*; and (e) *characteristics*.

There are partial differential equations whose solutions cannot be obtained by use of the above methods; constructing the solutions for such differential equations is beyond the scope of this book. However, many partial differential equations used in the mathematical modeling of physical problems can be solved by use of these five methods.

Appropriate boundary (space) and/or initial (time) conditions must be applied to the general solution of a partial differential equation to obtain a suitable solution for the problem under investigation. Three common types of boundary conditions are

- 1. Dirichlet: specification of the solution at each point on the boundary;
- 2. Neumann: specification of the normal derivative of the solution at each point on the boundary; and
- 3. Cauchy: specification of appropriate initial value(s), Dirichlet and Neumann conditions when appropriate.

The following equations are examples of important partial differential equations in physics involving the Laplacian operator.

$$\nabla^2 u = 0;$$
 Laplace's equation. (8.1)

The function u(x, y, z) in Eq.(8.1) may represent electric potential in a charge-free region, gravitational potential in a region free of matter, or steady-state (time-independent) temperature in a region without a heat source.

$$\nabla^2 u = f(x, y, z);$$
 Poisson's equation. (8.2)

The function u(x, y, z) in Eq.(8.2) may represent electric potential, gravitational potential, or steady-state temperature in regions with respective sources denoted by f(x, y, z).

$$\nabla^2 u = \frac{1}{\sigma} \frac{\partial u}{\partial t};$$
 heat conduction (or diffusion) equation. (8.3)

In Eq.(8.3), the function u(x, y, z, t) may represent a time-dependent temperature in a region without a heat source or concentration of a diffusing substance. The constant σ is called the **diffusivity**.

$$abla^2 u = rac{1}{v^2} rac{\partial^2 u}{\partial t^2};$$
 mechanical wave equation. (8.4)

The function u(x, y, z, t) in Eq.(8.4) may represent the motion of a vibrating string or membrane, and v is the speed of the wave motion.

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)\right\}\Psi = i\hbar\frac{\partial\Psi}{\partial t}; \quad \text{Schrödinger's equation.}$$
(8.5)

In quantum mechanics, Schrödinger's (wave) equation is the basic equation of motion of a microscopic particle of mass m, and $\Psi(x, y, z, t)$ is called the **wave function**. The potential energy of the particle is represented by V(x, y, z), and other quantities in this equation have their usual meaning.

This chapter is mainly devoted to the physical applications of linear second-order homogeneous partial differential equations in two independent variables; the general form for equations in this category is

$$A\frac{\partial^2 u}{\partial x^2} + 2B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial t^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu = 0.$$
(8.6)

In Eq.(8.6), the coefficients may be a function of x and y, and properties of the solution of the differential equation depend on the relative magnitudes of the coefficients. Based on the coefficients in Eq.(8.6), partial differential equations are classified as follows.

$$AC - B^2 \begin{cases} > 0; & \text{elliptic,} \\ < 0; & \text{hyperbolic, and} \\ = 0; & \text{parabolic.} \end{cases}$$

The general equation of a conic section $(Ax^2 + 2Bxy + Cy^2 = 1)$ representing an ellipse, a hyperbola, or a parabola is the basis for above classification. According to these classifications, note that the (a) two-dimensional Laplace equation is elliptic; (b) one-dimensional mechanical wave equation is hyperbolic; and (c) one-dimensional heat conduction (diffusion) and Schrödinger equations are parabolic. The geometrically related classifications are not of primary importance when solving the differential equation by use of analytic methods but do reflect the nature of the boundary conditions. For example, solutions of elliptic equations must satisfy conditions on a closed boundary. In this Section, the focus will be on direct integration and separation of variables methods for solving the partial differentials involved in physical applications. In Section 8.2, the separation of variables and Fourier transform methods are illustrated. Example 84 By use of direct integration, solve

$$\frac{\partial^2 u(x,y)}{\partial x \partial y} = x^2 y; \quad u(x,0) = x^2 \quad and \quad u(1,y) = \cos y.$$

Solution : On integrating the original partial differential with respect to x, we obtain

$$\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = x^2 y$$
 or $\frac{\partial u}{\partial y} = \frac{1}{3}x^3 y + f(y)$.

Integrating the above first-order ODE with respect to y, we obtain

$$u(x,y) = \frac{1}{6}x^{3}y^{2} + \int f(y)dy + g(x) = \frac{1}{6}x^{3}y^{2} + F(y) + g(x)$$

where $F(y) = \int f(y)dy$.

Condition 1:

$$u(x,0) = x^{2} = F(0) + g(x) \Longrightarrow g(x) = x^{2} - F(0)$$

$$u(x,y) = x^{3}y^{2}/6 + F(y) + x^{2} - F(0).$$

Condition 2:

$$u(1, y) = \cos y = \frac{y^2}{6} + F(y) + 1 - F(0)$$

$$\implies F(y) = \cos y - \frac{y^2}{6} - 1 - F(0).$$

The required solution is therefore

$$u(x,y) = \frac{1}{6}x^{3}y^{2} + \cos y - \frac{1}{6}y^{2} - 1 + x^{2}.$$

8.2 The Method of Separation of Variables

The method of separation of variables was introduced and developed by d'Alembert, D. Bernoulli, and Euler during the middle of the eighteenth century. It is the oldest systematic technique (and still the most useful) for solving partial differential equations. The twodimensional Laplace equation is an example of an elliptic differential equation, and solutions of the two-dimensional Laplace equation are called **harmonic functions**. To illustrate the separation of variables method, we solve the two-dimensional Laplace equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0. \tag{8.7}$$

The separation of variables method is illustrated by use of the following three-step process. Step 1 Assume that the solution u(x, y) can be written as

$$u(x,y) = X(x)Y(y)$$

where X is a function of x only and Y is a function of y only.

Step 2 Substitute the right-hand side of Step 1 into the original differential equation.

$$X''Y + XY'' = 0.$$

Step 3 Divide the equation in Step 2 by the right-hand side of Step 1.

$$\frac{X''}{X} + \frac{Y''}{Y} = 0$$
 or $\frac{X''}{X} = -\frac{Y''}{Y}$.

Note that the left-hand side of the above equation is a function x of only and the right-hand side is a function of y only (i.e., the variables have been separated). Since

$$\frac{d}{dx}\left(\frac{X''}{X}\right) = -\frac{d}{dx}\left(\frac{Y''}{Y}\right) = 0 \quad \text{and} \quad \frac{d}{dy}\left(\frac{X''}{X}\right) = -\frac{d}{dy}\left(\frac{Y''}{Y}\right) = 0,$$

it follows that

$$rac{X''}{X} = \lambda \quad ext{and} \quad rac{Y''}{Y} = -\lambda \Longrightarrow X'' - \lambda X = 0 \quad ext{and} \quad Y'' + \lambda Y = 0.$$

The parameter λ is called the separation constant and is independent of x and y, in this example. In general, the separation of variables method reduces a partial differential equation with n independent variables to n ordinary differential equations involving (n-1) separation constants. The above two ordinary differential equations can be solved by use of techniques developed in the Chapter 7. The general solution of the two-dimensional Laplace equation is the product of the solutions of the ordinary differential equations for X and Y, u(x, y) = X(x)Y(y).

Example 85 The electric potential u(x, y) at points inside a rectangle (see Fig. 8.1) is characterized by the solution of the two-dimensional Laplace equation. For boundary conditions given by $u(x, 0) = u_0$ and $u(0, y) = u(a, y) = u(x, \infty) = 0$, find u(x, y).



Solution : We must find the solution to the following differential equation subject to the given conditions:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0. \tag{8.7'}$$

Separation of variables in the above differential equation with separation constant λ^2 (the square is for convenience as will be seen below) yields

$$\frac{d^2X}{dx^2} + \lambda^2 X = 0 \quad \text{with solution} \quad X(x) = A \cos \lambda x + B \sin \lambda x$$

and

$$\frac{d^2Y}{dy^2} - \lambda^2 Y = 0 \quad \text{with solution} \quad Y(y) = Ce^{\lambda y} + De^{-\lambda y}.$$

The general solution of the two-dimensional Laplace equation is

$$u(x,y) = \{A\cos\lambda x + B\sin\lambda x\} \{Ce^{\lambda y} + De^{-\lambda y}\}$$

Condition $u(x, \infty) = 0$ requires that C = 0; condition u(0, y) = 0 leads to A = 0, and condition u(a, y) = 0 gives $\lambda_n = n\pi/a$ for $n = 1, 2, 3, \ldots$ Now, the general solution reduces to

$$u(x,y) = \sum_{n=1}^{\infty} B'_n \sin\left(\frac{n\pi x}{a}\right) e^{-n\pi y/a} \quad \text{where} \quad B'_n = B_n D_n$$

The final condition is used to determine the values of B'_n as follows.

$$u(x,0) = u_0 = \sum_{n=1}^{\infty} B'_n \sin\left(\frac{n\pi x}{a}\right).$$

The above equation is just a Fourier sine series, and the B'_n are given by

$$B'_n = \frac{2}{a} \int_0^a u_0 \sin\left(\frac{n\pi x}{a}\right) dx = -\frac{4u_0}{n\pi} \quad \text{for } n \text{ odd.}$$

The equation for the potential at points within the rectangle in Fig. 8.1, particular solution, is therefore

$$u(x,y) = -rac{4u_0}{\pi}\sum_{\substack{n=1\ \mathrm{odd}}}^{\infty}rac{1}{n}\sin\left(rac{n\pi x}{a}
ight)e^{-n\pi y/a}.$$

The extension of the above analysis to three independent variables is straight forward. While this presentation made use of Cartesian coordinates, inclusion of other coordinates systems (for example, cylindrical and spherical) may be carried out in a similar manner. In general, time-independent equations involving the Laplacian operator may be put in the form of Helmholtz's differential equation, $\nabla^2 u + k^2 u = 0$, when the appropriate k is used. Hence, solutions of Helmholtz's equation in various coordinate systems apply to all problems involving the Laplacian operator. In spherical coordinates (r, θ, ϕ) , use of (a) separation of variables; (b) the power series method; and (c) the appropriate k for Helmholtz's differential equation lead to the following special functions: (a) spherical harmonics; (b) Legendre polynomials and associated Legendre functions; (c) Laguerre polynomials and associated Laguerre polynomials; and (d) spherical Bessel functions. Bessel functions result when cylindrical coordinates (ρ, ϕ, z) are used in Helmholtz's differential equation. These special functions are discussed in Chapter 9.

8.2.1 The One-Dimensional Heat Conduction Equation

The method of separation of variables will now be applied to separate the space and time variables in the one-dimensional heat conduction equation.

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\sigma} \frac{\partial u}{\partial t}.$$
(8.8)

In Eq.(8,8), substitute u(x,t) = X(x)T(t) and divide by XT; the resulting two ordinary differential equations for separation constant $-\lambda^2$ are

$$\frac{d^2X}{dx^2} + \lambda^2 X = 0 \quad \text{with solution} \quad X(x) = A \cos \lambda x + B \sin \lambda x$$

and

$$\frac{dT}{dt} + \lambda^2 T = 0$$
 with solution $T(t) = C \exp(-\lambda^2 \sigma t)$.

The general solution of the one-dimensional heat conduction equation is

$$u(x,t) = (A\cos\lambda x + B\sin\lambda x)C\exp(-\lambda^2\sigma t).$$
(8.9)

Example 86 Solve the one-dimensional heat conduction equation for the temperature distribution u(x,t) in a rod of length ℓ such that $u(0,t) = u(\ell,t) = 0$ and $u(x,0) = T_0 \exp(-ax^2)$.

Solution : We have shown that the separation of variables method applied to the onedimensional heat conduction equation yields the following general solution:

$$u(x,t) = (A \cos \lambda x + B \sin \lambda x) C \exp(-\lambda^2 \sigma t).$$

The square on the separation constant, $-\lambda^2$, is selected for convenience, and the negative sign is used in anticipation of an oscillatory solution; boundary and initial conditions will determine the actual sign of the separation constant.

Conditions $u(0,t) = u(\ell,t) = 0$ lead to A = 0 and $\lambda_n = n\pi/\ell$ for n = 1, 2, ..., respectively. The final condition yields

$$u(x,0) = T_0 e^{-ax^2} = \sum_{n=1}^{\infty} B'_n \sin\left(\frac{n\pi x}{\ell}\right).$$

The above equation is just a Fourier sine series, and the coefficients B'_n are given by

$$B'_n = \frac{2}{\ell} \int_0^\ell T_0 e^{-ax^2} \sin\left(\frac{n\pi x}{\ell}\right) dx = \frac{4T_0}{n\pi} \quad \text{for } n \text{ odd.}$$

The particular relation for the temperature distribution in the rod is therefore given by

$$u(x,t) = \frac{4T_0}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi x}{\ell}\right) e^{-n^2 \pi^2 \sigma t/\ell}.$$

Example 87 By use of the Fourier transform method, solve the one-dimensional heat conduction equation for the temperature distribution T(x,t) such that T(x,t) and $T_x(x,t)$ approach zero as x approaches plus and minus infinity. In addition, the initial condition $T(x,0) = T_0 \exp(-ax^2)$ for constant a is imposed.

Solution : Here, one transforms out the space variable so that the resulting equation will be a first-order ordinary differential equation in t. On taking the Fourier transform of each term in the one-dimensional heat conduction equation, one obtains

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\partial^2 T}{\partial x^2}e^{ikx}dx = \frac{1}{\sigma}\frac{1}{\sqrt{2\pi}}\frac{\partial}{\partial t}\int_{-\infty}^{\infty}T(x,t)e^{ikx}dx.$$

By use of partial integration and the conditions that T(x,t) and $T_x(x,t)$ approach zero as x approaches plus and minus infinity, the above equation reduces to

$$\frac{\partial T(k,t)}{\partial t} + \sigma k^2 T(k,t) = 0.$$

The solution of the above first-order ordinary differential with independent variable t is

$$T(k,t) = A(k)e^{-\sigma k^2 t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} T(x,t)e^{ikx} dx$$

Substituting the initial condition $T(x,0) = T_0 \exp(-ax^2)$ into the above equation yields

$$A(k)=rac{T_0}{\sqrt{2a}}e^{-k^2/4a}$$

The solution in transform space (k-space) is therefore

$$T(k,t) = \frac{T_0}{\sqrt{2a}} \exp\left[\left(-\frac{1+4\sigma at}{4a}\right)k^2\right].$$

The solution in x-space is obtained when the k-space solution in the above equation is inverted; the result is

$$\begin{split} T(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} T(k,t) e^{-ikx} dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\{ \frac{T_0}{\sqrt{2a}} \exp\left[\left(-\frac{1+4\sigma at}{4a} \right) k^2 \right] \right\} e^{-ikx} dk \\ &= \frac{T_0}{\sqrt{1+4\sigma at}} \exp\left[-\frac{ax^2}{1+4\sigma at} \right]. \end{split}$$

8.2.2 The One-Dimensional Mechanical Wave Equation

Here, we consider the one-dimensional mechanical wave equation characterizing the motion of a string and use the method of separation of variables to separate the space and time variables.

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2}.$$
(8.10)

Assume u(x,t) = X(x)T(t) in the above equation and divide the resulting equation by XT. The result is

$$\frac{1}{X}\frac{d^{2}X}{dx^{2}} = \frac{1}{v^{2}}\frac{1}{T}\frac{d^{2}T}{dt^{2}}$$

The above equation leads to the following two ordinary differential equations

$$rac{d^2X}{dx^2} + \lambda^2 X = 0$$
 with solution $X(x) = A \cos \lambda x + B \sin \lambda x$

and

$$rac{d^2T}{dt^2}+\lambda^2 v^2T=0 \quad ext{with solution} \quad T(t)=C\cos\lambda vt+D\sin\lambda vt.$$

The general solution of the one-dimensional mechanical wave equation is

$$u(x,t) = (A\cos\lambda x + B\sin\lambda x) (C\cos\lambda vt + D\sin\lambda vt).$$
(8.11)

In our example of the separation of variables in the heat conduction equation and in the mechanical wave equation, the separation constant is denoted by $-\lambda^2$. The square is used for convenience as seen above. The negative sign is selected since an oscillatory solution is anticipated. Boundary conditions, however, will determine the required sign for the separation.

Example 88 Solve the one-dimensional mechanical wave equation for the motion of a string fixed at the ends $u(0,t) = u(\ell,t) = 0$ with initial configuration such that $u(x,0) = 2hx/\ell$ for x in the interval $(0,\ell/2)$ and $u(x,0) = 2h(\ell-x)/\ell$ for x in the interval $(\ell/2,\ell)$. The string is initially at rest which means that the partial derivative of u(x,t) with respect to t evaluated at t = 0 equals zero, $u_t(x,0) = 0$ (see Fig. 8.2).



Figure 8.2

Solution : The general solution of the one-dimensional mechanical wave equation is

$$u(x,t) = (A\cos\lambda x + B\sin\lambda x) (C\cos\lambda vt + D\sin\lambda vt).$$

Boundary and initial conditions will now be used to determined the values of the arbitrary constants in the above general solution. The first end point condition u(0,t) = 0 in the general solution leads to A = 0. The second end point condition $u(\ell, t) = 0$ requires that $\sin \lambda \ell = 0$ for a nontrivial solution or $\lambda_n = n\pi/\ell$ where n ranges from unity to infinity. The solution now reduces to

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{\ell}\right) \left\{ C_n \cos\left(\frac{n\pi vt}{\ell}\right) + D_n \sin\left(\frac{n\pi vt}{\ell}\right) \right\}.$$

Condition $u_t(x,0) = 0$ substituted into the partial derivative of u(x,t) with respect to t requires that $D_n = 0$ for all n, and the resulting solution becomes

$$u(x,t) = \sum_{n=1}^{\infty} B'_n \sin\left(\frac{n\pi x}{\ell}\right) \cos\left(\frac{n\pi vt}{\ell}\right) \quad \text{where} \quad B'_n = B_n C_n.$$

The final condition for the above equation, u(x,0) equals $2hx/\ell$ for $(0,\ell/2)$ and u(x,0) equals $2h(\ell-x)/\ell$ for $(\ell/2,\ell)$, leads to a Fourier sine series from which the B'_n may be obtained. The expression for the coefficients is

$$B'_{n} = \frac{2}{\ell} \int_{0}^{\ell} f(x) \sin\left(\frac{n\pi x}{\ell}\right) dx$$

= $\frac{4h}{\ell^{2}} \left[\int_{0}^{\ell/2} x \sin\left(\frac{n\pi x}{\ell}\right) dx + \ell \int_{\ell/2}^{\ell} \sin\left(\frac{n\pi x}{\ell}\right) dx - \int_{\ell/2}^{\ell} x \sin\left(\frac{n\pi x}{\ell}\right) dx \right]$
= $\frac{8h}{n^{2}\pi^{2}} \sin\left(\frac{n\pi}{2}\right)$ for n odd.

The particular solution of the mechanical wave equation subject to the given boundary and initial conditions reduces to

$$u(x,t) = \frac{8h}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^{(n-1)/2}}{n^2} \sin\left(\frac{n\pi x}{\ell}\right) \cos\left(\frac{n\pi vt}{\ell}\right).$$

The motion of the string is such that only odd harmonics occur and is symmetrical about the midpoint.

Example 89 By use of the Fourier transform method, find the solution of the one-dimensional mechanical wave equation,

$$rac{\partial^2 u}{\partial x^2} = rac{1}{v^2} rac{\partial^2 u}{\partial t^2},$$

for a very long (infinite) elastic string subject to the following boundary and initial conditions:

$$u(x,t) \to 0$$
 and $\frac{\partial u}{\partial x} \to 0$ as $x \to \pm \infty$;
 $u(x,0) = f(x)$ and $u_t(x,0) = 0$.

Solution : If we write the Fourier transform of u(x,t) in the form

$$U(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t) e^{ikx} dx$$

then the Fourier transform of the one-dimensional mechanical wave equation subject to the above two boundary conditions reduces to

$$-k^2 U(k,t) = \frac{1}{v^2} \frac{\partial^2 U(k,t)}{\partial t^2}$$

The solution of the above ordinary differential equation with independent variable t is

$$U(k,t) = c_1 e^{ikvt} + c_2 e^{-ikvt}$$

On applying the first initial condition u(x, 0) = f(x), we obtain

$$U(k,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,0)e^{ikx}dx = c_1 + c_2$$

= $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{ikx}dx = F(k).$

The result from the first initial condition is that $c_1 + c_2 = F(k)$. The second initial condition, $u_t(x, 0) = 0$, leads to

$$U(k,0) == \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u_t(x,0) e^{ikx} dx = ikvc_1 - ikvc_2 = 0.$$

The result from the second initial condition is that $c_1 = c_2$. The k-space solution is therefore

$$U(k,t) = rac{F(k)}{2}e^{ikvt} + rac{F(k)}{2}e^{-ikvt}.$$

The required x-space solution is obtained by taking the inverse transform of U(k,t); the result is

$$\begin{split} u(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} U(k,t) e^{-ikx} dk \\ &= \frac{1}{\sqrt{2\pi}} \left\{ \frac{1}{2} \int_{-\infty}^{\infty} \left[F(k) e^{ikvt} \right] e^{-ikx} dk + \frac{1}{2} \int_{-\infty}^{\infty} \left[F(k) e^{-ikvt} \right] e^{-ikx} dk \right\} \\ &= \frac{1}{2} f(x-vt) + \frac{1}{2} f(x+vt). \end{split}$$

There are many important cases where the above inverse transform would be extremely difficult to evaluate directly, as was done in this case; in such cases, the convolution theorem (e.g., see page 165) is used to find the inverse transform of the product of two k-space functions. We use the above case to outline the procedure for applying the convolution theorem; the second step above becomes

$$\begin{split} u(x,t) &= \frac{1}{2} \frac{1}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} \left[F(k) e^{ikvt} \right] e^{-ikx} dk + \int_{-\infty}^{\infty} \left[F(k) e^{-ikvt} \right] e^{-ikx} dk \right\} \\ &= \frac{1}{2} \frac{1}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} f(\xi) g_{+}(x-\xi) d\xi + \int_{-\infty}^{\infty} f(\xi) g_{-}(x-\xi) d\xi \right\}. \end{split}$$

The x-space forms of $g_+(x-\xi)$ is obtained as follows.

$$g_{+}(x-\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[e^{ikvt} \right] e^{-ik(x-\xi)} dk$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(x-vt-\xi)} dk = \sqrt{2\pi} \delta(x-vt-\xi).$$

Similarly, we find that

$$g_{-}(x-\xi) = \sqrt{2\pi}\delta(x+vt-\xi).$$

On substituting g_+ and g_- into the above equation for u(x,t), we obtain

$$u(x,t) = \frac{1}{2} \left\{ \int_{-\infty}^{\infty} f(\xi)\delta(x-vt-\xi)d\xi + \int_{-\infty}^{\infty} f(\xi)\delta(x+vt-\xi)d\xi \right\}$$
$$= \frac{1}{2}f(x-vt) + \frac{1}{2}f(x+vt).$$

Use of the convolution theorem, as expected, leads to the same solution as obtained by use of direct integration. Let us examine the behavior of f(x - vt) at time $t + \Delta t$ and position $x + \Delta x$; we obtain

$$f[x + v\Delta t - v(t + \Delta t)] = f(x - vt).$$

Here it is seen that f(x - vt) represents a wave motion (signal or pulse) traveling in the positive x-direction with speed v, and this motion repeats itself at $t + \Delta t$ and $x + \Delta x$. Similarly, f(x + vt) represents a signal traveling in the negative x-direction that repeats itself at $t + \Delta t$ and $x - \Delta x$.

8.2.3 The Time-Independent Schrödinger Wave Equation

Here, the method of separation of variables will be used to obtain the time-independent Schrödinger equation. We had

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)\right\}\Psi = i\hbar\frac{\partial\Psi}{\partial t}; \quad \text{Schrödinger's equation.}$$
(8.5')

Step 1 Assume that $\Psi(x, y, z, t) = \psi(x, y, z)T(t)$ in Eq.(8.5') Step 2 Substitute the right-hand side of Step 1 into Eq.(8.5')

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)\right\}\psi T = i\hbar\psi\frac{dT}{dt}.$$

Step 3 Divide both sides of the equation in Step 2 by the right-hand side of Step 1.

$$\frac{1}{\psi}\left\{-\frac{\hbar^2}{2m}\right\}\nabla^2\psi + V(x, y, z) = \frac{i\hbar}{T}\frac{dT}{dt} \equiv E.$$
(8.12)

Since the left-hand side of Eq.(8.12) is a function of space only and the right-hand side is a function of time only (Time has been separated from the space variables.), each side

must equal a constant (separation constant) that is independent of space and time. From a mathematical point of view, the separation constant is simply an arbitrary parameter in the general solution. The separation constant is an arbitrary physical parameter when solving physical problems. In Eq. (8.12), the separation constant has the same dimensions as energy and is denoted by E. Equation (8.12) leads to

$$T(t) = C \exp\left(-\frac{iEt}{\hbar}\right) \tag{8.13}$$

and

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)\right\}\psi = E\psi.$$
(8.14)

The function T(t) above is the solution of the time-dependent part of the Schrödinger equation, and Eq.(8.14) is the time-independent (steady-state) Schrödinger wave equation. Analyses of solutions of Eq. (8.14) for various potentials and use of the fundamental postulates of quantum theory form the major part of the study of quantum mechanics.

8.3 Green's Functions in Potential Theory

In this Section, the three-dimensional Fourier transform method will be used to solve Poisson's equation for the electric potential $\phi(\mathbf{r})$ due to a volume charge density $\rho(\mathbf{r})$, and the three-dimensional Green's function will be defined. Poisson's equation is written as

$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0}.$$
(8.15)

The quantity ϵ_0 is the permittivity of free space. The Fourier transform of $\phi(\mathbf{r})$ has the form

$$\Phi(\mathbf{k}) = \frac{1}{\left(2\pi\right)^{2/3}} \int_{-\infty}^{\infty} \phi(\mathbf{r}) \exp\left(i\mathbf{k}\cdot\mathbf{r}\right) d^3r.$$
(8.16)

A shorthand notation for triple integral, $d^3r = dxdydz$, is used in the above equation. On taking the Fourier transform of both sides of Poisson's equation, its solution in transform space (subject to the conditions that $\phi(r)$ and $\partial \phi/\partial r$ approach zero as r approaches plus and minus infinity) becomes

$$\Phi(\mathbf{k}) = \frac{P(\mathbf{k})}{k^2 \epsilon_0}.$$
(8.17)

The Fourier transform $P(\mathbf{k})$ is given by

$$P(\mathbf{k}) = \frac{1}{(2\pi)^{2/3}} \int_{-\infty}^{\infty} \rho(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} d^3r'.$$
(8.18)

The inverse transform of $\Phi(\mathbf{k})$ yields the solution in configuration space, $\phi(\mathbf{r})$; the result is

$$\begin{split} \phi(\mathbf{r}) &= \frac{1}{(2\pi)^{2/3}} \int_{-\infty}^{\infty} \Phi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3k \\ &= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}')}{k^2 \epsilon_0} \exp\left[-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')\right] d^3k d^3r' \\ &= \frac{1}{(2\pi)^3 \epsilon_0} \int_{-\infty}^{\infty} \rho(\mathbf{r}') G(\mathbf{r}-\mathbf{r}') d^3r'. \end{split}$$
(8.19)

The function $G(\mathbf{r} - \mathbf{r}')$, the Green's function for the operator ∇^2 , is given by

$$G(\mathbf{r} - \mathbf{r}') = \int_{-\infty}^{\infty} \frac{\exp\left[-i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')\right]}{k^2} d^3k.$$
(8.20)

When spherical coordinates are chosen for the variables in k-space, we have

$$d^{3}k = k^{2}\sin\theta dk d\theta d\phi = -k^{2}d(\cos\theta)d\phi dk$$

The polar axis is in the direction of $\mathbf{r} - \mathbf{r}'$. The equation for $G(\mathbf{r} - \mathbf{r}')$ becomes

$$G(\mathbf{r} - \mathbf{r}') = -\int_{+1}^{-1} \int_{0}^{2\pi} \int_{0}^{\infty} \frac{k^{2} \exp\left[-i\mathbf{k} |\mathbf{r} - \mathbf{r}'| \cos\theta\right] d(\cos\theta) d\phi dk}{k^{2}}$$
$$= 2\pi \int_{0}^{\infty} \frac{e^{-ik|\mathbf{r} - \mathbf{r}'|} - e^{ik|\mathbf{r} - \mathbf{r}'|}}{-ik|\mathbf{r} - \mathbf{r}'|} dk = 4\pi \int_{0}^{\infty} \frac{\sin k |\mathbf{r} - \mathbf{r}'|}{k|\mathbf{r} - \mathbf{r}'|} dk$$
$$= \frac{2\pi^{2}}{|\mathbf{r} - \mathbf{r}'|}.$$
(8.21)

The final form for $\phi(\mathbf{r})$ is

$$\phi(\mathbf{r}) = \left\{ \frac{1}{(2\pi)^3 \epsilon_0} \right\} (2\pi^2) \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}') d^3 r'}{|\mathbf{r} - \mathbf{r}'|}$$
$$= \frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}') d^3 r'}{|\mathbf{r} - \mathbf{r}'|}.$$
(8.22)

Physically, the Green's function $G(\mathbf{r} - \mathbf{r'})$ is the electric potential at point \mathbf{r} due to a point charge located at $\mathbf{r'}$. For a volume charge density $\rho(\mathbf{r'})$, the potential at \mathbf{r} is given by

$$\int_{-\infty}^{\infty} \rho(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r'.$$
(8.23)

In differential equation form, this analysis may be written as

$$\nabla^2 G(\mathbf{r} - \mathbf{r}') = -4\pi\delta\left(\mathbf{r} - \mathbf{r}'\right). \tag{8.24}$$

The above partial differential equation is subject to appropriate boundary conditions for $G(\mathbf{r} - \mathbf{r}')$. The Dirac delta function $\delta(\mathbf{r} - \mathbf{r}')$ means $\delta(x - x') \delta(y - y') \delta(z - z')$ with properties

(a)
$$\delta(\mathbf{r}-\mathbf{r}')=0$$
 for $\mathbf{r}-\mathbf{r}'\neq 0$ and $\int_{-\infty}^{\infty}\delta(\mathbf{r}-\mathbf{r}')\,d^3r'=1.$

For Dirichlet boundary conditions, $G(\mathbf{r} - \mathbf{r}') = 0$ on the boundary surface enclosing the charge distribution $\rho(\mathbf{r}')$. It can be shown that the Neumann problem requires appropriate non-zero values for the normal derivative of the Green's function on the boundary surface. Use of the Green's function method simplifies the problem of applying boundary conditions.

8.4 Some Numerical Methods

Numerical methods in partial differential equations form a vast subject and are treated in details in numerous textbooks on the subject. Here the focus is on essential concepts involved in converting a partial differential equation to its corresponding difference equation by use of finite difference methods. One should consult the references for a detailed discussion of (a) the various special techniques for finding numerical solutions; (b) convergence of solutions; and (c) stability of the various methods.

8.4.1 Fundamental Relations in Finite Differences

First differences $\Delta_x u$ and $\Delta_y u$ for positive h and k are defined by

$$\Delta_x u = \frac{u(x+h,y) - u(x,y)}{h} \quad \text{and} \quad \Delta_y u = \frac{u(x,y+k) - u(x,y)}{k}.$$
 (8.25)

The corresponding second differences are defined by

$$\Delta_{xx}u = \frac{u(x+h,y) - 2u(x,y) + u(x-h,y)}{h^2}$$
(8.26)

$$\Delta_{yy}u = \frac{u(x,y+k) - 2u(x,y) + u(x,y-k)}{k^2}.$$
(8.27)

For convenience, Δx and Δy are replaced with h and k, respectively, in the above finite difference equations, and k replaces Δt in the following two Sections.

8.4.2 The Two-Dimensional Laplace Equation: Elliptic Equation

The two-dimensional Laplace equation in terms of finite differences reduces to

$$u(x,y) = \frac{1}{4} \left\{ u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) \right\}.$$
 (8.28)

The computational procedure involves replacing u(x, y), for example a potential, at a particular grid point (see Fig. 8.3) by the average value of its four closest neighbors. The function u(x, y) or its derivative must by specified at all points surrounding a given region.

8.4.3 The One-Dimensional Heat Conduction Equation: Parabolic Equation

In terms of finite differences, the one-dimensional heat conduction equation becomes

$$u(x,t+k) = \frac{\sigma k}{h^2} \left\{ u(x+h,t) - 2u(x,t) + u(x-h,t) \right\} + u(x,t).$$
(8.29)



Figure 8.3

The numerical solution involves determining the initial values of u(x,t) at various x locations (see Fig. 8.4 for the space-time grid) and applying the above equation to obtain the u(x,t) at other times.

8.4.4 The One-Dimensional Wave Equation: Hyperbolic Equation

The finite difference representation of the one-dimensional mechanical wave equation reduces to

$$u(x,t+k) = \frac{k^2 v^2}{h^2} \{ u(x+h,t) - 2u(x,t) + u(x-h,t) \} + 2u(x,t) - u(x,t-k).$$
(8.30)

The starting value for u(x, t+k) is determined from the initial conditions (see Fig. 8.5), and remaining values are determined by use of the above equation.





8.5 Problems

8.1 Show that $u = \cos x \cos at$ is a solution of $u_{tt} = a^2 u_{xx}$. 8.2 By use of the separation of variables method, solve $u_x = 4u_y$; $u(0, y) = 8e^{-3y}$. 8.3 Consider the one-dimensional heat equation,

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma} \frac{\partial T}{\partial t}$$

If b^2 is the separation constant, discuss the nature of the solution for (a) $b^2 > 0$; (b) $b^2 = 0$; and (c) $b^2 < 0$. (d) Find the particular solution for and

$$T(0,t) = T(\ell,t) = 0$$
 and $T(x,0) = T_0 \sin\left(\frac{n\pi x}{\ell}\right)$ (for $0 < x < \ell$)

if the general solution is

$$T(x,t) = Ce^{-b^2\sigma t} (A\cos bx + B\sin bx).$$

8.4 Solve

$$\left. rac{\partial^2 I}{\partial x^2} - rac{2}{k} rac{\partial I}{\partial t} + I = 0 \quad ext{where} \quad I(\ell,t) = 0 \quad ext{and} \quad \left. rac{\partial I}{\partial x} \right|_{x=0} = -ae^{-kt}.$$

8.5 Solve

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma} \frac{\partial T}{\partial t}$$

where $T(x, t \to 0)$ tends to a finite value, T(0, t) = 0, and $\partial T/\partial x|_{x=\ell} = 0$.

			← h →	
		(x, t+k)		
	(x-h, t)	•	(x+h,t)	
 	(x-n, t)		(x + n, t)	
 		(x, t-k)		

Figure 8.5

8.6 The one-dimensional motion of a transverse wave in a string is characterized by

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \varphi}{\partial t^2}.$$

(a) Discuss the nature of the solution for $k^2 > 0, k^2 = 0$, and $k^2 < 0$ where is the separation constant. (b) Find the general periodic motion solution of this wave equation. (c) For

$$\left. arphi(0,t) = arphi(\ell,t) = \left. rac{\partial arphi}{\partial t}
ight|_{t=0} = 0 \quad ext{and} \quad arphi(x,0) = Y,$$

show that the solution for periodic motion is

$$\varphi(x,t) = \sum_{n=1}^{\infty} Y_n \sin\left(\frac{n\pi x}{\ell}\right) \cos\left(\frac{n\pi vt}{\ell}\right).$$

8.7 Consider the two-dimensional Laplace equation,

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0.$$

(a) For separation constant b^2 , show that the general solution is given by

$$\varphi(x, y) = (A\cos bx + B\sin bx) (C\cosh by + D\sinh by)$$

(b) Find $\varphi(x, y)$ subject to the following conditions:

$$\varphi(x,0) = \varphi(0,y) = \varphi(\ell,y) \text{ and } \varphi(x,h) = \varphi_0 \sin \frac{n\pi x}{\ell}.$$

8.8 Develop the solution of the three-dimensional Laplace equation in Cartesian coordinates; for separation constants a and b, show that it can be written as

$$\varphi(x, y, z) = \sum_{p, j, k=1}^{2} c_{pjk} \exp\left\{(-1)^{p} \sqrt{a}x\right\} \exp\left\{(-1)^{j} \sqrt{b}y\right\}$$
$$\times \exp\left\{(-1)^{k} i \sqrt{a+b}z\right\}.$$

8.9 By separating the variables in Laplace's equation in cylindrical coordinates, show that

$$u(
ho,\phi,z)=P(
ho)\Phi(\phi)Z(z)$$

where $Z = Ae^{\sqrt{a}x} + Be^{-\sqrt{a}z}$, $\Phi = C \cos n\phi + D \sin n\phi$ and $P(\rho)$ is the solution of

$$\frac{d^2P}{d\rho^2} + \frac{1}{\rho}\frac{dP}{d\rho} + \left(a - \frac{n^2}{\rho^2}\right)P = 0.$$

8.10 Show that the solution of Laplace's equation in spherical polar coordinates is

$$\cdot u = R(r)\Theta(\theta)\Phi(\phi)$$

where $\Phi = A \cos m\phi + B \sin m\phi$, R is a solution of

$$\frac{1}{R}\frac{d}{dr}\left(r^{2}\frac{dR}{dr}\right) = \ell\left(\ell+1\right),$$

and Θ is a solution of

$$\left[\ell\left(\ell+1\right)\sin^2\theta - m^2\right]\Theta + \sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = 0.$$

8.11 (a) By use of the sine transform method, solve the one-dimensional heat conduction equation,

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma} \frac{\partial T}{\partial t},$$

subject to T(x,0) = 0 and $T(0,t) = T_0$ where $T(x,t) \to 0$ and $\partial T/\partial x \to 0$ as $x \to \infty$. (b) Show that $T(x,t) \to T_0$ as $t \to \infty$.

 $8.12~\mathrm{By}$ use of the cosine transform method, solve the one-dimensional heat conduction equation,

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma} \frac{\partial T}{\partial t},$$

subject to the following conditions T(x,0) = 0 and $\partial T/\partial x \to Q_0$ as $x \to 0$, where $T(x,0) \to 0$ and $\partial T/\partial x \to 0$ as $x \to \infty$.

8.13 By use of the Fourier transform method, solve the one-dimensional heat conduction equation,

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma} \frac{\partial T}{\partial t},$$

subject to $T(x,t) \to 0$ and $\partial T/\partial x \to 0$ as $x \to \pm \infty$; $T(x,0) = e^{-a^2x^2}$ where a is a positive constant.

8.14 By use of the Fourier transform method, solve the infinite string problem when $u(x,t) \to 0$ and $\partial u/\partial x \to 0$ as $x \to \pm \infty$; subject to u(x,0) = f(x) and $\partial u/\partial x = g(x)$ as $x \to 0$.

8.15 (a) By use of the Fourier transform method, solve the one-dimensional Schrödinger wave equation for a free particle,

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

(b) Write the solution of Part (a) in the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p_x) \exp\left[i\left(p_x x - p_x^2 t/2m\right)/\hbar\right] dp_x.$$

In the above equation, $\Psi(p_x, 0) = \phi(p_x)$. (c) For $\Psi(x, 0) = e^{-x^2/2a^2}$, calculate $\phi(p_x)$. (d) Obtain the explicit expression for $\Psi(x, t)$. The real quantity $\Psi^*\Psi$ has a physical interpretation in quantum mechanics. (e) Obtain the explicit expression for $|\Psi|^2$ and show that the width of this Gaussian form increases with time; that is to say, the wave packet spreads in x-space as time increases.

8.16 Obtain (a) Eq.(8.28), (b) Eq.(8.29), and (c) Eq.(8.30).

Chapter 9

Special Functions

9.1 Introduction

This chapter is devoted to the theory and applications of a set of higher transcendental functions that arise naturally in mathematical physics. These higher transcendental functions are referred to as **special functions**, and they arise (a) when solving, in certain curvilinear coordinate systems, partial differential equations that are defined by physical problems and/or (b) when finding eigenfunctions and eigenvalues of differential operators. The partial differential equations approach to special functions involves use of the separation of variables method and (a) the Frobenius-Fuchs power series solutions of one or more resulting ordinary differential equations or (b) an Infeld-Hull type factorization procedure for finding eigenfunctions and eigenvalues of second-order ordinary linear differential equations.

The focus is on a class of physical problems whose differential equation formulation involves the Laplacian operator, ∇^2 . The resulting partial differential equations include the Laplace equation, heat conduction equation (diffusion equation), mechanical wave motion equation, and Schrödinger wave equation. After applying the separation of variables method, the resulting time-independent parts of all these partial differential equations may be written in the form of the Helmholtz differential equation, $\nabla^2 u + k^2 u = 0$. Problems involving the Helmholtz differential equation in spherical coordinates lead to spherical harmonics, Legendre polynomials and associated Legendre functions, Laguerre and associated Laguerre polynomials, and spherical Bessel functions. Problems modeled by use of Helmholtz's differential equation in cylindrical coordinates involve the various types of Bessel functions. Solutions of the Schrödinger wave equation for a linear harmonic oscillator are expressed in terms of Hermite polynomials.

Special functions such as Hermite polynomials, Legendre polynomials and associated Legendre functions, spherical harmonics, Laguerre and associated Laguerre polynomials and Bessel functions are widely used in mathematical physics and are the main focus of this chapter; these special functions are special cases of the hypergeometric functions, ${}_2F_1(a, b, c; z)$, or confluent hypergeometric functions, ${}_1F_1(a, c; z)$. There exist other useful special functions in mathematical physics that are not expressible in terms of ${}_2F_1$ or ${}_1F_1$. The functions ${}_2F_1$ and ${}_1F_1$ may be developed from the following main viewpoints: (a) ordinary differential equations and the Frobenius-Fuchs power series method; (b) factorization of ordinary differential equations; and (c) representation theory of local Lie groups.

9.2 The Sturm-Liouville Theory

9.2.1 Introduction

This Section is devoted to a treatment of the Sturm-Liouville theory and orthogonal polynomials since these concepts provide insight into properties of solutions of the second-order ordinary linear differential equations in which we are interested.

Linear operators are basic to linear differential equations, and the solutions of each of the differential equations we will consider form a vector space (see page 71). In mathematical physics, the (a) linear operator is normally a differential operator; (b) eigenvalue equation is a differential equation; and (c) eigenfunctions (solutions) form a vector space and satisfy certain imposed Dirichlet, Neumann, or Cauchy boundary conditions. Typically, the actual physical problem is used as a guide for the formulation of boundary conditions. Sometimes, however, it is difficult to formulate the appropriate boundary conditions for a problem. Hence, it is important to understand what conditions are appropriate for a particular type of differential equation (see, e.g., Chapter 8).

The Laplace equation, the time-independent heat conduction (diffusion) equation, and the time-independent mechanical wave equation may be put into the form of the Helmholtz differential equation. The Helmholtz differential equation, $\nabla^2 u + k^2 u = 0$, for constant k^2 is an eigenvalue equation where (a) $-k^2$ is the eigenvalue; (b) u is the eigenfunction and is subject to boundary conditions; and (c) ∇^2 is the operator. The time-independent Schrödinger wave equation contains the operator ∇^2 and is an eigenvalue equation of the form $H\psi = E\psi$ where $H = (-\hbar^2/2m)\nabla^2 + V(x, y, z)$.

The separation of variables method applied to Helmholtz's differential equation and to the time-independent Schrödinger's wave equation in various coordinate systems leads to ordinary differential equations that may be written in the following general form.

$$\frac{d}{dx}\left\{p(x)\frac{du}{dx}\right\} - q(x)u + \lambda\rho(x)u = 0.$$
(9.1)

The parameter λ is a separation constant (In some cases, more than one separation constant may appear.); we will focus on the case of one separation constant. Equation (9.1) is the well-known **Sturm¹-Liouville² equation**, and it may be written in the following operator form.

$$\mathcal{L}(u) + \lambda \rho(x)u = 0. \tag{9.2}$$

The Liouville operator, a linear operator, is defined by use of the following equation.

$$\mathcal{L}(u) = \frac{d}{dx} \left\{ p(x) \frac{du}{dx} \right\} - q(x)u.$$
(9.3)

For the general differential operator M(u) = p(x)u'' + r(x)u' + q(x)u, the operator $\overline{M}(u) = (pu)'' - (ru)' + qu$ is defined as the **adjoint** of M(u). Note that $M(u) = \overline{M}(u)$ when

¹Jacques Charles Francois Sturm (1803–1855), Swiss physicist who became a French citizen in 1833. He is best known for the Sturm-Liouville problem. Also, he did work on infinitesimal geometry, differential equations and differential geometry.

²Joseph Liouville (1809–1882), French mathematician and scientist who is known for his mathematical work which ranges from mathematical physics to astronomy to pure mathematics.

p' = r, and M(u) is said to be a **self-adjoint operator** in this case. On applying the general definition for the adjoint of an operator to Eq.(9.3), we find that $\mathcal{L}(u) = \overline{\mathcal{L}}(u)$ which means that the Liouville operator is a self-adjoint operator. In fact, it can be shown that every second order differential operator can be transformed to the self-adjoint form (see Problem 9.16).

In the Sturm-Liouville equation, the function $\rho(x)$ (also, w(x) and r(x) are used) is called the density or weight. This name for $\rho(x)$ is related to the historical origin of the Sturm-Liouville equation which involved finding the solution for the one-dimensional mechanical wave equation, $[p(x)u_x]_x = \rho(x)u_{tt}$, representing the motion of a nonhomogeneous string. In the mechanical wave equation, u(x,t) is the displacement of the string from its equilibrium position, p(x) is proportional to the modulus of elasticity and $\rho(x)$ is the mass per unit length of the string. Separation of variables leads to the following ordinary differential equations: $(pX')' + \lambda\rho X = 0$ and $\ddot{T} + \lambda T = 0$ where λ is the separation constant and u(x,t) is assumed to equal the product X(x)T(t) with typical boundary conditions given by X(a) = X(b) and p(a)X'(a) = p(b)X'(b).

In Eq.(9.1), the functions, p(x), q(x), and $\rho(x)$ are assumed to be (a) real (b) continuous with continuous derivatives; and (c) nonzero in the region of interest [a, b]. Moreover, it is assumed that p(x) and $\rho(x)$ are always positive in [a, b]. The Sturm-Liouville equation is a generalized form of the usual eigenvalue equation since the eigenvalue is multiplied by the density function, $\rho(x)$, which may be different from unity. The sign convention for q(x) in Eqs.(9.1) and (9.3) conforms to the usage of Courant and Hilbert; some authors use a plus sign for in these equations. The function u(x) is subject to appropriate boundary conditions. With appropriate substitutions, the following differential equations are among the list of important differential equations in mathematical physics that may be put in the Sturm-Liouville form: Legendre and associated Legendre, Laguerre and associated Laguerre, Schrödinger equation for the linear harmonic oscillator, and Bessel. Hence, a study of the general properties of the Sturm-Liouville equation is extremely useful in mathematical physics. A summary of the relations between the differential equations for many important special functions and the Sturm-Liouville equation is given in Table 9.1.

The problem of determining the dependence of the (a) eigenfunction u(x) on the eigenvalue λ and (b) eigenvalue λ on the boundary conditions imposed on u(x) is often referred to as the **Sturm-Liouville problem**. The Sturm-Liouville problem is important in both classical and quantum theory. Sturm-Liouville theory unites properties of the solutions of second-order ordinary linear differential equations related to

- (a) Hermitian and self-adjoint operators;
- (b) reality of eigenvalues of Hermitian and self-adjoint operators;
- (c) orthogonality and completeness of eigenfunctions;
- (d) degeneracy of eigenvalues (If N linearly independent eigenfunctions correspond to the same eigenvalue, then the eigenvalue is said to be N-fold degenerate.);
- (e) the fact that eigenvalues of the Sturm-Liouville equation form a discrete set of values such that ... λ₁ ≤ λ₂ ≤ λ₃....

These properties are important in the study of problems that lead to each of the differential equations we will analyze in this chapter.

Table 9.1 Relation to the Sturm-Liouville Equation

 $\frac{d}{dx}\left\{p(x)\frac{du}{dx}\right\} - q(x)u + \lambda\rho(x)u = 0$

	(
Equation	p(x)	q(x)	$\rho(x)$	λ
Legendre, $P_n(x)$	$1 - x^2$	0	1	n(n+1)
Associated Legendre, $P_{n}^{m}\left(x\right)$	$1-x^2$	$rac{m^2}{1-x^2}$	1	$n\left(n+1 ight)$
Laguerre, $L_n(x)$	xe^{-x}	0	e^{-x}	n
Associated Laguerre, $L_n^k(x)$	$x^{k+1}e^{-x}$	0	$x^k e^{-x}$	n-k
Bessel, $J_{n}(x)$, $Y_{n}(x)$, $H_{n}(x)$,	x	$\frac{n^2}{x}$	x	1
Hermite, $H_n(x)$	e^{-x^2}	0	e^{-x^2}	2n
Quantum Oscillator, $\psi_{n}\left(x ight)$	1	x^2	1	λ
Jacobi, $P_{n}^{(\alpha,\beta)}(x); \alpha, \beta > -1$	$rac{1-x^2}{\left(1-x ight)^{-lpha}\left(1+x ight)^{eta}} \\ \left(1-x^2 ight)^{1/2}$	0	$rac{{\left({1 - x} ight)^lpha }}{{\left({1 + x} ight)^{ - eta } }}}{{\left({1 - {x^2}} ight)^{ - 1/2} }}$	$n\left(n+lpha+eta+1 ight)$
Chebyshev, $T_n(x)$	$\left(1-x^2\right)^{1/2}$	0	$(1-x^2)^{-1/2}$	n^2
Gegenbauer, $C_{n}^{\left(lpha ight)}\left(x ight) ;lpha >-rac{1}{2}$	$\left(1-x^2\right)^{lpha+1/2}$	0	$\left(1-x^2\right)^{lpha-1/2}$	$n\left(n+2lpha ight)$

9.2.2 Hermitian Operators and Their Eigenvalues

Consider two twice differentiable functions u_i and u_j . By use of Eqs.(9.1 and 9.2), we obtain

$$u_i^* \mathcal{L}(u_j) - \left[\mathcal{L}(u_i)\right]^* u_j = \frac{d}{dx} \left\{ p\left(u_i^* \frac{du_j}{dx} - u_j \frac{du_i^*}{dx}\right) \right\}.$$
(9.4)

In Eq.(9.4), the asterisk is used to denote complex conjugate of the respective functions. Integrating both sides of Eq.(9.4) over the range of interest yields

$$\begin{aligned} &\int_{a}^{b} \left\{ u_{i}^{*} \mathcal{L}(u_{j}) - \left[\mathcal{L}(u_{i})\right]^{*} u_{j} \right\} dx \\ &= \left\{ p \left(u_{i}^{*} \frac{du_{j}}{dx} - u_{j} \frac{du_{i}^{*}}{dx} \right) \right\}_{x=b} - \left\{ p \left(u_{i}^{*} \frac{du_{j}}{dx} - u_{j} \frac{du_{i}^{*}}{dx} \right) \right\}_{x=a} \end{aligned}$$

Note that the above equation results from the fact that \mathcal{L} is self-adjoint. The operator \mathcal{L} is said to be Hermitian if the following endpoints boundary conditions are imposed on the two functions and their derivatives:

$$\left\{ p\left(u_i^* \frac{du_j}{dx} - u_j \frac{du_i^*}{dx}\right) \right\}_{x=b} = \left\{ p\left(u_i^* \frac{du_j}{dx} - u_j \frac{du_i^*}{dx}\right) \right\}_{x=a}.$$
(9.5)

By use of the boundary conditions in Eq.(9.5), the **Hermitian relation** may be written as

$$\int_{a}^{b} \{u_{i}^{*}\mathcal{L}(u_{j}) - [\mathcal{L}(u_{i})]^{*} u_{j}\} dx = \int_{a}^{b} [\mathcal{L}(u_{i})]^{*} u_{j} dx.$$
(9.6)

Thus far, the Liouville operator has been assumed to be real. In quantum mechanics, operators are generally complex (For example, the *x*-component of the linear momentum operator is given by $p_x = -i\hbar\partial/\partial x$.), and it is assumed that wave functions satisfy the boundary conditions in Eq.(9.5). The Hermitian relation in quantum mechanics for linear operator \hat{A} takes the form

$$\int_{-\infty}^{\infty} \psi_i^* \hat{A} \psi_j d\tau = \int_{-\infty}^{\infty} \left(\hat{A} \psi_i \right)^{\dagger} \psi_j d\tau.$$
(9.7)

An arbitrary linear operator may be put in matrix form, and the notation \hat{A}^{\dagger} means (a) to interchange rows with columns and (b) to take the complex conjugate of each element (this process is called the **Hermitian conjugate**); in this connection, note that $(\hat{A}\psi_i)^{\dagger} = \psi_i^* \hat{A}^{\dagger}$. When an operator satisfies the condition $\hat{A} = \hat{A}^{\dagger}$, the operator is said to be Hermitian. In the bra and ket vector notation, Eq.(9.7) becomes $\langle \psi_i | \hat{A}\psi_j \rangle = \langle \hat{A}\psi_i | \psi_j \rangle$. For solution $u_i = u_j$ in Eq.(9.6) and use of Eq.(9.2), we obtain

$$\int_{a}^{b} \left[u^{*} \mathcal{L}(u) - u \mathcal{L}(u^{*}) \right] dx = \left(\lambda - \lambda^{*} \right) \int_{a}^{b} \rho(x) u^{*} u dx = 0.$$
(9.8)

The result in Eq.(9.8) means that eigenvalues of Hermitian operators are real, $\lambda = \lambda^*$.

9.2.3 Orthogonality Condition and Completeness of Eigenfunctions

By use of Eq.(9.2) for distinct eigenfunctions and with distinct eigenvalues, the Hermitian relation in Eq.(9.6) may be written as

$$\int_{a}^{b} \left\{ u_{i}^{*}\mathcal{L}(u_{j}) - \left[\mathcal{L}(u_{i})\right]^{*}u_{j} \right\} = \int_{-\infty}^{\infty} \left[u_{i}^{*}(-\lambda_{j}\rho u_{j}) + \lambda_{i}^{*}\rho u_{i}^{*}u_{j} \right] dx$$
$$= \left(\lambda_{i}^{*} - \lambda_{j}\right) \int_{a}^{b} u_{i}^{*}u_{j}\rho(x) dx = 0.$$

Since $\lambda_i \neq \lambda_j$ and λ_i is real, the above equation implies that

$$\int_{a}^{b} u_{i}^{*} u_{j} \rho(x) dx = 0.$$
(9.9)

Equation (9.9) shows that eigenfunctions corresponding to distinct eigenvalues are orthogonal in the interval [a, b] with respect to the weight function $\rho(x)$.

An orthonormal set of Sturm-Liouville eigenfunctions, $\{u_k(x)\}$, forms a complete set of functions (cf. Courant and Hilbert, 1953; Chapter 6, Section 3). This completeness property

means that the following equation is valid for any function f(x) which is at least piece-wise continuous in the interval [a, b].

$$\lim_{n \to \infty} \int_{a}^{b} \left| f(x) - \sum_{k=1}^{n} c_{k} u_{k}(x) \right|^{2} \rho(x) dx = 0.$$
(9.10)

The notation $|...|^2$ means the product of the enclosed quantity and its complex conjugate, $|z|^2 = z^*z$. Equation (9.10) and the orthogonality relation in Eq.(9.9) lead to

$$f(x) = \sum_{k=1}^{\infty} c_k u_k(x)$$
 where $c_k = \int_a^b f(x) u_k^*(x) \rho(x) dx$ (9.11)

and

$$\sum_{k=1}^{\infty} |c_k|^2 = \int_a^b |f(x)|^2 \,\rho(x) dx. \tag{9.12}$$

Equation (9.12) is referred to as **the completeness relation**. By use of Eq.(9.11) with the appropriate orthogonality relation and weight, one may obtain series expansions for f(x) in terms of any complete set of orthogonal polynomials (or orthogonal functions); for example, the Fourier series, Legendre series, and Hermite series may be written respectively as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/\ell}; \qquad -\ell \le x \le \ell$$

where $c_n = \frac{1}{2\ell} \int_{-\ell}^{\ell} f(x) e^{-in\pi x/\ell};$

$$\begin{split} f(x) &= \sum_{n=0}^{\infty} c_n P_n(x); \qquad -1 \leq x \leq 1 \\ \text{where} \qquad c_n &= \frac{2n+1}{2} \int_{-1}^1 f(x) P_n(x) dx; \quad \text{and} \end{split}$$

$$f(x) = \sum_{n=0}^{\infty} c_n H_n(x); \qquad -\infty \le x \le \infty$$

where
$$c_n = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2} dx.$$

The above expansions are three of a large number in important expansions involving orthogonal polynomials that are used in many areas of mathematical physics.

9.2.4 Orthogonal Polynomials and Functions

The power series solutions of many second-order ordinary linear differential equations in mathematical physics such as the Legendre, Laguerre, and Hermite differential equations may be written as an orthogonal polynomial plus an orthogonal function. The set of real polynomials $\{f_n(x)\}$ is said to be **orthogonal** with respect to the weight function $\rho(x)$ over the interval [a, b] if the following relations are valid.

$$\int_{a}^{b} \rho(x) f_{n}(x) f_{m}(x) dx = \begin{cases} 0 & \text{if } m \neq n \\ h_{n}^{2} & \text{if } m = n. \end{cases}$$

$$(9.13)$$

If $h_n^2 = 1$ for all *n*, then the system of orthogonal polynomials in Eq.(9.13) is said to be **orthonormal**. Note that the weight determines the system of polynomials up to a constant factor (the value of h_n) in each polynomial; the specification of this constant factor for each polynomial is referred to a **standardization** (or standard convention). Summarized in Table 9.2 are some frequently used orthogonality relations.

Table 9.2 Some Orthogonality Relations

$$\int_{-1}^{1} P_n(x) P_k(x) dx = \frac{2}{2n+1} \delta_{nk}$$
$$\int_{-1}^{1} P_n^m(x) P_k^m(x) dx = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_{nk}$$
$$\int_{0}^{\infty} e^{-x} L_n(x) L_m(x) dx = \delta_{nm}$$
$$\int_{0}^{\infty} e^{-x} x^k L_n^k(x) L_m^k(x) dx = \frac{(n!)^3}{(n-k)!} \delta_{nm}$$
$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi} \delta_{nm}$$

Recurrence Formula for Orthogonal Polynomials In many cases, three consecutive orthogonal polynomials, f_{n+1} , f_n , and f_{n-1} satisfy a **recurrence formula** of the form

$$A_n f_{n+1}(x) = (B_n + C_n x) f_n(x) - D_n f_{n-1}(x).$$
(9.14)

The recurrence relations for some of the frequently used orthogonal polynomials are listed in Table 9.3.

$f_{n}(x)$	A _n	B_n	C_n	D_n
$P_{n}(x)$	n+1	0	2n + 1	n
$P_n^m(x)$	n-m+1	0	2n+1	n+m
$L_{n}(x)$	n+1	2n+1	-1	n
$L_{n}^{k}\left(x ight)$	n + 1	2n+k+1	-1	n+k
$H_{n}\left(x ight)$	1	0	2	2n

Table 9.3 Recurrence Relations for Some Polynomials
Rodrigues's Formula Formulas, involving the *n*-th derivative of an elementary function, that can be used to generate orthogonal polynomials, f_n , are called **Rodrigues³ formulas**. It can be shown that the Rodrigues formulas for many orthogonal polynomials may be combined into the following general Rodrigues formula.

$$f_n = \frac{1}{a_n \rho(x)} \frac{d^n \left\{ \rho(x) \left[g(x) \right]^n \right\}}{dx^n}.$$
(9.15)

The quantity g(x) is a polynomial whose coefficients are independent of n and the a_n factor is determined by the standardization of the orthogonal polynomial system. The **Leibniz** formula for the *n*-th derivative of a product should be used to evaluate the right-hand side of Eq.(9.15); this formula is

$$\frac{d^n}{dx^n} \left\{ A(x)B(x) \right\} = \sum_{s=0}^n \left\{ \frac{n!}{(n-s)!s!} \frac{d^{n-s}A(x)}{dx^{n-s}} \frac{d^s B(x)}{dx^s} \right\}.$$
(9.16)

Rodrigues's formulas for some important orthogonal polynomials are given in Table 9.4.

Table 9.4 Rodrigues Formulas for Some Polynomials

	$a_{np}(x)$ au		
$f_{n}\left(x\right)$	an	$g\left(x ight)$	$\rho(x)$
$P_{n}\left(x\right)$	$2^n n!$	$x^2 - 1$	1
$L_{n}^{k}\left(x ight)$	n!	x	$x^k e^{-x}$
$H_{n}\left(x ight)$	$(-1)^{n}$	1	e^{-x^2}
$P_n^{(\alpha,\beta)}(x)$	$(-1)^n 2^n n!$	$1-x^2$	$(1-x)^{\alpha} \left(1+x\right)^{\beta}$
$C_{n}^{\left(lpha ight) }\left(x ight)$	$(-1)^n 2^2 n! \frac{\Gamma(2\alpha) \Gamma(\alpha+n+1/2)}{\Gamma(\alpha+1/2) \Gamma(n+2\alpha)}$	$1 - x^2$	$\left(1-x^2\right)^{\alpha-1/2}$
$T_{n}\left(x ight)$	$(-1)^n 2^{n+1} \frac{\Gamma(n+1/2)}{\sqrt{\pi}}$	$1 - x^2$	$(1-x^2)^{-1/2}$

 $f_n = \frac{1}{a_n \rho(x)} \frac{d^n \left\{ \rho(x) \left[g(x) \right]^n \right\}}{dx^n}$

The Generating Function: The function G(x,t) is said to be a generating function of the sequence of functions $\{f_n(x)\}$ if the $f_n(x)$ are, up to a constant, the coefficients of t^n in the expansion of G(x,t) in powers of t. Such an expansion is valid for orthogonal polynomials and most orthogonal functions, and it may be written in the form

$$G(x,t) = \sum_{n=0}^{\infty} a_n f_n(x) t^n.$$
 (9.17)

In Eq.(9.17), the a_n are independent of x and t. The generating functions for certain orthogonal polynomials that will be used in other sections are given in Table 9.5.

 $^{^{3}}$ Benjamin Olinde Rodrigues (1794–1851), French mathematician who known for the formula that carries his name.

Table 9.5 Some Generating Functions

G(x,t)	$=\sum_{n=0}^{\infty}a_n$	$f_n(x) t^n; R = \sqrt{1 - 2xt + t^2}$
$f_{n}\left(x ight)$	an	$G\left(x,t ight)$
$P_{n}(x)$	1	R^{-1}
$L_{n}\left(x ight)$	1	$(1-t)^{-1} \exp \{-xt/(1-t)\}$
$L_{n}^{k}\left(x ight)$	1	$(1-t)^{-(k+1)} \exp \{xt/(t-1)\}$
$H_{n}\left(x ight)$	1/n!	$\exp\left(2xt-t^2\right)$
$P_{n}^{\left(lpha,eta ight) }\left(x ight)$	$2^{-lpha-eta}$	$R^{-1}\left(1-t+R\right)^{-\alpha}\left(1+t+r\right)^{-\beta}$
$C_{n}^{\left(lpha ight) }\left(x ight)$	1	R^{-2lpha}
$T_{n}\left(x ight)$	2	$1 + (1 - t^2) / R^2$

9.3 The Hermite Polynomials

The Hermite differential equation,

$$y'' - 2xy' + 2ny = 0; \quad n = \text{constant},$$
 (9.18)

is a special case of the Sturm-Liouville differential equation and a special case of the confluent hypergeometric differential equation. The polynomial, $H_n(x)$, solution of the Hermite differential equation may be obtained by use of the Frobenius-Fuchs power series method (see Worksheet in Section 9.9.1 at the end of this Chapter); it has the form

$$y_n(x) \equiv H_n(x) = \sum_{j=0}^{N} \frac{(-1)^j n! (2x)^{n-2j}}{j! (n-2j)!}$$
(9.19)
where $N = \begin{cases} n/2 & \text{for } n \text{ even} \\ (n-1/2) & \text{for } n \text{ odd.} \end{cases}$

The orthogonality relation, recurrence relation, Rodrigues formula, and generating function for $H_n(x)$ are respectively given in Tables 9.2, 9.3, 9.4, and 9.5. A representative sketch of $H_1(x)$ is given in Fig. 9.1.

Example 90 The Quantum Mechanical Linear Harmonic Oscillator

Solution: The problem of describing the small oscillation of a mass m attached to the end of a spring with force constant k and potential energy $V(x) = kx^2/2$ can be solved exactly in both classical and quantum mechanics. This system is referred to as a linear harmonic oscillator and is used to represent and analyze more complex physical systems such as (a) vibrations of individual atoms in molecules and in crystals and (b) classical and quantum theories of radiation. The solution of Schrödinger's wave equation for the linear harmonic



Figure 9.1: Hermite polynomials $H_n(x)/n^3$ (Abramowitz and Stegun, 1964)

oscillator is expressed in terms of Hermite polynomials, $H_n(x)$. The equation to be solved is the one-dimensional Schrödinger wave equation for the linear harmonic oscillator which has the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{kx^2}{2}\psi = E\psi.$$
(9.20)

Note that Eq.(9.20) is just the one-dimensional Helmholtz equation for which k^2 equals $2m \left(E - kx^2/2\right)/\hbar^2$. Solving a problem in quantum mechanics involves finding the wave functions, ψ_n , and the corresponding eigenenergy, E_n . In dimensionless form, Eq.(9.20) becomes (see Worksheet in Section 9.9.1)

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0 \tag{9.21}$$

where
$$\xi = \left(\frac{m\omega}{\hbar}\right)^{1/2} x$$
, $\omega^2 = \frac{k}{m}$, and $\lambda = \frac{2E}{\hbar\omega}$.

On substituting $\lambda = 1 + 2n$ into Eq.(9.21), we obtain the Weber⁴ differential equation, and the transformation

$$\psi = \exp\left(-\xi^2/2\right)y(\xi)$$
 (9.22)

reduces the Weber differential equation to the Hermite differential equation. The transformation equation, Eq.(9.22), leading to Hermite's differential equation is motivated by use of the Sommerfeld⁵ polynomial method (see Schiff, 1968; Section 13, page 66) for solving certain differential equations. By use of the Sommerfeld method, the solution of Eq.(9.21) is the product of the physically acceptable asymptotic solution times a polynomial. The

⁴Wilhelm Edward Weber (1804–1891), German physicist who is known for his work in electromagnetism and for the Weber equation. He was Chair of physics at the University of Gottingen and collaborated with Gauss on numerous problems.

⁵Arnold Johannes Wilhelm Sommerfeld (1868–1951), German physicist who was born in Königsberg, Prussia. He is known for his work in many areas of physics, especially in quantum theory. He developed a very famous school of theoretical physics in Munich.

resulting asymptotic, $|\xi|$ approaches infinity, differential equation is $\psi'' - \xi^2 \psi = 0$, and the physically acceptable solution of this differential equation is given by $\exp(-\xi^2/2)$. In this case, the polynomial part of the solution of Eq.(9.21) comes from solving Hermite's differential equation. The eigenfunctions and eigenenergy for the linear harmonic oscillator, Eq.(9.21), are respectively given by

$$\psi_n = N_n e^{-\xi^2/2} H_n(\xi)$$
 and $\lambda_n = 1 + 2n = \frac{2E_n}{\hbar\omega}$. (9.23)

The eigenenergy reduces to the familiar form $E_n = \hbar \omega (n + 1/2)$. The behavior of ψ_n for the first six values of n is illustrated in the sketches in Fig. 9.2.



Figure 9.2: Harmonic oscillator wave functions $\psi_n(\xi)$

9.4 The Helmholtz Differential Equation in Spherical Coordinates

9.4.1 Introduction

The Laplacian operator in spherical coordinates (r, θ, ϕ) has the form

$$\nabla^2 = \nabla_r^2 + \frac{1}{r^2} \nabla_{\theta,\phi}^2. \tag{9.24}$$

The radial and angular parts of the Laplacian are given respectively by

$$\nabla_r^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \tag{9.25}$$

and

$$\nabla_{\theta,\phi}^2 = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}.$$
(9.26)

The Helmholtz differential equation in spherical coordinates has the form

$$\left\{\nabla_{r}^{2} + \frac{1}{r^{2}}\nabla_{\theta,\phi}^{2}\right\}u + k^{2}u = 0.$$
(9.27)

The solution of Eq.(9.27) involves (a) symmetry-type information in terms of the angular parts θ and ϕ which is common to all problems with spherical symmetry and (b) dynamical information in terms of the radial part which characterizes the particular problem under investigation. In this connection, the Helmholtz differential equation reduces to the (a) Laplace differential equation for $k^2 = 0$, (b) time-independent heat conduction (diffusion) or time-independent mechanical wave differential equations for $k^2 = \text{constant}$, and (c) time-independent Schrödinger wave equation for $k^2 = (2m/\hbar^2) \{E - V(r)\}$. Separating the angular parts from the radial part in Eq.(9.27) for $u(r, \theta, \phi) = R(r)Y(\theta, \phi)$, the corresponding differential equations for R(r) and $Y(\theta, \phi)$ with separation constant λ are

$$\nabla_r^2 R(r) + \left\{ k^2 - \frac{\lambda}{r^2} \right\} R(r) = 0$$
(9.28)

and

$$\nabla^2_{\theta,\phi} Y(\theta,\phi) + \lambda Y(\theta,\phi) = 0. \tag{9.29}$$

Note that the general solutions of Eq.(9.29) are independent of the specific problem under investigation but are common to all problems that involve the Laplacian operator in spherical coordinates. The solutions of Eq.(9.29) with separation constant $-m^2$ are called **spherical harmonics** (also known as surface harmonics of the first kind), $Y_{\lambda}^{m}(\theta,\phi)$. It is shown in Worksheet in Section 9.9.2 that a replacement of the form $\lambda = \ell(\ell+1)$ is required for square integrable solutions of the theta part of Eq.(9.29). Tesseral harmonics is the name given to $Y_{\ell}^{m}(\theta,\phi)$ when $m < \ell$, and the term **sectoral harmonics** is used when m = l. Tesseral and sectoral harmonics may be written as $C_{\ell}e^{im\phi}P_{\ell}^{m}(\cos\theta)$ where $P_{\ell}^{m}(\cos\theta)$ are associated Legendre functions of the first kind. When m = 0, the spherical functions are called **Legendre polynomials** of the first kind (also known as zonal harmonics and Legendre coefficients).

On substituting Eqs.(9.25 and 9.26) into Eqs.(9.28 and 9.29) respectively and separating the variables in Eq.(9.29) $\{Y(\theta, \phi) = \Theta(\theta)\Phi(\phi) \text{ with separation constant } -m^2\}$, we obtain the following three ordinary differential equations.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \left[k^2 - \frac{\ell\left(\ell+1\right)}{r^2}\right]R = 0 \quad \text{Radial equation,} \tag{9.30}$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \left[\ell\left(\ell+1\right) - \frac{m^2}{\sin^2\theta}\right]\Theta = 0 \quad \text{Theta equation,} \tag{9.31}$$

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0.$$
 Azimuthal equation. (9.32)

The general solution of the azimuthal equation is $\Phi = c_1 e^{im\phi} + c_2 e^{-im\phi}$. In solving physical problems, the requirement that $\Phi(\phi)$ be a single-valued function is imposed. That is to

say, we require that $\Phi(\phi) = \Phi(\phi + 2\pi)$ which leads to the following acceptable values for $m: 0, \pm 1, \pm 2, \ldots$, and the solution may be written in the form $\Phi(\phi) = Ae^{im\phi}$. In quantum mechanics, the single-valued function requirement is referred to as Born's⁶ periodic boundary condition, and m is the **magnetic quantum number**.

9.4.2 Legendre Polynomials and Associated Legendre Functions

Solutions of the theta equation, Eq.(9.31), involve the Legendre polynomials and associated Legendre functions. The traditional treatment of the theta equation involves introducing a new independent variable by use of the transformation $w = \cos \theta$ (also, the notation $x = \cos \theta$ is used; here, x is not the usual Cartesian coordinate); this transformation yields the **associated Legendre differential equation**

$$(1 - w^2) \frac{d^2 \Theta}{dw^2} - 2w \frac{d\Theta}{dw} + \left\{ \ell \left(\ell + 1\right) - \frac{m^2}{1 - m^2} \right\} \Theta = 0.$$
(9.33)

The **Legendre differential equation** is the result when m = 0 in Eq.(9.33); it is written as

$$\left(1-w^2\right)\frac{d^2\Theta}{dw^2} - 2w\frac{d\Theta}{dw} + \ell\left(\ell+1\right)\Theta = 0.$$
(9.34)

The solution of the Legendre differential equation may be obtained by use of the power series method, and the solution of the associated Legendre differential equation may be obtained from the solution of the Legendre differential equation by means of differentiation (see Worksheet in Section 9.9.2). The general solution of the Legendre differential equation has the form

$$\Theta_{\ell}(w) = A_{\ell} P_{\ell}(w) + B_{\ell} Q_{\ell}(w); \quad A_{\ell} \text{ and } B_{\ell} \text{ are constants.}$$
(9.35)

In Eq.(9.35), $P_{\ell}(w)$ are called the **Legendre polynomials of the first kind** of order ℓ ; the $Q_{\ell}(w)$ are known as **Legendre functions of the second kind** and are seldom used in solving physical problems. The series form for $P_{\ell}(w)$ is

$$P_{\ell}(w) = \sum_{r=0}^{N} \frac{(-1)^{r} (2\ell - 2r)! w^{\ell - 2r}}{2^{\ell} r! (\ell - r)! (\ell - 2r)!}$$
(9.36)

where
$$N = \begin{cases} \ell/2 & \text{for } \ell \text{ even} \\ (\ell - 1)/2 & \text{for } \ell \text{ odd.} \end{cases}$$

The orthoganality relation, recurrence relation, Rodrigues formula, and generating function for the Legendre polynomials are given in Tables 9.2, 9.3, 9.4, and 9.5.

The Legendre functions of the second kind, $Q_{\ell}(w)$, satisfy a recursion relation of the same form as the one for $P_{\ell}(w)$. Graphical illustrations of Legendre polynomials are given in Figs 9.3-9.5, and Legendre functions of the second kind are illustrated in Figs.9.6 and 9.7.

 $^{^{6}}$ Max Born (1882–1970), German physicist who is best known for his mathematical description of observables in quantum theory. He was awarded the 1954 Nobel Prize in physics for his statistical studies of wave functions.



Figure 9.3: Legendre polynomials, $P_n(\cos\theta)$ (Abramowitz and Stegun, 1964)

Associated Legendre functions result when Legendre polynomials are differentiated m times (see Worksheet in Section 9.9.2)

$$P_{\ell}^{m}(w) = \left(1 - w^{2}\right)^{m/2} \frac{d^{m} P_{\ell}(w)}{dw^{m}}.$$
(9.37)

The two linearly independent solutions of the associated Legendre differential equation are

$$\Theta_{\ell}^{m}(w) = A_{\ell}^{m} P_{\ell}^{m}(w) + B_{\ell}^{m} Q_{\ell}^{m}(w).$$
(9.38)

The quantities $P_{\ell}^{m}(w)$ and $Q_{\ell}^{m}(w)$ are associated Legendre functions of the first and second kind respectively. The orthogonality relation, recurrence relation, and Rodrigues formula for the associated Legendre functions are given in Tables 9.2, 9.3, and 9.4. Graphical illustrations of associated Legendre functions are given in Fig 9.8.

The radial equation, Eq.(9.30), characterizes the dynamical information of specific problems or classes of problems. The Laplace equation leads to a simple radial equation when $k^2 = 0$; for this case, the solution characterizes such steady-state problems as potentials in electrostatics and temperatures in heat conduction. The time-independent Schrödinger equation results when $k^2 = 2\mu [E - V(r)/\hbar^2]$ for a class of two-body central force problems; the reduced mass of such a system is given by $\mu = m_1 m_2/(m_1 + m_2)$ where m_1 and m_2 are the masses of constituent particles.

Example 91 Calculate the steady-state temperature distribution $T(r, \theta)$ within a sphere of radius b when the temperature over the surface of the sphere is independent of ϕ . That is to say, $T(b, \theta) = f(\theta)$ where $f(\theta)$ is a known function.

Solution : The general solution of Laplace's differential equation for this problem is independent of ϕ (circular symmetry) and has the form $T(r, \theta) = R(r)\Theta(\theta)$. The radial and theta equations for this problem reduce to

$$r^{2}R'' + 2rR' - \ell(\ell+1)R = 0$$
 and



Figure 9.4: Legendre polynomials, $P_n(x)$ (Abramowitz and Stegun, 1964)

$$\sin\theta\Theta'' + \cos\theta\Theta' + \ell(\ell+1)\sin\theta\Theta = 0.$$

The general solution of the above equation for R is

$$R(r) = Ar^{\ell} + \frac{B}{r^{\ell+1}}, \quad A \text{ and } B \text{ are constants.}$$

The general solution of the above theta equation (the Legendre differential equation) is $P_{\ell}(\cos \theta)$. We set the *B* coefficient to zero since a finite solution at every point within the sphere is required. The general solution of the problem is a superposition of the product of radial and theta solutions; we write

$$T(r,\theta) = \sum_{\ell=0}^{\infty} A_{\ell} r^{\ell} P_{\ell}(\cos \theta).$$

Values of the coefficients are obtained by use of the boundary condition $T(b, \theta) = f(\theta)$ and the orthogonality relations for the Legendre polynomials. The specific form for $f(\theta)$ must be given if the specific values for are required.



Figure 9.5: Legendre polynomials, $P_n(x)$ (Abramowitz and Stegun, 1964)

9.4.3 Laguerre Polynomials and Associated Laguerre Polynomials

The Laguerre⁷ differential equation,

$$xy'' + (1 - x^2)y' + ny = 0;$$
 $n = \text{constant},$ (9.39)

is a special case of the Sturm-Liouville differential equation as well as a special case of the confluent hypergeometric differential equation; its solution may be obtained by relation to $_{1}F_{1}$ or by use of the Frobenius-Fuchs power series method (see Worksheet in Section 9.9.3),

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{k+\lambda}; \qquad a_0 \neq 0.$$
(9.40)

The indicial equation in the above power series has a double root at k = 0, and the power series method yields only one of the two linearly independent solutions of the Laguerre differential equation; this solution, however, is extremely important in mathematical physics.

⁷Edmond Nicolas Laguerre (1834–1886), French mathematician who is known for his work in analysis and geometry. He is best known for the differential equation and polynomials named for him.



Figure 9.6: Legendre functions of the second kind, $Q_n(x)$ (Abramowitz and Stegun, 1964)

The finite solutions of the Laguerre differential equation, $L_n(x)$, are called Laguerre polynomials. The solution in series form is

$$L_n(x) = \sum_{j=0}^{\infty} \frac{(-1)^j \, n! x^j}{(n-j)! \, (j!)^2}.$$
(9.41)

The orthogonality and recurrence relations for the Laguerre polynomials are given in Tables 9.2 and 9.3; the generating function and the Rodrigues formula are respectively given by

$$\frac{\exp\left[-xt/(1-t)\right]}{1-t} = \sum_{n=0}^{\infty} \frac{L_n(x)t^n}{n!} \quad \text{and}$$
(9.42)

$$L_n(x) = \frac{1}{n!} e^x \frac{d^n \left(x^n e^x\right)}{dx^n}.$$
(9.43)

Note that $L_n(0) = 1, L_0(x) = 1 - x$, and $L_2(x) = 2 - 4x + x^2$. A sketch of Laguerre polynomials is given in Fig. 9.9.

Note that the k-th derivative of the Laguerre differential equation yields the associated Laguerre differential equation,

$$x\frac{d^2L_n^k(x)}{dx^2} + (k+1-x)\frac{dL_n^k(x)}{dx} + (n-k)L_n^k(x) = 0.$$
(9.44)

In obtaining Eq.(9.44), the Leibniz formula, Eq.(9.16), for finding the k-th derivative of a product was used; note that the associated Laguerre polynomials, $L_n^k(x)$, are related to the Laguerre polynomials by use of the following relation

$$L_{n}^{k}(x) = \frac{d^{k}L_{n}(x)}{dx^{k}}.$$
(9.45)

The orthogonality relation, recurrence relation, Rodrigues formula, and generating function for associated Laguerre polynomials are respectively given in Tables 9.2, 9.3, 9.4, and 9.5.

Example 92 A Central Force Problem in Quantum Mechanics

Solution : The time-independent Schrödinger wave equation is used to study the mechanics of two microscopic particles moving under the influence of a central force (that is to say, the force and potential depend only on the distance between the two particles). This problem provides the basis for the quantum mechanical treatment of a fundamental class of problems such as (a) the rigid rotator which is of considerable importance in the study of the spectra of diatomic molecules; (b) the theory of the hydrogen atom; and (c) the nonrelativistic theory of the deuteron. For an attractive inverse square force law, we substitute $k^2 = 2\mu (E - A/r)/\hbar^2$ into the radial equation, Eq.(9.30); the quantity A is a positive constant. Anticipating use of the well-known solution of the associated Laguerre differential equation, the following substitutions are made in the radial equation for inverse square force problems.

$$\xi = \beta r, \ \ \beta^2 \equiv \frac{8\mu \left|E\right|}{\hbar^2}, \ \ \text{and} \ \ \gamma \equiv \frac{2\mu A}{\beta \hbar^2} = \frac{A}{\hbar} \left(\frac{\mu}{2\left|E\right|}\right)^{1/2}.$$
 (9.46)

By use of the substitutions in Eq.(9.46), the radial equation, Eq.(9.30), reduces to

$$\xi \frac{d^2 R}{d\xi^2} + 2\frac{dR}{d\xi} + \left\{\gamma - \frac{\xi}{4} - \frac{\ell(\ell+1)}{\xi}\right\}R = 0.$$
(9.47)

The symbol ℓ represents the **angular momentum quantum number**. Equation (9.47) is reduced to the associated Laguerre differential equation by use of the following transformation:

$$R_{n\ell}(\xi) = \exp\left(-\xi/2\right)\xi^{\ell}L_{n+1}^{2\ell+1}(\xi).$$
(9.48)

The desired solution of the equation to be solved, Eq.(9.47), is a normalization constant times $R_{n\ell}(\xi)$. A polynomial solution of the associated Laguerre differential equation is obtained when $\gamma = n = \ell + k + 1$ for k = 0, 1, 2, ..., n - 1. The **principal quantum number** is represented by n.

Example 93 The Hydrogen Atom Obtain the eigenfunction and eigenenergy for the hydrogen atom.

Solution : The hydrogen atom represents a two-body central force problem in quantum mechanics where the electron and proton are the two particles under investigation. The Coulomb potential is the central potential for the hydrogen atom. Here, the total energy is negative for bound states, E < 0, and the attractive potential energy is given by $V = -e^2/(4\pi\epsilon_0 r) = -A/r$ where $A = e^2/4\pi\epsilon_0$. The eigenenergy, E_n , is obtain from Eq.(9.46); we obtain the familiar Bohr⁸ result,

$$E_n = -\frac{\mu A^2}{2\hbar^2 n^2}.$$

 $^{^{8}}$ Niels Henrik David Bohr (1885–1962) was born in Copenhagen, Denmark. He is known for his many fundamental contributions to atomic theory and quantum theory. He was awarded the 1922 Nobel Prize for physics.

The corresponding steady-state wave function is the product of solution of the radial part and the angular part which is $Y_{\ell}^{m}(\theta, \phi)$ times a normalization constant, $C_{n\ell}$; the result is

$$\psi(r,\theta,\phi) = -C_{n\ell}R_{n\ell}(\xi)Y_{\ell}^{m}(\theta,\phi).$$
(9.49)

The eigenfunction solution, Eq.(9.49), is given in most quantum mechanics books, and the normalization constant is obtained in the usual manner.

9.5 The Helmholtz Differential Equation in Cylindrical Coordinates

9.5.1 Introduction

Problems in mathematical physics that involve cylindrical geometry are in general simpler to solve in cylindrical coordinates (ρ, ϕ, z) than in Cartesian coordinates. The Helmholtz differential equation in cylindrical coordinates has the form

$$\rho \frac{\partial^2 u}{\partial \rho^2} + \frac{\partial u}{\partial \rho} + \frac{1}{\rho} \frac{\partial^2 u}{\partial \phi^2} + \rho \frac{\partial^2 u}{\partial z^2} + k^2 \rho u = 0.$$
(9.50)

By use of the separation of variables method for with separation constants $-\lambda^2$ and $-n^2$, the following three ordinary differential equations are obtained.

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -\lambda^2 \quad \text{where} \quad Z(z) = A\cos(\lambda z) + B\sin(\lambda z) ,$$
$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -n^2 \quad \text{where} \quad \Phi(\phi) = C\cos(n\phi) + D\sin(n\phi) , \text{ and}$$

$$\rho^{2} \frac{d^{2} l}{d\rho^{2}} + \rho \frac{d^{2}}{d\rho} + \left\{ \rho^{2} \left(k^{2} - \lambda^{2} \right) - n^{2} \right\} P = 0.$$
(9.51)

Equation (9.51) may be put into the form of Bessel's differential equation by use of the following substitutions $\xi = \alpha \rho$ and $k^2 - \lambda^2 \equiv \alpha^2$. We obtain

$$\xi^2 \frac{d^2 P}{d\xi^2} + \xi \frac{dP}{d\xi} + \left\{\xi^2 - n^2\right\} P = 0.$$
(9.52)

9.5.2 Solutions of Bessel's Differential Equation

Bessel's⁹ differential equation,

$$x^{2}y'' + xy' + (x^{2} - n^{2})y = 0; \quad n = \text{constant},$$
 (9.53)

⁹Friedrich Wilhelm Bessel (1784–1846), German mathematician and scientist whose formal education ended at age 14 but made major contributions in mathematics and astronomy. Functions now known as Bessel functions resulted from his work in astronomy.

may be solved by use of the power series method (see Worksheet in Section 9.9.4); we obtain

$$J_n(x) = \sum_{j=0}^{\infty} \frac{(-1)^j (x/2)^{2j+n}}{j! \Gamma(n+j+1)}.$$
(9.54)

The gamma function is defined on page 242. Note that $J_{-n}(x) = (-1)^n J_n(x)$. General solutions of Bessel's differential equation when n is an integer are

$$y_n(x) = AJ_n(x) + BN_n(x); \quad n \text{ integer.}$$
(9.55)

The functions $J_n(x)$ and $N_n(x)$ are explained in the following sections.

9.5.3 Bessel Functions of the First Kind

The functions $J_n(x)$ are called **Bessel functions of the first kind**; the generating function, and recurrence relation for $J_n(x)$ are respectively given by

$$\exp\left\{\frac{1}{2}x\left(t-\frac{1}{t}\right)\right\} = \sum_{n=-\infty}^{\infty} J_n(x)t^n \quad \text{and} \tag{9.56}$$

$$J_{n-1}(x) + J_{n+1}(x) = \frac{2n}{x} J_n(x).$$
(9.57)

The orthogonality relation for the interval [0, a] may be written in the following

$$\int_{0}^{a} J_{n}\left(\beta_{ni}\frac{x}{a}\right) J_{n}\left(\beta_{nj}\frac{x}{a}\right) x dx = \begin{cases} 0 \text{ for } i \neq j \\ a^{2}/2 \left[J_{n+1}(\beta_{nj})\right]^{2} \text{ otherwise.} \end{cases}$$
(9.58)

In Eq.(9.58), n > -1, the parameter β_{ni} is the *i*-th-zero of J_n , and $0 \le x \le a$. The general solutions of Bessel's differential equation when n is not an integer are

$$y_n(x) = CJ_n(x) + DJ_{-n}(x); \quad n \text{ not integer.}$$

$$(9.59)$$

Sketches of several Bessel functions of the first kind are given in Fig. 9.10.

9.5.4 Neumann Functions

The Neumann¹⁰ functions are defined by

$$N_n(x) \equiv \frac{J_n(x)\cos n\pi - J_{-n}(x)}{\sin n\pi}; \quad n = \text{integer.}$$
(9.60)

Sometimes the notation $Y_n(x)$ is used to represent Neumann functions. The Neumann functions are called **Bessel functions of the second kind**. L'Hospital's¹¹ rule should be used to evaluate $N_n(x)$. Sketches of several Neumann functions are given in Fig. 9.10.

¹⁰Carl Gottfried Neumann (1832–1925), German mathematician and physicist was born in Königsberg, Prussia. He worked on topics ranging from applied mathematics to electrodynamics to pure mathematics.

¹¹Guillaume Francois Antoine Marquis de L'Hospital (1661–1704), French mathematician who wrote the first book on calculus (1696). He is best known for the rule named for him.

Example 94 Vibrations of a Circular Membrane. The displacement $u(r, \theta, t)$ of a stretched circular membrane with mass per unit area μ and under tension T satisfies the two-dimensional mechanical wave equation in plane polar coordinates (r, θ) which may be written in the following form.

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\frac{1}{r}\frac{\partial u}{\partial \theta}\right)\right\} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}.$$

The speed of the wave motion is defined by $v = \sqrt{T/\mu}$. Develop the solution of this equation for a vibrating drum head.

Solution : Separating the variables $u(r, \theta, t) = R(r)\Theta(\theta)T(t)$ with separation constants $-\alpha^2$ and $-n^2$ yields the following three ordinary differential equations.

$$\begin{aligned} \frac{d^2T}{dt^2} + \omega^2 T &= 0, \quad \text{or} \quad T(t) = A \cos \omega t + B \sin \omega t \quad \text{where} \quad \omega^2 \equiv v^2 \alpha^2, \\ \frac{d^2\Theta}{d\theta^2} + n^2\Theta &= 0, \quad \text{or} \quad \Theta(\theta) = C \cos n\theta + D \sin n\theta, \quad \text{and} \\ \xi^2 \frac{d^2R}{d\xi^2} + \xi \frac{dR}{d\xi} + \left(\xi^2 - n^2\right)R = 0 \quad \text{where} \quad \xi \equiv \alpha r. \end{aligned}$$

The solution of the above equation is $R(\xi) = EJ_n(\xi) + FN_n(\xi)$ since it is of the Bessel differential equation form. In addition, it is required that the solution be finite at $\xi = 0$; hence, F is set to zero since $N_n(\xi)$ approaches infinity as ξ approaches zero. The general solution for the motion of the drum head is therefore given by

$$u = [A\cos\omega t + B\sin\omega t] [C\cos n\theta + D\sin n\theta] EJ_n(\xi).$$

Since the membrane is fixed (no vibration, u = 0) around the edge where r = b (radius of the head), the drum head vibrates in circular modes such that $EJ_n(\xi) = 0$. The nodes are located at $\alpha r = \xi_k$ where ξ_k are the values of ξ for which $J_n(\xi)$ has a zero. A single term in the solution corresponds to a standing wave whose modes are concentric circles, and the complete solution is obtained by summing over all such modes of vibration.

9.5.5 Hankel Functions

Hankel¹² functions of the first and second kind are respectively defined by

$$H_n^{(1)}(x) \equiv \frac{i}{\sin n\pi} \left\{ e^{-in\pi} J_n(x) - J_{-n}(x) \right\}$$

= $J_n(x) + iN_n(x)$ and (9.61a)

$$H_n^{(2)}(x) \equiv -\frac{i}{\sin n\pi} \left\{ e^{in\pi} J_n(x) - J_{-n}(x) \right\} = J_n(x) - iN_n(x).$$
(9.61b)

The Hankel functions are independent solutions of the Bessel differential equation, and they are useful in connection with their behavior for large values of x since they are infinite at x = 0. Hankel functions are sometimes referred to as Bessel functions of the third kind.

 $^{^{12}}$ Hermann Hankel (1839–1873), German mathematician who worked on the theory of complex numbers, the theory of functions, and the history of mathematics.

9.5.6 Modified Bessel Functions

The modified Bessel differential equation is obtained when x is replaced with (*it*) in Eq.(9.53); the result is

$$t^{2}y'' + ty' + (t^{2} + n^{2}) y = 0.$$
(9.62)

The solutions of Eq. (9.62) are called **modified Bessel functions** of the first kind and are denoted by $I_n(t)$; they are given by

$$I_n(t) \equiv i^{-n} J_n(it) = \sum_{j=0}^{\infty} \frac{(t/2)^{2j+n}}{j! (j+n)!}; \quad n \text{ integer.}$$
(9.63)

When n is not an integer, $I_n(t)$ and $I_{-n}(t)$ are linearly independent solutions of the modified Bessel differential equation, Eq.(9.62). When n is an integer, $I_n(t) = I_{-n}(t)$. The modified Bessel functions of the second kind, $K_n(t)$, are defined by

$$K_n(t) \equiv \frac{\pi}{2} \left\{ \frac{I_n(t) - I_{-n}(t)}{\sin n\pi} \right\}.$$
 (9.64)

The modified Bessel functions of the second kind are well behaved for all values of n. Sketches of several modified Bessel functions are given in Fig. 9.11.

9.5.7 Spherical Bessel Functions

Solutions of the radial equation, Eq.(9.30), for $k^2 = \text{constant}$ are obtained by comparing the radial equation with the Bessel differential equation; these solutions are called **spherical Bessel functions** and have the form

$$R(\zeta) = Aj_n(\zeta) = \left(\frac{\pi}{2\zeta}\right)^{1/2} J_{n+1/2}(\zeta) \text{ for } \zeta = kr.$$
(9.65)

Spherical Bessel functions are often used in quantum mechanics and in other areas of physics. Sketches of several spherical Bessel functions, spherical Neumann functions, and spherical modified Bessel functions are respectively given in Figs. 9.12, 9.13, and 9.14.

9.6 The Hypergeometric Function

Important members of a large subset of special functions are related to a class of functions called hypergeometric functions which are solutions of the hypergeometric differential equation (also known as the Gauss differential equation). The hypergeometric differential equation has three regular singular points, and it can be shown that any second-order ordinary linear differential equation with three regular singular points can be transformed (reduced) to the hypergeometric differential equation form. The solutions of many physical problems involve special functions that result from solving second-order ordinary linear differential equations with regular singular points. It is, therefore, natural to expect a connection among hypergeometric functions and certain special functions. The **hypergeometric differential equation** has the form

$$x(1-x)y'' + [c - (a+b+1)x]y' - aby = 0.$$
(9.66)

Note that Eq.(9.66) has regular singular points at $x = 0, 1, \infty$. In Eq.(9.66), parameters a, b, and c are arbitrary constants. The hypergeometric differential equation can be solved by use of the Frobenius-Fuchs power series method (see Worksheet in Section 9.9.5); here the form of the solution is

$$y = \sum_{j=0}^{\infty} a_j x^{k+j}; \quad a_0 \neq 0.$$
(9.67)

In general, the solutions of Eq. (9.66) are the various forms of the Gauss hypergeometric series; they are $\{y(x) = {}_{2}F_{1}(a, b, c; x) = F(a, b, c; x)\}$

$${}_{2}F_{1}(a,b,c;x) = \sum_{n=0}^{\infty} \frac{(a)_{n}(b)_{n}}{n!(c)_{n}} x^{n}.$$
(9.68)

The factorial function in Eq.(9.68) is defined by

$$(\lambda)_{n} = \prod_{k=1}^{n} (\lambda + k - 1) = \lambda (\lambda + 1) (\lambda + 2) \dots (\lambda + n - 1)$$
$$= \frac{\Gamma(\lambda + n)}{\Gamma(\lambda)}$$
(9.69)

for $\lambda = a, b$, and c respectively. This notation for the factorial function is called a **Pochhammer symbol**. The notation ${}_2F_1$ means that there are two factorial functions in the numerator of the series and one factorial function in the denominator of the series in Eq.(9.20). The gamma function $\Gamma(\lambda)$ is defined on page 242.

For convenience, we will write F(a, b, c; x) for $_2F_1(a, b, c; x)$ since the three parameters in the parentheses are sufficient to avoid confusion with the notation for the confluent hypergeometric function. Originally, the notation $_2F_1(a, b; c; x)$ was used to represent the hypergeometric function. One, however, finds a variety of combinations of commas and/or semicolons used in the literature to represent the hypergeometric function. We will use a comma to separate constants and use a semicolon to separate the variable from the constants.

The hypergeometric series F(-m, b, -n; x) is not defined if n < m. The hypergeometric series converges if |x| < 1 and diverges if |x| > 1. For x = 1, the series converges if c > a + b, and it converges for x = -1 if c > a + b - 1. The hypergeometric series becomes a polynomial of degree n in x when a or b equals a negative integer.

Note that F(a, b, c; 0) = 1 and F(a, b, c; x) = F(b, a, c; x). Also, note that many elementary transcendental functions may be expressed in terms of a hypergeometric series; two example are $\ln(1+x) = xF(1, 1, 2; -x)$ and $(1+x)^a = F(-a, b, b; -x)$. The geometric series is a special case of the hypergeometric series since

$$F(1,1,1;x) = \sum_{n=0}^{\infty} x^n.$$

The numerous properties of F(a, b, c; x) summarized in this chapter as well as in many other places were developed by Euler and Gauss.

Solutions of the hypergeometric differential equation that are orthogonal polynomials are of particular interest in this chapter, and polynomial solutions occur when a or b is a negative integer. Examples of the connections of F(a, b, c; x) with some special polynomials of interest are given in the Table 9.6.

Table 9.6 Connections of F(a, b, c; x) with Special Polynomials

Chebyshev	$T_n(1-2x) = F(-n, n, 1/2; x)$
Gegenbauer	$n!/\left(2\alpha\right)_{n}C_{n}^{\left(\alpha\right)}\left(1-2x\right)=F\left(-n,n+2\alpha,\alpha+1/2;x\right)$
Jacobi	$n!/(\alpha+1)_n P_n^{(\alpha,\beta)}(1-2x) = F(-n,\alpha+1+\beta+n,\alpha+1;x)$
Legendre	$P_n(1-2x) = F(-n, n+1, 1; x)$

The Gegenbauer¹³ (also known as ultraspherical), Legendre and associated Legendre, and Chebyshev polynomials are special cases of the Jacobi polynomial (sometime called hypergeometric polynomial). Chebyshev¹⁴ (Tschebyscheff, Tchebichef, and Tchebicheff are other spellings found in the literature) polynomials involve solutions of separated equations in spherical, parabolic, prolate, and oblate spheroidal coordinates. Chebyshev polynomials converge rapidly and have the special property that $\max T_n(x) = +1$ and $\min T_n(x) = -1$; because of this property, Chebyshev polynomials are useful in numerical analysis. Gegenbauer functions result from separated equations in circular cylinder and spherical coordinates with two regular singular points at ± 1 rather than at 0 and 1.

We now summarize some of the basic properties of the solutions of the Jacobi differential equation (see Table 9.1) and express these solutions in terms of $_2F_1$. The solutions of the Jacobi differential equation may be written as

$$y = c_1 P_n^{(\alpha,\beta)}(x) + c_2 Q_n^{(\alpha,\beta)}(x).$$

The quantity $P_n^{(\alpha,\beta)}(x)$ is a polynomial and is called Jacobi polynomial of the first kind. The quantity $Q_n^{(\alpha,\beta)}(x)$ is not a polynomial and is called Jacobi functions of the second kind. In terms of hypergeometric functions, we write

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+1)_n}{n!} F\left(-n, n+\alpha+\beta+1, \alpha+1; \left[1-x\right]/2\right) \quad \text{and}$$

$$Q_{n}^{(\alpha,\beta)}(x) = \frac{C(\alpha,\beta)}{(x-1)^{n+\alpha+1} (x+1)^{\beta}} F(n+1, n+\alpha+1, 2n+\alpha+\beta+2; 2/[1-x])$$

The symbol $C(\alpha, \beta)$ in the above equation represents the following quantity

$$C(\alpha,\beta) = \frac{2^{n+\alpha+\beta}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(2n+\alpha+\beta+2)(x-1)^{n+\alpha+1}}.$$

¹³Leopold Bernhard Gegenbauer (1849–1903), Austrian mathematician who is best known for the polynomials now named for him.

¹⁴Pafnuty Lvovich Chebyshev (1821–1894), Russian mathematician who is known for his work in number theory and for the polynomials named for him.

The standardization for the Jacobi polynomial is given by

$$P_n^{(\alpha,\beta)}(1) = \frac{(\alpha+1)_n}{n!}.$$

Rodrigues's formula and the generating function for the Jacobi polynomial are given in Tables 9.4 and 9.5 respectively. The form of the recursion formula for the Jacobi polynomial is given by

$$2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)P_{n+1}^{(\alpha,\beta)}(x)$$

= $(2n+\alpha+\beta+1)\left[(2n+\alpha+\beta)(2n+\alpha+\beta)x+\alpha^2-\beta^2\right]P_n^{(\alpha,\beta)}(x)$
- $2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1}^{(\alpha,\beta)}(x).$

The integral representation of the Jacobi polynomial may be written as

$$P_{n}^{(\alpha,\beta)}(x) = \frac{1}{2\pi i} \oint_{C} \frac{1}{2} \left(\frac{t^{2}-1}{t-x}\right)^{n} \left(\frac{1-t}{1-x}\right)^{\alpha} \left(\frac{1+t}{1+x}\right)^{\beta} dt; \quad x \neq \pm 1.$$
(9.70)

The contour in Eq.(9.70) is a simple closed contour in a positive sense around t = x; the points $t = \pm 1$ are outside of the contour. In Eq.(9.70), the quantities raised to the α and β power are defined to be unity when t = x. Graphical illustrations of Jacobi, Chebyshev, and Gegenbauer polynomials are given in Figs. 9.15-9.17.

9.7 The Confluent Hypergeometric Function

The confluent hypergeometric differential equation (also called the Kummer¹⁵ differential equation) has the form

$$xy'' + (c - x)y' - ay = 0. (9.71)$$

Equation (9.71) may be obtained from the hypergeometric differential equation by a merging (a confluence) of the two upper singular points. In the confluent hypergeometric differential equation, there is a regular singularity at x = 0 and an irregular singularity at $x = \infty$. By use of the power series method in the neighborhood of x = 0, we find that one solution of Eq.(9.71) has the form (confluent hypergeometric functions or Kummer functions)

$$y(x) = {}_{1}F_{1}(a,c;x) = 1 + \frac{ax}{c} \frac{a(a+1)x}{2!c(c+1)} + \dots = \sum_{n=0}^{\infty} \frac{(a)_{n} x^{n}}{(c)_{n}}.$$
(9.72)

The confluent hypergeometric series converges for all values of x. In Table 9.7, we give the connection of certain orthogonal polynomials with the confluent hypergeometric functions.

¹⁵Ernst Eduard Kummer (1810–1893), German (Prussian) mathematician who worked on function theory and extended the work of Gauss on the hypergeometric series.

Table 9.7 Connections of with Certain Special Polynomials

Bessel Functions	$J_n(x) = (e^{-ix}/n!) (x/2)^n F(n+1/2, 2n+1; 2ix)$
Modified Bessel Functions	$I_n(x) = (e^{-x}/n!) (x/n!)^n F(n+1/2, 2n+1; 2x)$
Laguerre Polynomials	$L_n(x) = F\left(-n, 1; x\right)$
Associated Laguerre Polynomials	$L_n^m(x) = (n+m)!/n!m!F\left(-n,m+1;x\right)$
Hermite Polynomials	$H_{2n}(x) = (-1)^n (2n)! / n! F(-n, 1/2; x^2)$

The error function and complementary error function are respectively defined by

$$\operatorname{er} f(x) = rac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$
 where $\operatorname{er} f(\infty) = 1$ and
 $\operatorname{er} f_C(x) = 1 - \operatorname{er} f(x) = rac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt.$

The Hermite polynomials may be obtained from derivatives of the error function as follows.

$$\frac{d^{n+1}\mathrm{er}f(x)}{dx^{n+1}} = \frac{2\,(-1)^n}{\sqrt{\pi}}H_n(x)e^{-x^2}$$

In addition, the error function is related to the confluent hypergeometric function by use of the following equation.

$$\mathrm{er} f(x) = rac{2x}{\sqrt{\pi}} {}_1F_1\left(rac{1}{2},rac{3}{2};-x^2
ight).$$

9.8 Other Special Functions used in Physics

As explained in the introduction of this chapter, the list of special functions is extensive. The Handbook of Mathematical Functions (Abramowitz and Stegun, 1964) contains a fairly comprehensive list of special functions and their basic properties. The focus in this chapter has been on special functions that are widely used in mathematical physics to solve classes of problems whose formulations involve special cases of the Helmholtz differential equation. In general, special functions may be classified as Type 1: those special functions that satisfy a differential equation or Type 2: special functions that do not satisfy a differential equation; for example, the gamma function is a Type 2 special function. In the sections below, we summarize some other special functions that are used in mathematical physics but are not covered in the above sections.

9.8.1 Some Other Special Functions of Type 1

Some other special functions that satisfy a differential equation are (a) Airy¹⁶ functions are solutions of the Airy differential equation which has the form y'' - xy = 0; the Airy differential equation characterizes constant force-type problems in quantum mechanical and

¹⁶George Biddel Airy (1801–1892), English mathematician and astronomer who is known for his many contributions to mathematics and astronomy.

in elementary particle physics; (b) Mathieu¹⁷ functions are solutions of the **Mathieu dif**ferential equation which has the form $y'' + (a - 2b\cos 2x) y = 0$; the Mathieu differential equation results when a cosine-type potential is substituted into the one-dimensional timeindependent Schrödinger wave equation; and (c) parabolic cylinder functions are connected with confluent hypergeometric functions and with Hermite polynomials; they are solutions of differential equations of the general form given by $y'' + (ax^2 + bx + c) y = 0$.

Many bound state and collision problems in classical and quantum mechanics as well as in other areas of physics involve integrals of the form

$$\int R(x,y)dx.$$
(9.73)

When R(x, y) is a rational function and $y^2 = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$ where $a_4 \neq 0$ or $a_4 = 0$ and $a_3 \neq 0$, the integral in Eq.(9.73) is called an **elliptic integral**. Complete elliptic integrals of the first and second kind are respectively defined as

$$K(m) = \int_0^{\pi/2} \left(1 - m\sin^2\theta\right)^{-1/2} d\theta \quad \text{and}$$
(9.74)

$$E(m) = \int_0^{\pi/2} \left(1 - m\sin^2\theta\right)^{1/2} d\theta.$$
 (9.75)

Analyzing the motion of a simple pendulum involves an elliptic integral of the first kind. Elliptic integrals can be evaluated directly by use of series expansions or computers. Their importance in mathematical physics, however, is related to their appearance when solving physical problem involving certain nonlinear differential equations. Elliptic integrals are special cases of the hypergeometric functions since

$$K(m) = rac{\pi}{2} F\left(rac{1}{2},rac{1}{2},1;m
ight) \quad ext{and} \quad E(m) = rac{\pi}{2} F\left(-rac{1}{2},rac{1}{2},1;m
ight).$$

The Handbook of Mathematical Functions (Abramowitz and Stegun, 1964) is a good reference for additional information on elliptic integrals.

9.8.2 Some Other Special Functions of Type 2

Some special functions used in mathematical physics that do not satisfy a differential equation are (a) Einstein and Debye functions which are used in representing the specific heats of solids due to lattice vibrations; (b) error function; (c) gamma function; and (d) beta function. The latter two functions are widely used in many areas of mathematical physics and are now summarized.

The factorial, n!, is defined as

$$n! \equiv n(n-1)\dots 2 \cdot 1 = \int_0^\infty e^{-t} t^n dt; \quad n \text{ integer.}$$
(9.76)

¹⁷Claude Louis Mathieu (1783–1875), French scientist and mathematician known for his work in mathematics and astronomy.

Note that 0! = 1, and $n! = \pm \infty$ if *n* equals a negative integer. The gamma function, Γ , is a generalization of the factorial to cases of noninteger values for *n*. The Euler definition of the gamma function is

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt \quad \text{for } \operatorname{Re}(z) > 0.$$
(9.77)

In Eq.(9.77), Re(z) denotes the real part of z = x + iy. Note that $\Gamma(1/2) = \sqrt{\pi}$. Evaluating the integral in Eq.(9.77) by parts yields the recurrence relation for the gamma function, $\Gamma(z+1) = z\Gamma(z)$. If z is a positive integer n, then $\Gamma(z+1)$ equals n!.

The gamma function is used to express, in compact form, solutions of many problems of mathematical physics. The gamma function, however, does not satisfy a differential equation that is related to a physical problem; in fact, the gamma function does not satisfy any differential equation with rational coefficients. A sketch of $\Gamma(x)$ for some positive and negative values is given in Fig. 9.18.

The **beta function**, B(p,q), is defined by use of an integral, and it involves a simple and useful combination of gamma functions; it has the form

$$B(p,q) = \int_0^1 t^{p-1} (1-t)^{q-1} dt$$
 for $p > 0$ and $q > 0$.

It can be shown that B(p,q) = B(q,p). The beta function is frequently used in high energy particle physics as well as other areas of mathematical physics.

9.9 Problems

9.1 If u(x) is a complex eigenfunction, show that the real and imaginary parts satisfy the Sturm-Liouville equation. Discuss degeneracy for this case.

9.2 The differential equation p(x)u'' + q(x)u' + r(x)u = 0 is self-adjoint if q = p'. (a) Show that a self-adjoint differential equation can be expressed in the Sturm-Liouville form. (b) Show that if this differential equation is not self-adjoint (i.e., $q \neq p'$), it can be put into the self-adjoint form by multiplying through by $\exp \left[\int (q - p') dx/p\right]$. 9.3 Show that

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

Hint: Differentiate both sides of the equation for the generating function for Hermite polynomials with respect to t and equate coefficients of like powers of t. 9.4 Show that

$$H_n'(x) = 2nH_{n-1}(x).$$

Hint: Differentiate both sides of the equation for the generating function for Hermite polynomials with respect to x and equate coefficients of like powers of t. 9.5 (a) Show that

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \begin{cases} 2^n n! \sqrt{\pi} & \text{for } n = m \\ 0 & \text{for } n \neq m. \end{cases}$$

9.9. PROBLEMS

(b) Evaluate

$$\int_{-\infty}^{\infty} \left\{ H_0(x) \right\}^2 x e^{-x^2} dx.$$

9.6 By use of the generating function, evaluate

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) x H_m(x) dx.$$

9.7 Show that the series for $H_n(x)$ in Eq.(9.19) satisfies the Hermite differential equation. 9.8 For $x = \cos \theta$, show that

$$\int_{-1}^{1} P_n(x) P_m(x) dx = \begin{cases} 0 & \text{for } n \neq m \\ 2/(2n+1) & \text{for } n = m. \end{cases}$$

9.9 Show that

(a)
$$P_{\ell}(-x) = (-1)^{\ell} P_{\ell}(x)$$
 and (b) $L''_{n}(0) = n (n-1)/2$.

9.10 Show that

$$J_{n-1}(x) + J_{n+1}(x) = \frac{2n}{x} J_n(x).$$

Hint: Differentiate both sides of the equation for the generating function for Bessel functions and equate coefficients of like powers of t.

9.11 Show that

$$J_{n-1}(x) - J_{n+1}(x) = 2J'_n(x).$$

Hint: Differentiate both sides of the generating function for $J_n(x)$ with respect to x and equate coefficients of corresponding powers of t.

9.12 Show that $J_n(-x) = J_n(x)$ for n even and $J_n(-x) = -J_n(x)$ for n odd.

9.13 Show that $N_n(x)$ and $J_n(x)$ are linearly independent for n = integer.

9.14 Show that $N_n(x)$ is a solution of the Bessel differential equation for n = integer. 9.15 Show that $J_1(x) = -J'_0(x)$.

9.16 Show that the Hankel functions, $H_n^{(1)}(x)$ and $H_n^{(2)}(x)$, satisfy the Bessel differential equation.

9.17 Develop the Wronskian for $J_n(x)$ and $J_{-n}(x)$.

9.18 Show that the series in Eq.(9.54) for $J_n(x)$ satisfies the Bessel differential equation.

9.19 For the error function, show that (a)
$$\operatorname{er} f(x) = -\operatorname{er} f(-x)$$
 and (b) $\operatorname{er} f(\infty) = 1$

- 9.20 Show that (a) $\Gamma(1) = 1$ and (b) $\Gamma(n) = (n-1)!$.
- 9.21 Show that $2 \cdot 4 \cdot 6 \cdots 2n = 2^n \Gamma(n+1)$.

9.22 Show that $1 \cdot 3 \cdot 5 \cdots (2n-1) = 2^{1-n} \Gamma(2n) / \Gamma(n)$.

9.23 By use of the definition of the beta function

$$B(p,q) \equiv \int_0^1 t^{p-1} (1-t)^{q-1} dt \quad p \text{ and } q > 0,$$

show that B(p,q) = B(q,p). Hint: Let t = 1 - u.

9.24 Let t = x/(1+x) in the definition for the beta function and show that

$$B(p,q) = \int_0^\infty \frac{x^{p-1}dx}{(1+x)^{p+q}}$$

9.25 Show that $B(p, 1-p) = \pi/\sin \pi p$. Hint: See Example on page 139. 9.26 Let t = s + y(x - s) and show that

$$\int_s^x \frac{dt}{\left(x-t\right)^{1-\alpha} \left(t-x\right)^{\alpha}} = \int_0^1 \frac{dy}{y^{\alpha} \left(1-y\right)^{1-\alpha}}.$$

Note that

$$\int_0^1 \frac{dy}{y^{\alpha} (1-y)^{1-\alpha}} = B(1-\alpha, \alpha) = \frac{\pi}{\sin \alpha \pi}.$$

9.27 Show that $B(p,q) = \Gamma(p) \Gamma(q) / \Gamma(p+q)$.

9.9.1 Worksheet: The Quantum Mechanical Linear Harmonic Oscillator

The time-independent Schrödinger wave equation for the linear harmonic oscillator with potential $V(x) = kx^2/2$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi.$$
 (W1)

On making the change of variable $\xi = \alpha x$ (for constant α), note that

$$\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \alpha \frac{d}{d\xi} \quad \text{and} \quad \frac{d^2}{dx^2} = \frac{d}{dx}\left(\frac{d}{dx}\right) = \alpha^2 \frac{d^2}{d\xi^2}$$

Equation (W1) reduces to

$$\frac{d^2\psi}{d\xi^2} + \frac{2mE}{\hbar^2}\psi - \frac{2mk}{\hbar^2\alpha^4}\xi^2\psi = 0.$$
 (W2)

Now let

$$\alpha^4 = \frac{mk}{\hbar^2}$$
 and $\lambda = \frac{2E}{\hbar} \left(\frac{m}{k}\right)^{1/2} = \frac{2E}{\hbar\omega}$

Equation (W2) in dimensionless form becomes

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0. \tag{W3}$$

The plan is to solve Eq.(W3), directly or indirectly, by use of the power series method. Hence, the dimensionless form is very desirable since there is no need to keep track of dimensions of the various coefficients involved in the series method.

(A) Explore using the power series method directly on Eq.(W3). That is to say, assume that the solution of Eq.(W3) has the form

$$\psi = \sum_{r=0}^{\infty} a_r \xi^{k+r} \qquad a_0 \neq 0. \tag{W4}$$

(B) Write down the indicial equation. (C) Try to write down the recursion formula.

(D) Explain the difficulty encountered.

(E) By replacing λ with 1 + 2n for n = constant, show that Eq.(W3) reduces to the well-known Weber differential equation,

$$\frac{d^2\psi}{d\xi^2} + (1+2n-\xi^2)\,\psi = 0. \tag{W5}$$

(F) In Eq.(W5), show that the transformation

$$\psi(\xi) = e^{-\xi^2/2} y(\xi) \tag{W6}$$

leads to the well-known Hermite differential equation

$$\frac{d^2y}{d\xi^2} - 2\xi \frac{dy}{d\xi} + 2ny = 0. \tag{W7}$$

The Hermite differential equation is normally written as y'' - 2xy' + 2ny = 0. The solution of Hermite's differential equation by use of the power series method is well-known. Our plan for solving Eq.(W3) is to solve the Hermite differential equation and use the transformation in Eq.(W6).

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Assume the following form for the solution of Eq.(W7)

$$y = \sum_{r=0}^{\infty} a_r \xi^{k+r} \qquad a_0 \neq 0.$$

(A) By use of the power series method, show that

$$\begin{array}{ll} a_0k\,(k-1)=0 & \mbox{indicial equation} \\ a_1k\,(k+1)=0 & \\ a_{r+2}\,(k+r+2)\,(k+r+1)-2\,(k+r-n)\,a_r=0 & \mbox{recursion formula.} \end{array}$$

(B) For k = 0, show that the recursion formula may be written as

$$a_{r+2} = \frac{2(n-r)a_r}{(r+2)(r+1)}.$$

(C) Show that the case k = 1 leads to a redundant set of terms; hence, only the case k = 0 is needed. (D) Show that the general even and odd terms in the series solution may be written respectively as

$$a_{2j} = \frac{(-2)^j n (n-2) \cdots (n-2j+2) a_0}{(2j)!} \quad j = 0, 1, 2, \dots \text{ and}$$
$$a_{2j+1} = \frac{(-2)^j (n-1) (n-3) \cdots (n-2j+1) a_1}{(2j+1)!} \quad j = 0, 1, 2, \dots$$

(E) Show that the general solution of the Hermite differential equation, Eq.(W7), has the form

$$y(\xi) = \sum_{j \text{ even}}^{\infty} a_j \xi^j + \sum_{j \text{ odd}}^{\infty} a_j \xi^j$$

= $a_0 \sum_{j=0}^{\infty} \frac{(-2)^j n (n-2) \cdots (n-2j+2) \xi^{2j}}{(2j)!}$
+ $a_1 \xi \left[1 + \sum_{j=1}^{\infty} \frac{(-2)^j (n-1) (n-3) \cdots (n-2j+1) \xi^{2j}}{(2j+1)!} \right]$

Note that both terms in the general solution of the Hermite differential equation are infinite series. We have a physical requirement that $y(\xi)$ tends to a finite number as ξ tends to infinity. To satisfy this physical requirement, we must terminate each series; note that

- 1. the first infinite series becomes an even polynomial of degree n when n-2j+2=0and
- 2. the second infinite series becomes an odd polynomial of degree n when n-2j+1=0.

The even and odd polynomials may be combined to obtain a single polynomial in descending powers of n; the first term of this polynomial is $a_n \xi^n$ and subsequent terms are given by the recursion formula in the following form

$$a_r=-rac{\left(r+2
ight)\left(r+1
ight)a_{r+2}}{2\left(n-r
ight)}.$$

For r = n - 2, we obtain

$$a_{n-2} = \frac{n(n-1)a_n}{2\cdot 2}$$
 and $a_{n-4} = \frac{n(n-1)(n-2)(n-3)a_n}{2^2\cdot 2\cdot 4}$.

The general term is

$$a_{n-2j} = \frac{(-1)^j n (n-1) (n-2) \cdots (n-2j+1) a_n}{2^2 \cdot 2 \cdot 4 \cdots 2j}.$$
 (W8)

(A) Show that

$$n(n-1)\cdots(n-2j+1) = n(n-1)\cdots(n-2j+1)\cdot\frac{(n-2)(n-2j-1)\cdots 3\cdot 2\cdot 1}{(n-2j)(n-2j-1)\cdots 3\cdot 2\cdot 1} = \frac{n!}{(n-2j)!}$$

(B) Show that $2 \cdot 4 \cdots 2 = (2 \cdot 1) (2 \cdot 2) (2 \cdot 3) \cdots = 2^j j!$. (C) Show that the general term in Eq.(W8) reduces to

$$a_{n-2j} = \frac{(-1)^j \, n! a_n}{j! 2^{2j} \, (n-2j)!}$$

The polynomial solution (finite) solution is Hermite's differential equation becomes

$$y(\xi) = a_n \sum_{j=0}^{N} \frac{(-1)^j n! \xi^{n-2j}}{2^{2j} j! (n-2j)!}; \quad N = \begin{cases} n/2 & \text{for } n \text{ even} \\ (n-1)/2 & \text{for } n \text{ odd} \end{cases}$$

With the standardization $a_n = 2^n, y(\xi)$ becomes the Hermite polynomials

$$y(\xi) = H_n(\xi) = \sum_{j=0}^{N} \frac{(-1)^j n! (2\xi)^{n-2j}}{j! (n-2j)!}$$

The solution of the quantum mechanical equation for the linear harmonic oscillator, Eq.(W3), is $\psi(\xi) = N_n e^{-\xi^2/2} H_n(\xi)$ where the N_n are normalization constants. The eigenenergy is obtained as follows.

$$\lambda = 1 + 2n = \frac{2E_n}{\hbar\omega} \Longrightarrow E_n = \hbar\omega \left(n + 1/2\right); \quad n = 0, 1, 2, \dots$$

9.9.2 Worksheet: The Legendre Differential Equation

Assume the solution of the Legendre differential equation

$$\left(1 - w^2\right)\frac{d\Theta}{dw^2} - 2w\frac{d\Theta}{dw} + \lambda\Theta = 0 \tag{W9}$$

has the form

$$\Theta(w) = \sum_{n=0}^{\infty} a_n w^{k+n} ; \quad a_0 \neq 0.$$
 (W10)

On substituting Eq.(W10) into Eq.(W9), show that (A) $k(k-1)a_0 = 0$ (indicial equation); (B) $k(k+1)a_1 = 0$ (Note that a_0 and a_1 are arbitrary for k = 0.); and (C)

$$a_{n+2} = \frac{\left[\left(k+n\right)\left(k+n-1\right)+2\left(k+n\right)-\lambda\right]a_n}{\left(k+n+2\right)\left(k+n+1\right)} \qquad (\text{recursion formula}).$$

(D) Show that the general solution of Eq.(W9) reduces to

$$\Theta(w) = a_0 \left[1 - \frac{\lambda}{2!} w^2 - \frac{\lambda (6-\lambda)}{4!} w^4 - \frac{\lambda (6-\lambda) (20-\lambda)}{6!} w^6 + \cdots \right] + a_1 \left[w + \frac{(2-\lambda)}{3!} w^3 + \frac{(2-\lambda) (12-\lambda)}{5!} W^5 + \cdots \right].$$

(E) By use of the Gauss test (see page 116) for convergence (use the recursion formula for k = 0 as the coefficients), show that the series for $\Theta(w)$ diverges for $w = \pm 1$. Since $w = \cos \theta$, it is important to construct a solution that converges for $-1 \le w \le 1$; such a solution is obtained when λ is replaced with $\ell(\ell+1)$ and the coefficients are rewritten in terms of $\ell(\ell+1)$. (F) For this replacement, show that the recursion formula becomes

$$a_{n+2} = \frac{\left[n\left(n+1\right) - \ell\left(\ell+1\right)\right]a_n}{(n+2)\left(n+1\right)} = -\frac{\left(\ell-n\right)\left(\ell+n+1\right)a_n}{(n+2)\left(n+1\right)}$$

(G) For n even, write out a few terms of the above recursion formula and show that the coefficients of the general term are given by

$$a_{2j} = \frac{(-1)^j \ell (\ell - 2) (\ell - 4) \cdots (\ell - 2j + 2) (\ell + 1) (\ell + 3) \cdots (\ell + 2j - 1) a_0}{(2j)!}.$$

(H) For n odd, write out a few terms of the recursion formula and show that the coefficients of the general term are given by

$$a_{2j+1} = \frac{(-1)^{j} (\ell - 1) (\ell - 3) \cdots (\ell - 2j + 1) (\ell + 2) (\ell + 4) \cdots (\ell + 2j) a_{1}}{(2j + 1)!}.$$

When $\ell = 2j$, the even part of the solution becomes a finite series (an even polynomial of degree ℓ) since $a_{2j} \neq 0$ but $a_{2j+1} = 0$ where $\ell - (2j+2) + 2 = 0$. Similarly, the odd part of the solution becomes an odd polynomial of degree ℓ for $\ell = 2j + 1$ since $a_{2j+1} \neq 0$ but $a_{2j+3} = 0$. A single finite series (polynomial), in descending powers of w, that is valid for both even and odd ℓ will now be obtained. The first term of this polynomial is $a_{\ell}w^{\ell}$, and subsequent terms are given by the recursion formula

$$a_{j+2} = \frac{[j(j+1) - \ell(\ell+1)]a_j}{(j+2)(j+1)} = -\frac{(\ell-j)(\ell+j+1)a_j}{(j+2)(j+1)}$$

(I) Solve the above equation for a_j and write out terms for $j = \ell - 2$ and $j = \ell - 4$ and show that the general term is

$$a_{\ell-2r} = \frac{(-1)^r \ell (\ell-1) (\ell-2) \cdots (\ell-2r+1) a_{\ell}}{2 \cdot 4 \cdots 2r (2\ell-1) \cdots (2\ell-2r+1)}.$$
 (W11)

Equation (W11) can be written in a compact form if we note that following three relations

$$\ell (\ell - 1) \cdots (\ell - 2r + 1) = \ell (\ell - 1) \cdots (\ell - 2r + 1) \cdot \frac{(\ell - 2r) (\ell - 2r - 1) \cdots 3 \cdot 2 \cdot 1}{(\ell - 2r) (\ell - 2r - 1) \cdots 3 \cdot 2 \cdot 1} = \frac{\ell!}{(\ell - 2r)!};$$
(W12)

$$2 \cdot 4 \cdot 6 \cdots 2r = (2 \cdot 1) (2 \cdot 2) (2 \cdot 3) \cdots (2 \cdot r) = 2^{r} r!;$$
 and (W13)

$$\begin{aligned} &(2\ell-1)\left(2\ell-3\right)\cdots\left(2\ell-2r+1\right)\\ &=\frac{2\ell\left(2\ell-1\right)\left(2\ell-2\right)\left(2\ell-3\right)\cdots\left(2\ell-2r+1\right)}{2\ell\left(2\ell-2\right)\left(2\ell-4\right)\cdots\left(2\ell-2r+2\right)}\cdot\frac{(2\ell-2r)!}{(2\ell-2r)!}\\ &=\frac{(2\ell)!}{2^{r}\ell\left(\ell-1\right)\cdots\left(\ell-r+1\right)\left(2\ell-2r\right)!}=\frac{(2\ell)!\left(\ell-r\right)!}{2^{r}\left(2\ell-2r\right)!\ell!}.\end{aligned}$$

$$(W14)$$

By use of Eq.(W14, W13, and W12), the general term, Eq.(W11) becomes

$$a_{\ell-2r} = (-1)^r \left[\frac{(\ell!)^2 (2\ell - 2r)!}{r! (2\ell)! (\ell - 2r) (\ell - r)!} \right] a_{\ell}.$$

The solution of the Legendre differential equation now has a finite series part and an infinite series part and may be written in the form

$$\Theta_{\ell}(w) = a_{\ell} \sum_{r=0}^{N} \frac{(-1)^{r} (\ell!)^{2} (2\ell - 2r)! w^{\ell - 2r}}{r! (2\ell)! (\ell - r)!} + Q_{\ell}(w)$$

where $N = \begin{cases} \ell/2 & \text{for } \ell \text{ even} \\ (\ell - 2)/2 & \text{for } \ell \text{ odd.} \end{cases}$

For standardization,

$$a_{\ell} = \frac{(2\ell)!}{2^{\ell} \left(\ell!\right)^2},$$

the finite series part of the solution reduces to the Legendre polynomials of the first kind

$$P_{\ell}(w) = \sum_{r=0}^{N} \frac{(-1)^{r} (2\ell - 2r)! w^{\ell - 2r}}{2^{r} r! (\ell - 2r)! (\ell - r)!}.$$

9.9.3 Worksheet: The Laguerre Differential Equation

The power series solution of the Laguerre differential equation

$$xy'' + (1 - x)y' + \alpha y = 0; \quad \alpha = \text{constant}$$
 (W15)

will be developed. Assume the following series form for the solution of Eq.(W15)

$$y(x) = \sum_{j=0}^{\infty} a_j x^{k+j}; \quad a_0 \neq 0.$$

(A) Show that the indicial equation and the recursion formula are respectively given by

$$\left[k\left(k-1\right)+k\right]a_{0}=0$$

and

$$a_{j+1} = \frac{(k+j-\alpha) a_j}{(k+j+1) (k+j) + k + j + 1}.$$

The indicial equation has a double root, k = 0; this results from the fact that the Laguerre differential equation has a nonessential singularity at the origin. Hence the power series method yields only one solution that is finite for all values of x. This solution, however, is extremely important in physics.

(B) For k = 0, write out a few terms using the recursion formula and show that one solution of the Laguerre differential equation has the form

$$y(x) = a_0 \left[1 - \frac{\alpha}{1^2} x + \frac{\alpha (\alpha - 1)}{(2!)^2} x^2 + \dots + \frac{(-1)^j \alpha (\alpha - 1) \cdots (\alpha - j + 1) x^j}{(j!)^2} + \dots \right]$$

mit $j = 1, 2, 3, \ldots$

The above solution becomes finite (a polynomial of degree n) when $\alpha - j + 1 = 0$ or α equals a positive integer. With standardization $a_0 = 1$ and $\alpha = n$, this finite solution becomes the Laguerre polynomials of order n; they are given by

$$L_n(x) = a_0 \sum_{j=0}^n \frac{(-1)^j \alpha (\alpha - 1) \cdots (\alpha - j + 1) x^j}{(j!)^2}$$
$$= \sum_{j=0}^n \frac{(-1)^j n! x^j}{(n-j)! (j!)^2}.$$

(C) Differentiate the Laguerre differential equation k times with respect to x and show that the associated Laguerre differential equation is obtained

$$xrac{d^2L_n^k(x)}{dx^2} + (k+1-x)\,rac{dL_n^k(x)}{dx}_{-}(n-k)\,L_n^k(x) = 0$$

where $L_n^k(x) = rac{d^kL_n(x)}{dx^k}.$

9.9.4 Worksheet: The Bessel Differential Equation

Assume that the solution of the Bessel differential equation

$$x^{2}y'' + xy' + (x^{2} - n^{2})y = 0$$

has the form

$$y(x) = \sum_{j=0}^{\infty} a_j x^{k+j}; \quad a_0 \neq 0$$

Show that (A) $(k^2 - n^2) a_0 = 0$ (indicial equation); (B) $[(k+1)^2 - n^2] a_1 = 0$; and (C)

$$a_j = -rac{a_{j-2}}{\left(k+j\right)^2 - n^2}; \quad j \ge 2 \quad (ext{recursion formula}).$$

(D) Consider the case k = n, $a_0 \neq 0$, and $a_1 = 0$; write out a few terms of the recursion formula and show that the general term is

$$a_{2j} = \frac{(-1)^j a_0}{2^{2j} j! (n+1) (n+2) \cdots (n+j)}$$

Note that

$$(n+1)(n+2)\cdots(n+j) = (n+j)(n+j-1)\cdots(n+2)(n+1)\cdot\frac{\Gamma(n+1)}{\Gamma(n+1)}$$
$$= \frac{\Gamma(n+j+1)}{\Gamma(n+1)}.$$

With standardization

$$a_0 = \frac{1}{2^n \Gamma\left(n+1\right)},$$

the solution of the Bessel differential equation for k = n and n = integer becomes the Bessel functions of the first kind of order n

$$J_n(x) = \sum_{j=0}^{\infty} \frac{(-1)^j x^{2j+n}}{2^{2j+n} j! \Gamma(n+j+1)}$$
$$= \sum_{j=0}^{\infty} \frac{(-1)^j (x/2)^{2j+n}}{j! \Gamma(n+j+1)}.$$

9.9.5 Worksheet: The Hypergeometric Differential Equation

Consider the hypergeometric differential equation

$$x(1-x)y'' + [c - (a+b+1)x]y' - aby = 0.$$
 (W16)

Assume that the solution has the form

$$y(x) = \sum_{\lambda=0}^{\infty} a_{\lambda} x^{k+\lambda}; \quad a_0 \neq 0.$$

- (A) Show that the indicial equation is $[k(k-1)+ck]a_0 = 0$.
- (B) Obtain the recursion formula.
- (C) For k = 0, show that the solution of Eq.(W16) is

$$y_{1} = a_{0} \left[1 + \frac{ab}{c} x + \left(\frac{ab}{c} \right) \frac{(1+a)(a+b)}{2(1+c)} x^{2} + \cdots + \frac{a(a+1)\cdots(a+r-1)\cdot b(b+1)\cdots(b+r-1)}{r!c(c+1)\cdots(c+r-1)} x^{r} + \cdots \right].$$
(W17)

The above series is called the hypergeometric series since it reduces to the ordinary geometric series for a = 1 and b = c; this solution is denoted by $y_1 = a_0 F(a, b, c; x)$. Note that the right-hand side of Eq.(W17) becomes a polynomial when a + r - 1 = 0 or a = 1 - r = -n (n > 0). For k = 1 - c, the solution of Eq.(W16) becomes

$$y_2 = a_0 x^{1-c} F(a-c, b-c+1, 2-c, x).$$



Figure 9.7: Legendre Functions of the second kind, $Q_n(x)$ (Abramowitz and Stegun, 1964)



Figure 9.8: Associated Legendre functions, $P_n^1(x)$ (Abramowitz and Stegun, 1964)



Figure 9.9: Laguerre polynomials, $L_n(x)$, (Abramowitz and Stegun, 1964)



Figure 9.10: Bessel functions of the first and second kinds, $J_n(x)$ and $Y_n(x)$ (Abramowitz and Stegun, 1964)

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Figure 9.11: Modified Bessel functions, $K_n(x)$ and $I_n(x)$ (Abramowitz and Stegun, 1964)



Figure 9.12: Spherical Bessel functions of the first kind, $j_n(x)$ (Abramowitz and Stegun, 1964)


Figure 9.13: Spherical bessel functions of the second kind, $y_n(x)$ (Abramowitz and Stegun, 1964)



Figure 9.14: Modified spherical Bessel functions of the first and second kinds (Abramowitz and Stegun, 1964)



Figure 9.15: Jacobi polynomials, $P_n^{(1.5,-0.5)}(x)$ (Abramowitz and Stegun, 1964)



Figure 9.16: Chebyshev polynomials, $T_n(x)$ (Abramowitz and Stegun, 1964)



Figure 9.17: Gegenbauer polynomials, $C_n^{(0.5)}(x)$ (Abramowitz and Stegun, 1964)



Figure 9.18: Gamma function, $\Gamma(x)$ and $1/\Gamma(x)$ (Abramowitz and Stegun, 1964)

Chapter 10

Integral Equations

10.1 Introduction

An integral equation is an equation in which an unknown function is under the sign of integration. In connection with his study of integral transforms in 1782, Laplace introduced integral equations into mathematical physics. Abel, in connection with a mechanical problem, and Liouville, in connection with differential equations, made important early contributions to the development of integral equations. The general form of an integral equation is as follows.

$$h(x)u(x) = f(x) + \lambda \int_{a}^{b(x)} K(x,s) G[u(s),s] ds.$$
(10.1)

In Eq.(10.1), (a) K(x, s) is called the kernel (nucleus or kern), (b) u(x) is the function to be determined, (c) h(x) and f(x) are known (given) functions, and (d) λ is a real or complex parameter (also called the eigenvalue when it is real). The classification of integral equations is given in Table 10.1.

Linear	$G\left[u(s), \overline{s}\right] = u\left(s\right)$
Fredholm	b(x) = b
volterra	b(x) = x
First kind	h(x) = 0
Second kind	h(x) = 1
Third kind	$h(x) \neq 0, 1$
Homogeneous	f(x) = 0
Singular	$a = -\infty$ and $b = \infty$

Table 10.1 Classification of Integral Equations

The classification of kernels of integral equations is given in Table 10.2.

Symmetric	$K\left(x,s\right) = K\left(s,x\right)$
Hermitian	$K(x,s) = K^*(s,x)$
Separable of degenerate	$K(x,s) = \sum_{i=1}^{n} g_i(x) \phi_i(s) n < \infty$
Difference	$K\left(x,s\right) = K\left(x-s\right)$
Cauchy	$K\left(x,s\right) = 1/\left(x-s\right)$
Singular	$K(x,s) \to \infty$ as $s \to x$
Hilbert-Schmidt	$\int_{a}^{b}\int_{a}^{b} K\left(x,s\right) ^{2}dxds<\infty$

Table 10.2 Classification of Kernals

This chapter is devoted to a brief introduction of solutions and applications of one-dimensional linear integral equations of the first and second kinds. The formulations of many problems in physics lead to either differential or integral equations. Certain problems (e.g., certain problems in transport theory) can only be represented by integral equations of the following general form

$$u(x) = f(x) + \lambda \int_{a}^{b} K(x,s) u(s) \, ds.$$
(10.2)

Equation (10.2) is an integral equation since the unknown function u(x) appears in the integrand. Functions f(x) and K(x,s) are to be given, and λ is a known parameter used here for convenience. The function f(x) is called the free term, and K(x,s) is the kernel. Quantities f(x), K(x,s), and λ may be either real or complex but are considered real in this chapter. Equation (10.2) is a linear integral equation since u is linear. An integral equation is singular if either (or both) of the limits of integration is infinite and/or if the kernel becomes infinite in the range of integration. When f(x) = 0, Eq. (10.2) is classified as a homogeneous integral equation. If the kernel is continuous in the closed region [a, b], then Eq. (10.2) is classified as a Fredholm¹ type integral equation of the second kind. Fourier transforms and dispersion relations are examples of singular integral equation (where the upper limit is a variable),

$$u(x) = f(x) + \lambda \int_{a}^{x} K(x, s) u(s) ds,$$
(10.3)

is known as a Volterra² type integral equation of the second kind. Fredholm integral equations of the first kind have the form

$$f(x) = \int_{a}^{b} K(x,s) u(s) ds.$$
 (10.4)

Volterra's type integral equations of the first kind have the form

$$f(x) = \int_{a}^{x} K(x,s) u(s) \, ds.$$
 (10.5)

¹Erik Ivar Fredholm (1866–1927) was born in Stockholm, Sweden. He is known for his contributions to mathematical physics and integral equations.

 $^{^{2}}$ Vito Volterra (1860–1940), Italian mathematician and physicist who is known for his work on partial differential equations and integral equations.

In summary, classifications are (a) Fredholm type if the limits of integration are fixed and Volterra type if one limit is variable and (b) first kind if the unknown function appears only in the integrand and second kind if the unknown function appears both in the integrand and outside the integrand.

Certain physical problems may be formulated as (a) differential equations with appropriate boundary and/or initial conditions, (b) integral equations, or (c) either differential or integral equations. An essential difference between the two formulations is that boundary conditions are imposed on general solutions of differential equations while boundary conditions are incorporated within the formulation of integral equations. While there exist procedures for converting differential equations to integral equations, use of integral equations seems more appropriate when (a) formulations of problems lead directly to integral equations or (b) solutions of the corresponding integral equations are easier to obtain than those for the corresponding differential equations.

It is important to note that certain problems in classical mechanics, transport and diffusion phenomena, scattering theory, and other areas of physics can be formulated only by use of integral equations; the number of such problems is very small when compared to those leading to differential equations. In general, the theory of solution techniques needed in solving integral equations is not as familiar to physicists as techniques for solving differential equations. Integral equations are seldom treated in details in introductory mathematical physics textbooks but are, however, discussed in advanced books in theoretical physics and mathematical physics. See the references for some excellent books on integral equations (e.g., Lovitt 1950, Mikhlin 1964, and Moiseiwitsch 1977). Many integral equations encountered in physics are normally solved by use of (a) intuitive analytical methods, (b) intuitive approximation methods and numerical techniques, or (c) integral transform methods.

Some systematic methods for solving nonsingular linear integral equations are (a) separable kernels, (b) transform theory, (c) Neumann series, (d) numerical, (e) Schmidt-Hilbert theory, and (f) Wiener-Hopf theory. The Wiener-Hopf method is a different type of transform method which may be applied to certain integral equations with displacement kernels, K(x,s) = K(x-s). Schmidt-Hilbert theory is an approach that applies to integral equations with Hermitian kernels, $K(x,s) = K^*(s,x)$. The Neumann series method involves developing the unknown function, u(x), as a power series in the parameter λ . Numerical solutions of Volterra equations involve (a) reducing the original equations to linear algebraic equations, (b) successive approximations, and (c) numerical evaluation of integrals. Numerical techniques for Fredholm equations involve solving a system of simultaneous equations.

10.2 Integral Equations with Separable Kernels

A subset of Fredholm equations of the first and second kinds with separable (degenerate) kernels can be solved by reducing them to a system of algebraic equations. In general, separable kernels may be written as

$$K(x,s) = \sum_{j=1}^{n} g_j(x)\phi_j(s) \qquad n < \infty.$$
(10.6)

In Eq. (10.6), it is assumed that $g_j(x)$ and $\phi_j(s)$ are linearly independent functions respectively. Substituting Eq.(10.6) into Eq.(10.2) yields

$$u(x) = f(x) + \lambda \sum_{j=1}^{n} g_j(x) C_j.$$
(10.7)

The C_j coefficients are given by

$$C_{j} = \int_{a}^{b} \phi_{j}(s) u(s) ds.$$
 (10.8)

The solution of Eq.(10.2) has now been reduced to finding the C_j from the indicated integrals in Eq.(10.8) and substituting the C_j into Eq.(10.7).

Example 102 By use of the separable kernel method, find the solution of

$$u(x) = x + \lambda \int_0^1 x s u(s) \, ds$$

Solution : The above integral equation becomes

$$u(x) = x + \lambda \int_0^1 x s u(s) ds = x + \lambda x \int_0^1 s u(s) ds$$

= x + \lambda x C. (10.9)

The C coefficient reduces to

$$C = \int_{0}^{1} su(s) ds = \int_{0}^{1} s(s + \lambda sC) ds \quad \text{(from Eq.(10.9))}$$
$$= \frac{1 + \lambda C}{3} \Longrightarrow C = \frac{1}{3 - \lambda}.$$
(10.10)

On substituting C from Eq.(10.10) into Eq.(10.9), we obtain the following solution of the original integral equation

$$u(x) = x + \lambda x C = x + \frac{\lambda x}{3 - \lambda} = \frac{3x}{3 - \lambda}.$$

Here, it is seen that solutions exist for values of λ different from 3.

Example 103 By use of the separable kernel method, find the solution of

$$u(x) = x + \frac{1}{2} \int_{-1}^{1} (s+x) \, ds.$$

Solution : Here the original integral becomes

$$u(x) = x + \frac{1}{2} \int_{-1}^{1} (s+x) ds$$

= $x + \frac{1}{2} \int_{-1}^{1} (s) ds + \frac{1}{2} \int_{-1}^{1} x ds$
= $x + \frac{1}{2} C_1 + \frac{1}{2} x C_2.$ (10.11)

The C_1 coefficient reduces to

$$C_{1} = \int_{-1}^{1} su(s) ds$$

= $\int_{-1}^{1} s\left(s + \frac{1}{2}C_{1} + \frac{1}{2}sC_{2}\right) ds$ (from Eq.(10.11))
= $\frac{2+C_{2}}{3}$.

The C_2 coefficient becomes

$$C_{2} = \int_{-1}^{1} u(s) ds$$

= $\int_{-1}^{1} \left(s + \frac{1}{2}C_{1} + \frac{1}{2}sC_{2} \right) ds$ (from Eq.(10.11))
= $C_{1} \Longrightarrow C_{1} = C_{2} = 1.$

On substituting the values for C_1 and C_2 into Eq.(10.11), the solution of the original equation becomes u(x) = (3x + 1)/2.

10.3 Integral Equations with Displacement Kernels

If the kernel of an integral equation is of the form K(x-s), it is referred to as a displacement kernel. Fredholm equations of the first and second kinds with displacement kernels and limits from minus infinity to plus infinity or from zero to plus infinity can normally be solved by use of Fourier and Laplace transform methods respectively (see Chapter 6). Here the Fourier transform approach for solving integral equations with displacement kernels will be illustrated. Taking the Fourier transform of each term in Eq.(10.2) yields

$$\int_{-\infty}^{\infty} u(x)e^{ikx}dx = \int_{-\infty}^{\infty} f(x)e^{ikx}dx + \lambda \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} K(x-s)u(s)ds\right)e^{ikx}dx.$$

In transform space (k-space), the above equation is

$$u(k) = F(k) + \lambda K(k)u(k).$$

The solution in x-space is obtained when the inverse transform of is taken, and the result becomes

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{F(k)e^{-ikx}dk}{1 - \lambda K(k)}.$$
 (10.12)

10.4 The Neumann Series Method

Consider the set of Fredholm equations of the second kind such that

$$\int_{a}^{b} |f(x)|^{2} dx$$
 and $\int_{a}^{b} |K(x,s)|^{2} ds$

are bounded. Assume the solution may be written as a power series, Neumann series (also known as Liouville-Neumann series), with form

$$u(x)\sum_{n=0}^{\infty}\lambda^{n}u_{n}(x).$$
(10.13)

Terms in the successive approximation are obtained by substituting the Neumann series into the Fredholm equation, Eq.(10.2), and equating coefficients of like powers of λ ; the results are

$$u_{0}(x) = f(x),$$

$$u_{1}(x) = \int_{a}^{b} K(x, s) u_{0}(s) ds, \dots,$$

$$u_{n}(x) = \int_{a}^{b} K(x, s) u_{n-1}(s) ds.$$
(10.14)

It can be shown that the Neumann series (a) converges for all values of λ for Volterra equations and (b) converges for small values of λ for Fredholm equations; techniques exist for improving the convergence in the Fredholm case. Numerical techniques may be used to evaluate terms in the Neumann series.

10.5 The Abel Problem

This brief introduction on integral equations is concluded with one of the earliest application (1833) of integral equations to a physical problem, the **Abel problem**. The Abel problem is as follows: Consider a bead sliding on a smooth wire under the influence of gravity and find the curve for which the time of descent is a given function the initial position.



Figure 10.1

Let the starting position of the bead be (x_0, y_0) and position of the bead at time t be (x, y) such that y equals zero at the end of the fall (see Fig. 10.1). The speed of the bead at (x, y), for an element of arc length along the path ds, is determined from the

conservation of energy principle and is given by

$$\frac{ds}{dt} = \sqrt{2g(y_0 - y)}.$$
(10.15)

If the shape of the curve is u(y), then ds = u(y) dy and the time of descent is given by

$$T = \int_0^{y_0} \frac{u(y) \, dy}{\sqrt{2g(y_0 - y)}}.$$
(10.16)

The Abel problem is to find the curve, u(y), for which the time, T, of descent is a given function, $f(y_0)$, of the initial vertical position, and the result is obtain from the solution of the following integral equation

$$f(y_0) = \int_0^{y_0} \frac{u(y) \, dy}{\sqrt{2g(y_0 - y)}}.$$
(10.17)

It can be shown that the curve in question is a portion of a cycloid (the curve traced out by a point on the circumference of a circle that is rolling along the x-axis). Equation (10.17) is called the **Abel equation**; in general form, the Abel equation is written as

$$f(x) = \int_{a}^{x} \frac{u(s) \, ds}{(x-s)^{\alpha}} \qquad 0 < \alpha < 1.$$
(10.18)

In Eq.(10.18), f(x) is a known function and u(s) is an unknown function.

The solution of the general Abel equation is obtained as follows. For clarity of notations, we first replace x with t in Eq.(10.18). Now multiply both sides of Eq.(10.18) by $(x - t)^{\alpha-1}$ and integrate both sides of the resulting equation with respect to t from a to x; the result is

$$\int_{a}^{x} \frac{f(t) dt}{(x-t)^{1-\alpha}} = \int_{a}^{x} \frac{dt}{(x-t)^{1-\alpha}} \int_{a}^{t} \frac{u(s) ds}{(t-s)^{\alpha}}.$$
 (10.19)

By use of the **Dirichlet formula** (for changing the order of integration)

$$\int_{a}^{b} d\xi \left\{ \int_{\xi}^{b} \varphi\left(\xi,\eta\right) d\eta \right\} = \int_{a}^{b} d\eta \left\{ \int_{a}^{\eta} \varphi\left(\xi,\eta\right) d\xi \right\},\tag{10.20}$$

the right-hand side of Eq.(10.19) may be written as

$$\int_{a}^{x} \frac{dt}{(x-t)^{1-\alpha}} \int_{a}^{t} \frac{u(s) \, ds}{(t-s)^{\alpha}} = \int_{a}^{x} u(s) \, ds \int_{s}^{x} \frac{dt}{(x-t)^{1-\alpha} \, (t-s)^{\alpha}}.$$
(10.21)

On making the substitution t = s + y(x - s) into the second integral on the right-hand side of Eq.(10.21), Eq.(10.21) reduces to (see Problem 9.26)

$$\int_{s}^{x} \frac{dt}{(x-t)^{1-\alpha} (t-s)^{\alpha}} = \int_{0}^{1} \frac{dy}{y^{\alpha} (1-y)^{1-\alpha}} = \frac{\pi}{\sin \alpha \pi}.$$
 (10.22)

Substituting Eq.(10.22) into Eq.(10.21) and substituting this result into Eq.(10.19), we obtain

$$\int_{a}^{x} \frac{f(t)dt}{\left(x-t\right)^{1-\alpha}} = \frac{\pi}{\sin\alpha\pi} \int_{a}^{x} u\left(s\right) ds.$$
(10.23)

Applying Leibniz's formula for the differentiation of an integral with variable limits (see Problem 7.20), Eq.(10.23) reduces to

$$\frac{\pi}{\sin \alpha \pi} u(x) = \frac{d}{dx} \int_{a}^{x} \frac{f(t)dt}{(x-t)^{1-\alpha}}.$$

Hence, the solution of the general Abel equation is

$$u(x) = \frac{\sin \alpha \pi}{\pi} \frac{d}{dx} \int_{a}^{x} \frac{f(t)dt}{\left(x-t\right)^{1-\alpha}}.$$
(10.24)

10.6 Problems

10.1 Find the solution of the following integral equation by converting it to a second-order differential equation and solving the resulting differential equation.

$$u(x) = e^{x} - 4x + \int_{0}^{x} (3 - 2x + 2s) \, ds.$$

Hint: Use Leibniz's formula for differentiating an integral with variable limits. 10.2 Consider the following integral equation

$$u(x) = x + \int_{0}^{x} xsu(s) ds = x + xg(x)$$

where $g(x) = \int_{0}^{x} su(s) ds$.

Find the solution of this integral equation by first finding the solution of the first-order differential equation for g(x).

10.3 By use of the separable kernel method, solve the following integral equations.

(a)
$$u(x) = x + \lambda \int_{0}^{1} e^{x} e^{s} u(s) ds$$

(b) $u(x) = x + \lambda \int_{0}^{1} (xs^{2} + x^{2}s) u(s) ds$
(c) $u(x) = \lambda \int_{0}^{1} e^{x} e^{s} u(s) ds$.

10.4 Solve the following integral equations.

(a)
$$u(x) = x + \int_{0}^{x} (t - x) u(t) dt$$

(b) $u(x) = 1 + \int_{0}^{x} (t - z) u(t) dt$
(c) $u(x) = e^{x} - \frac{e}{2} + \frac{1}{2} + \frac{1}{2} \int_{0}^{1} u(t) dt$
(d) $u(x) = \frac{3}{2}e^{x} - \frac{1}{2}xe^{x} - \frac{1}{2} + \frac{1}{2} \int_{0}^{1} tu(t) t$
(e) $u(x) = 1 + \int_{0}^{x} u(t) dt$

Chapter 11

Applied Functional Analysis

11.1 Introduction

Concepts of functions (of one variable) and operators were introduced into mathematics in connection with the development of calculus during the latter part of the seventeenth century. In general, an operator applied to a given function yields a new function. The problem of finding an extremum (maximum or minimum) of a function is carried out in the usual manner by use of ordinary calculus, but the general problem of finding the stationary value (an extremum) of certain definite integrals that occur in mathematical physics is the subject matter of the branch of mathematics called the **calculus of variations**.

In relation to the calculus of variations, the process of connecting (mapping) each function y(x) in [a, b] with a number represented by the definite integral

$$\int_{a}^{b} F(y, y', x) \, dx \quad \text{where} \quad y' = \frac{dy}{dx}$$

which depends on y(x) was given the name **functional** during the end of the nineteenth century. The basic idea of functional analysis is that problems are often easier to solve if a function is considered to be a member of a whole space of functions, X. The space X is assumed (a) to carry a metric, (b) to have a linear space structure, and (c) to be infinitely dimensional. The concept of a metric involves topological and geometrical language while linear operators on X involve concepts of linear algebra, and relations among these concepts constitute linear functional analysis.

A function which depends on one or more functions rather than on discrete variables is referred to as a **functional**. The domain of a functional is a space of admissible functions. More precisely, functionals are continuous linear maps from a normed space into itself or into some other normed space. The basic ingredient of the various definitions of a functional and of functional analysis is the existence of a linear space with a topology. The main topics in the previous chapters are technically topics in functional analysis even though the topology and geometry of the linear spaces involved were not stressed. Mathematically, a valid argument can be made that the placement of this chapter on functional analysis is analogous to putting the cart before the horse. This argument, however, neglects the applications of techniques approach which has been emphasized throughout the book. In mathematical physics, functional analysis often involves discussions connected with (a) the calculus of variations, (b) theory of ordinary and partial differential equations, (c) integral equations and transform theory, (d) spectral theory involving eigenvalues, eigenfunctions, and Fourier series expansion theory, (e) functional calculus used in the path integral formulation of quantum mechanics, quantum field theory, and statistical mechanics, and (f) the theory of distributions. In mathematics, functional analysis often involves (a) the general theory of linear normed spaces, (b) the topological structure of linear spaces and continuous transformations, (c) measure spaces and general theories of integration, (d) spectral theories, (e) distribution theory, and (f) number theory. In this chapter, the original problem of functional analysis (the calculus of variations) and applications of functional integration to quantum mechanics, quantum field theory, and statistical mechanics will be discussed.

11.2 Stationary Values of Certain Functions and Functionals

11.2.1 Maxima and Minima of Functions

For a continuous function, f(x), to have a maximum or a minimum (an extremum, stationary value) at x_0 , it is necessary that its first derivative vanish at x_0 . The necessary conditions for a continuous function f(x, y) to have an extremum at some point (x_0, y_0) are that

$$\frac{\partial f(x,y)}{\partial x}\bigg|_{(x,y)=(x_0,y_0)} = 0 \quad \text{and} \quad \frac{\partial f(x,y)}{\partial y}\bigg|_{(x,y)=(x_0,y_0)} = 0.$$
(11.1)

This procedure can be extended to functions of several variables $f(x^1, x^2, ..., x^n)$ as follows:

$$d f \left(x^{1}, x^{2}, \dots, x^{n}\right) = \frac{\partial f}{\partial x^{1}} dx^{1} + \frac{\partial f}{\partial x^{2}} dx^{2} + \dots + \frac{\partial f}{\partial x^{n}} dx^{n} = 0.$$
(11.2)

For an extremum at some point x_0^i , we require that

$$\frac{\partial f}{\partial x^1}\Big|_{x^i=x_0^i} = \left.\frac{\partial f}{\partial x^2}\right|_{x^i=x_0^i} = \cdots \left.\frac{\partial f}{\partial x^n}\right|_{x^i=x_0^i} = 0 \qquad (i=1,2,\ldots,n).$$
(11.3)

Equation (11.3) is valid since the $\{x^i\}$ and hence the $\{dx^i\}$ are assumed to be linearly independent.

11.2.2 Method of Lagrange's Multipliers

In certain situations, the variables $\{x^i\}$ may be subject to constraints given by an equation of the form

$$\varphi\left(x^1, x^2, \dots, x^n\right) = 0. \tag{11.4}$$

Because of the existence of an equation of constraints, the dx^i in Eq.(11.2) are not linearly independent (only n-1 are linearly independent), and the coefficients of the dx^i in Eq.(11.2) are not all equal zero. The method of Lagrange's (undetermined) multipliers may be used to find an extremum of $f(x^1, x^2, \ldots, x^n)$ subject to the equation of constraint in Eq.(11.4). The procedure is outlined in the following two steps. 1. Multiply the constraint condition, $d\varphi$, by a parameter λ that is independent of the coordinates. (This parameter is called a Lagrange multiplier.)

$$\lambda d\varphi = \lambda \sum_{i=1}^{n} \frac{\partial \varphi}{\partial x^{i}} dx^{i} = 0.$$
(11.5)

2. Add the result of Step 1 to the extremum condition

$$df + \lambda d\varphi = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x^{i}} + \lambda \frac{\partial \varphi}{\partial x^{i}} \right) dx^{i} = 0.$$
(11.6)

In Eq.(11.6), n-1 of the dx^i are linearly independent and the corresponding quantities in parenthesis are equal zero. The parameter λ can be selected so the remaining term in the parenthesis equals zero. The equations

$$\frac{\partial f}{\partial x^i} + \lambda \frac{\partial \varphi}{\partial x^i} = 0$$

and the equation of constraints, Eq.(11.4), are use to find the independent quantities $\{x^i\}$ and λ . The Lagrange multiplier method, however, fails if one of the partial derivatives of φ evaluated at the extremum point equals zero. If more than one equation of constraint exist (e.g., in statistical mechanics), then *Steps* 1 and 2 should be executed for each equation of constraint.

Example 104 A particle moves along the path $\varphi(x, y) = y + x^2 - 1 = 0$. By use of the method of Lagrange multipliers, calculate the minimum distance of the particle from the origin.

Solution : Here, we want to find the extremum of the distance (or square of the distance) function $f(x, y) = x^2 + y^2$ subject to the equation of constraint. For this simple problem, we could eliminate y from the two equations and find the extremum by use of elementary calculus. We use the method of Lagrange multipliers to illustrate the procedure. We find x, y, and λ from the following equations.

$$rac{\partial f}{\partial x} + \lambda rac{\partial arphi}{\partial x} = 0, \quad rac{\partial f}{\partial y} + \lambda rac{\partial arphi}{\partial y} = 0, \quad ext{and} \quad arphi\left(x,y
ight) = y + x^2 - 1 = 0.$$

The above equations reduce to

$$2x + \lambda 2x = 0 \begin{cases} x = 0 \text{ or} \\ \lambda = -1 \end{cases}$$
$$2y + \lambda = 0 \begin{cases} y = 1/2 \text{ when} \\ \lambda = -1 \end{cases}$$
$$y + x^{2} = 1 \begin{cases} y = 1 \text{ when } x = 0 \\ x^{2} = 1/2 \text{ when } y = 1/2. \end{cases}$$

The extremum points are (0,1) for a maximum, and $(\sqrt{1/2}, 1/2)$ for a minimum.

11.2.3 Maxima and Minima of a Certain Definite Integral

Consider the following definite integral of the functional F(y, y', x) where F is a known function of y, y' (where y' = dy/dx) and x, but y(x) is unknown

$$J = \int_{x_1}^{x_2} F(y, y', x) \, dx. \tag{11.7}$$



Figure 11.1

A fundamental problem in the calculus of variations (a problem which occurs frequently in mathematical physics) is that of finding a function such that the functional J is stationary (an extremum; this will be a minimum in most cases of physical interest). The basic procedure here is to evaluate the integral for a slightly modified path

$$y(x, \alpha) = y(x, 0) + \alpha \eta(x)$$
 where $\eta(x_1) = \eta(x_2) = 0$

and show that the change in the value of the integral due to the change in the path becomes zero. The condition $\eta(x_1) = \eta(x_2) = 0$ means that we consider only paths that pass through the end points. The function $\eta(x)$ is an arbitrary smooth (continuous with continuous derivatives) function, and α is a small parameter (see Fig. 11.1). The function $y(x, \alpha)$ describes neighboring paths where

$$\delta y = y(x, \alpha) - y(x, 0) = \alpha \eta(x)$$

is the variation (hence the name calculus of variations) of y(x,0) at some x. The delta symbol, δ , was introduced by Lagrange to denote a variation (a virtual change, in the sense of being a mathematical experiment), and it means a change is made in an arbitrary manner. Both dy and δy denote infinitesimal changes in y(x), but dy means an infinitesimal change in y(x) produced by dx while δy is an infinitesimal change which produces $y + \delta y$. Operationally, we have

$$\delta F(y, y', x) = \frac{\partial F}{\partial y} \delta y + \frac{\partial F}{\partial y'} \delta y'.$$

It is straight forward to show that

$$\frac{d\left(\delta y\right)}{dx} = \delta \frac{dy}{dx} \quad \text{and} \quad \delta \int_{x_1}^{x_2} F\left(y, y', x\right) dx = \int_{x_1}^{x_2} \delta F\left(y, y', x\right) dx.$$

In the integrand of Eq.(11.7), we replace y(x) and y'(x) with an arbitrary neighboring path $y(x, \alpha)$ and $y'(x, \alpha)$ and obtain

$$J(\alpha) = \int_{x_1}^{x_2} F[y(x,\alpha), y'(x,\alpha), x] \, dx.$$
 (11.8)

The condition for an extremum of $J(\alpha)$ is that

$$\left. \frac{\partial J}{\partial \alpha} \right|_{\alpha=0} = 0 \quad \text{for } \eta(x) \quad \text{arbitrary.}$$

The above condition may be written as

$$\left. lpha rac{\partial J}{\partial lpha}
ight|_{lpha = 0} = \delta J = 0 \quad ext{for} \;\; \delta y \;\; ext{arbitrary}.$$

On differentiating both sides of Eq.(11.8) with respect to α , we obtain

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left\{ \frac{\partial F}{\partial y} \frac{\partial y}{\partial \alpha} + \frac{\partial F}{\partial y'} \frac{\partial y'}{\partial \alpha} \right\} dx$$
$$= \int_{x_1}^{x_2} \left\{ \frac{\partial F}{\partial y} \eta(x) + \frac{\partial F}{\partial y'} \eta'(x) \right\} dx. \tag{11.9}$$

The last step in Eq.(11.9) results from the fact the α -dependence of F is in y and y' and that

$$rac{\partial y\left(x,lpha
ight)}{\partial lpha}=\eta\left(x
ight) \quad ext{and} \quad rac{\partial y'\left(x,lpha
ight)}{\partial lpha}=\eta'\left(x
ight).$$

Integrating the second term in Eq.(11.9) by parts, we obtain

$$\int_{x_1}^{x_2} \frac{\partial F}{\partial y'} \frac{\partial \eta'}{\partial x} dx = \eta \left(x \right) \left. \frac{\partial F}{\partial y'} \right|_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta \left(x \right) \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) dx$$
$$= -\int_{x_1}^{x_2} \eta \left(x \right) \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) dx. \tag{11.10}$$

The last step in Eq.(11.10) results from $\eta(x_1) = \eta(x_2) = 0$ since we consider only paths that pass through the end points. On substituting Eq.(11.10) into Eq.(11.9), we obtain

$$\frac{\partial J}{\partial \alpha}\Big|_{\alpha=0} = \int_{x_1}^{x_2} \left\{ \frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \right\} \eta(x) \, dx = 0.$$

Since the expression in brackets is a continuous function of x and $\eta(x)$ is an arbitrary smooth function, the fundamental theorem of the calculus of variations states that

$$\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = 0. \tag{11.11}$$

Equation (11.11) is known as Euler's equation and its solution yields the y(x) that makes J an extremum (minimum).

An alternate approach of finding the differential equation whose solution is the equation of the extremum path between x_1 and x_2 is the direct use of the variation process as follows.

$$\delta J = \delta \int_{x_1}^{x_2} F(y, y', x) \, dx = \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} \delta y + \frac{\partial F}{\partial y'} \delta y' \right] dx = 0.$$

On noting that $\delta y' = \delta dy/dx = d(\delta y/dx)$ and integrating the second term in the above equation by parts, we obtain

$$\delta J = \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \right] \delta y dx = 0$$

Since δy is arbitrary, the above equation leads to Euler's equation, Eq.(11.11). For several dependent variables $F(y_i, y'_i, x)$ where i = 1, 2, ..., n, we obtain

$$\delta J = \delta \int_{x_1}^{x_2} F(y_i, y'_i, x) \, dx = \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y_i} \delta y_i + \frac{\partial F}{\partial y'_i} \delta y'_i \right] \, dx = 0.$$

Integrating the second term in the above equation by parts leads to

$$\delta J = \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y_i} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'_i} \right) \right] \delta y_i dx = 0.$$

From the above equation, we obtain

$$\frac{\partial F}{\partial y_i} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'_i} \right) = 0 \qquad i = 1, 2, \dots, n.$$
(11.12)

Example 105 By use of the calculus of variations method (Euler's equation), determine the equation of the shortest distance between two points (x_1, y_1) and (x_2, y_2) in Cartesian coordinates.

Solution : The element of distance along the path between the two points is given by

$$ds = \sqrt{dx^2 + dy^2}.$$

The equation for the distance between the two points is therefore

$$s = \int_{x_1}^{x_2} \sqrt{1 + (y')^2} dx$$
 where $y' = \frac{dy}{dx}$.

For $F(y, y', x) = \sqrt{1 + (y')^2}$, the differential equation whose solution yields the equation for the shortest distance between the two points, Euler's equation, reduces to

$$rac{dy}{dx} = A \quad ext{since} \quad rac{\partial F}{\partial y} = 0 \quad ext{and} \quad rac{\partial F}{\partial y'} = rac{y'}{\sqrt{1 + \left(y'
ight)^2}}$$

The equation of the shortest path between the two points is therefore that of a straight line, y(x) = Ax + B.

Example 106 The Brachistochrone Problem The brachistochrone (shortest time) problem, first formulated and solved by Johann Bernoulli in 1696, is one of the first variational problems. The problem is as follows: (a) Consider a bead of mass which slides, under the influence of gravity, down a frictionless wire bent into the appropriate shape. (b) The goal is to find the equation (shape of the wire) of the path along which the bead travels so that the time is a minimum.



Figure 11.2:

Solution : For convenience, it is assumed that the bead starts from rest at the origin of a coordinate system (see Fig. 11.2). Since this is a conservative system, the following relations are valid

(a)
$$T_1 + V_1 = T_2 + V_2$$
; (b) $V_2 = -mgy$; (c) $T_1 = V_1 = 0$;
(d) $T_2 = \frac{1}{2}mv^2$; and (e) $v = \sqrt{2gy}$.

The expression for the time required for the bead to travel from the origin to point (x, y) is therefore given by

$$t = \int \frac{\sqrt{dx^2 + dy^2}}{\sqrt{2gy}}$$
$$= \int_0^{y_2} \frac{\sqrt{1 + (x')^2} dy}{\sqrt{2gy}} \quad \text{where} \quad x' = \frac{dx}{dy}.$$

The unknown function y(x) must be determined such that the time is a minimum. On applying Euler's equation with

$$F = \left(\frac{1 + (x')^2}{y}\right)^{1/2}$$

and independent variable y, one obtains

$$x = \int rac{Aydy}{\sqrt{y - A^2y^2}} \quad ext{since} \quad rac{\partial F}{\partial x} = 0 \quad ext{and} \quad rac{\partial F}{\partial x'} = rac{x'}{\sqrt{y\left(1 + x'
ight)^2}} = A$$

On letting $A = 1/\sqrt{2a}$ and making the change of variable $y = a(1 - \cos\theta)$, the above integral reduces to $x = a(\theta - \sin\theta) + \text{constant}$. The path that yields a minimum time of travel is in the form of parametric equations $x = a(\theta - \sin\theta)$ and $y = a(1 - \cos\theta)$, equations for a cycloid that passes through the origin.

11.3 Hamilton's Variational Principle in Mechanics

11.3.1 Introduction

Mechanics is the study of the motions (including rest) of physical objects. The laws of classical mechanics are valid for macroscopic objects (object size of order larger than 10^{-10} m), and the laws of quantum mechanics are valid in the microworld (object size of order smaller than 10^{-10} m). In this section, the focus is on the study of classical mechanics. Widely used equivalent formulations of classical mechanics are: (a) Newtonian mechanics (1687), (b) Lagrangian mechanics (1788), (c) Hamiltonian mechanics (1834), and (d) Hamilton-Jacobi theory (1837).

Formulations of classical mechanics developed since Newtonian mechanics are generalizations and equivalent forms of Newtonian mechanics. These generalizations do not lead to new information but offer different ways of approaching problems. Certain problems can be solved by use of all four approaches with equal amounts of ease (or difficulty). Other problems are more amenable to solution by use of one approach than by use of the others. The specific nature of the problem to be solved usually dictates the approach that should be used. Newton's second law is the basic equation of motion in the Newtonian picture of mechanics. In Lagrangian mechanics, Lagrange's equations are the required set of equations of motion for the system (particle or group of particles) under investigation. Hamilton's canonical equations are basic to Hamiltonian mechanics, and the Hamilton-Jacobi equation is the foundation of the Hamilton-Jacobi theory. The approach in this Section begins with Hamilton's variational principle for conservative systems (where the forces acting on the system may be derived from a potential function) from which Lagrange's equations will be developed by use of the variational calculus method. By use of a Legendre transformation, the Hamiltonian and subsequently Hamilton's canonical equations are obtained. The Hamilton-Jacobi theory will not be treated.

The variational technique used in mechanics was developed mainly by Euler and Lagrange and is a mathematical formulation of mechanics in which kinetic energy and potential energy play an essential role. In Newtonian mechanics, forces and other vector quantities play the central role.

11.3.2 Generalized Coordinates

Linearly independent quantities $\{q_k\} = q_1, q_2, \ldots, q_n$ that completely define the position (configuration) of a system as a function of time are called **generalized coordinates**.

Quantities $\{q_k\}$ are said to be linearly independent if the sum

$$\sum_{k=1}^{n} a_k q_k = 0$$

implies that $a_k = 0$ for all k. Generalized coordinates may be selected to match the conditions of the problem to be solved. The number of generalized coordinates that must be used to uniquely define the position of a system represents the number of **degrees** of freedom for the system. The corresponding quantities $\{\dot{q}_k\}$ are called generalized velocities.

The simultaneous specification of $\{q_k\}$ and $\{\dot{q}_k\}$ for a system determines the **mechanical** state of the system at that time, and subsequent motion is obtained from the solutions, $q_k(t)$, of the appropriate equations of motion. The appropriate second-order differential equations expressing the relations among generalized coordinates, q_k , generalized velocities, \dot{q}_k , and generalized accelerations, \ddot{q}_k , are called equations of motion for the system under investigation.

Although the set of generalized coordinates used to solve a problem is not unique, a proper set of generalized coordinates is that set which leads to an equation of motion whose solution has a straight forward physical interpretation. No general rule exists for obtaining a proper set of generalized coordinates.

11.3.3 Lagrange's Equations

Hamilton's variational principle asserts that the actual motion of a particle or system of particles (conservative system) from its initial configuration at time t_1 to its configuration at time t_2 is such that

$$\delta S = \delta \int_{t_1}^{t_2} L(q_k, \dot{q}_k) \, dt = 0. \tag{11.13}$$

In Eq.(11.13), L = T - V is defined as the Lagrangian for the system under investigation, Ldt is called the **action**, and

$$S = \int_{t_1}^{t_2} L dt$$

denotes the action integral. The quantities T and V are kinetic and potential energy respectively.

Among the infinite number of trajectories $q_k(t)$ that connect the end points $q_k(t_1)$ and $q_k(t_2)$, the physical (actual) path yields a stationary value for the action integral. The action is therefore a functional of the functions $q_k(t)$ satisfying the boundary conditions that all trajectories pass through the end points. By use of the variational technique leading to Eq.(11.12), one finds that $q_k(t)$ is obtained from the following set of differential equations.

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) = 0 \qquad k = 1, 2, \dots, n.$$
(11.14)

The equations in Eq.(11.14) are called Lagrange's (or Euler-Lagrange) equations for a particle or system of particles. Lagrange's equations, the equations of motion for the system under investigation, are a set of second-order ordinary differential equations. The general solutions of these equations contain 2n arbitrary constants of integration. The values of these 2n arbitrary constants are determined when the initial state (values for the q_k and \dot{q}_k at t = 0) of the system is specified.

Quantities $\partial L/\partial \dot{q}_k$ and $\partial L/\partial q_k$ are defined as canonical momenta (also called conjugate or generalized momenta) and generalized forces respectively

$$p_k = \frac{\partial L}{\partial \dot{q}_k}$$
 and $F_k = \frac{\partial L}{\partial q_k}$. (11.15)

By use of the definitions in Eq.(11.15), it is observed that Lagrange's equations may be considered a generalized version of Newton's second law where generalized forces equal the rate of change of canonical momenta.

Basic conservation laws of mechanics result from invariance of the Lagrangian under (a) time translation (homogeneous time) - conservation of energy, (b) coordinate translation (homogeneous space) - conservation of canonical momentum and conservation of total linear (mechanical) momentum, and (c) rotation in space (isotropic space) - conservation of angular momentum. In spite of the important role of the Lagrangian, it is not a unique function for a system since the equations of motion for the system, Lagrange's equations, are unchanged if the time derivative of an arbitrary function, $df(q_k, t)/dt$, is added to the Lagrangian.

11.3.4 Format for Solving Problems by Use of Lagrange's Equations

The following steps should be used when applying Lagrange's equations.

- 1. Draw a detailed diagram. Specify the degrees of freedom and the level where potential energy equals zero.
- 2. Write down the appropriate expressions for T, V and L.
- 3. Write down the specific set of Lagrange's equation(s).
- 4. Work out the terms in the set of equation(s) in Step 3.
- 5. Solve the resulting equation(s) of motion subject to the given initial conditions.

Example 107 By use Lagrangian mechanics, obtain the equation of motion for the linear harmonic oscillator.

Solution : The linear harmonic oscillator for this Example is illustrated in Fig. 11.3. We obtain the following quantities.

$$\begin{array}{l} q_1 = x \quad (\text{one degree of freedom}) \\ T = \frac{1}{2}m\dot{x}^2 \quad (\text{kinetic energy}) \\ V = \frac{1}{2}kx^2 \quad (\text{potential energy}) \\ L = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \quad (\text{Lagrangian}). \end{array}$$



Figure 11.3

Lagrange's equation reduces to

$$rac{\partial L}{\partial x} - rac{d}{dt} \left(rac{\partial L}{\partial \dot{x}}
ight) = 0 = \ddot{x} + \omega^2 x$$

where $rac{\partial L}{\partial x} = -kx$ and $rac{\partial L}{\partial \dot{x}} = m\dot{x}.$

The equation $\ddot{x} + \omega^2 x = 0$ is the familiar equation of motion for the classical linear harmonic oscillator; it is, of course, the same as the equation of motion obtained by use of Newtonian mechanics (see page 177; Hooke's law, $m\ddot{x} = -kx$).

11.4 Formulation of Hamiltonian Mechanics

It has been shown that Hamilton's variational principle combined with techniques of the calculus of variations transforms the process of finding the solution of a mechanical problem to that of obtaining solutions for Lagrange's equations. Hamilton developed a procedure for transforming Lagrange's equations to a canonical form by replacing them (a set of n second-order differential equations) with a set of 2n first-order differential equations now called Hamilton's canonical equations of motion.

11.4.1 Derivation of Hamilton's Canonical Equations

The Lagrangian is a function of q_k and \dot{q}_k ; now the change of variable $\dot{q}_k \rightarrow p_k$ where $p_k = \partial L/\partial \dot{q}_k$ will be made. By use of a Legendre transformation (see page 75), one obtains

$$-H = L - \sum_{k=1}^{n} p_k \dot{q}_k.$$
(11.16)

The negative sign on the left-hand side of Eq.(11.16) is by convention. The new function $H(q_k, p_k)$ contains the same geometrical and physical content as $L(q_k, \dot{q}_k)$ and is called

the Hamiltonian of the system. The total differential of the Hamiltonian is given by

$$\begin{split} dH &= \frac{\partial H}{\partial q_k} dq_k + \frac{\partial H}{\partial p_k} dp_k \\ &= \frac{\partial}{\partial q_k} \left(\sum_{k=1}^n p_k \dot{q}_k - L \right) dq_k + \frac{\partial}{\partial p_k} \left(\sum_{k=1}^n p_k \dot{q}_k - L \right) dp_k \\ &= -\frac{\partial L}{\partial q_k} dq_k + \dot{q}_k dp_k = -\dot{p}_k dq_k + \dot{q}_k dp_k. \end{split}$$

On comparing terms in the first and last steps in the above equations, we obtain

$$\dot{q}_k = \frac{\partial H}{\partial p_k}$$
 and $\dot{p}_k = -\frac{\partial H}{\partial q_k}$ $k = 1, 2, \dots, n.$ (11.17)

The equations in Eq.(11.17) are referred to as **Hamilton's canonical equations** of motion (or simply **Hamilton's equations**). Hamilton's equations can be used to develop the specific set of equations of motion for the particle or system of particles under investigation in terms of the phase space variables q_k and p_k . For a conservative system, it can be shown that the Hamiltonian equals the total energy of the system, H = T + V.

11.4.2 Format for Solving Problems by Use of Hamilton's Equations

In solving problems by use of Hamiltonian mechanics, the following five-step procedure is highly recommended.

- 1. Write out the Lagrangian, L = T V (see the previous Section).
- 2. Solve the equation $p_k = \partial L / \partial \dot{q}_k$ for \dot{q}_k and eliminate \dot{q}_k from the Lagrangian.
- 3. Construct the Hamiltonian for the system, $H = \sum_{k=1}^{n} p_k \dot{q}_k L$.
- 4. Obtain Hamilton's equations, $\dot{q}_k = \partial H / \partial p_k$ and $p_k = -\partial H / \partial \dot{q}_k$.
- 5. Solve the 2n first-order differential equations (equations of motion) developed in Step 4.

Example 108 By use of Hamiltonian mechanics, obtain the equation of motion for the linear harmonic oscillator (see Fig. 11.3).

Solution: In the previous Example, it was shown that the Lagrangian for the linear harmonic oscillator is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$

We now eliminate \dot{x} from the Lagrangian as follows.

$$p = \frac{\partial L}{\partial \dot{x}} = m \dot{x} \Longrightarrow \dot{x} = \frac{p}{m}.$$

The Lagrangian now becomes

$$L = \frac{p^2}{2m} - \frac{1}{2}kx^2.$$

The Hamiltonian reduces to

$$H = \sum_{k=1}^{n} p_k \dot{q}_k - L = \frac{p^2}{2m} + \frac{1}{2}kx^2 \quad \text{(total energy)}.$$

Hamilton's equations reduce to

$$\dot{x}=rac{\partial H}{\partial p}=rac{p}{m} \quad ext{and} \quad \dot{p}=-rac{\partial H}{\partial x}=-kx.$$

Note that

$$\ddot{x}=rac{\dot{p}}{m}=-rac{kx}{m} \quad ext{or} \quad \ddot{x}+\omega^2 x=0 \quad (ext{the required equation of motion}).$$

11.4.3 Poisson's Brackets

The total time derivative of an arbitrary function $f(q_k, p_k)$ is

$$\frac{df}{dt} = \sum_{k=1}^{n} \left(\frac{\partial f}{\partial q_k} \dot{q}_k + \frac{\partial f}{\partial p_k} \dot{p}_k \right) \\
= \sum_{k=1}^{n} \left(\frac{\partial f}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial H}{\partial q_k} \right) = \{f, H\}$$
(11.18)

Hamilton's equations were used in obtaining Eq.(11.18). The quantity on the right-hand side of Eq.(11.18) is called **Poisson brackets**. In general, the Poisson brackets of two functions $f(q_k, p_k)$ and $g(q_k, p_k)$ is defined as

$$\{f,g\} = \sum_{k=1}^{n} \left(\frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k} \right).$$

Hamilton's canonical equations in terms of Poisson's brackets are given by

$$\dot{q}_k = \frac{\partial H}{\partial p_k} = \{q_k, H\}$$
 and $\dot{p}_k = -\frac{\partial H}{\partial q_k} = \{p_k, H\}.$ (11.19)

Two variables ξ_i and φ_i are said to be **canonically conjugate** if

$$\{\xi_i,\xi_j\} = \{\varphi_i,\varphi_j\} = 0 \quad \text{and} \quad \{\xi_i,\varphi_j\} = \delta_{ij}. \tag{11.20}$$

In the last equation in Eq.(11.20), δ_{ij} is the Kronecker delta function. The quantities q_i and p_j are canonically conjugate variables since $\{q_i, q_j\} = \{p_i, p_j\} = 0$ and $\{q_i, p_j\} = \delta_{ij}$; these three Poisson brackets are referred to as fundamental Poisson brackets.

11.5 Continuous Media and Fields

Thus far, only conservative systems composed of discrete particles have been considered. The Lagrangian of a system composed of N free particles may be written as

$$L = \sum_{i=1}^{N} L_i\left(q_k, \dot{q}_k\right).$$

The extension of the above analysis to a system with an infinite number of degrees of freedom (a continuous medium) is achieved by

- 1. replacing the subscript k with a continuous variable (say x, meaning x, y, z);
- 2. replacing q_k with a new function $q_k \rightarrow Q(\mathbf{x}, t)$;
- 3. replacing the sum with an integral $\sum_i \rightarrow \int d^3x$; and
- 4. replacing canonical momenta with canonical momentum density given by

 $\pi(\mathbf{x}) = \partial \mathcal{L}/\partial \dot{Q}$ where \mathcal{L} is the Lagrangian density. The quantity $Q(\mathbf{x}, t)$ is called a field. To denote several fields, the notation $Q_{\alpha}(\mathbf{x}, t)$ may be used. The parameter α distinguishes among the different fields. In this context, a field is a set of functions of spacetime, and these functions satisfy a set of partial differential equations. The corresponding Hamilton's variational principle is

$$0 = \delta \int_{t_1}^{t_2} \sum_{\substack{i=1\\i=1}}^{N} L_i(q_k, \dot{q}_k) dt$$
$$= \delta \int_{t_1}^{t_2} \int_{\substack{\text{physical}\\\text{space}}} \mathcal{L}\left[Q_\alpha(\mathbf{x}, t), \dot{Q}_\alpha(\mathbf{x}, t)\right] d^4x.$$
(11.21)

Assuming that fields interact only with infinitesimal neighbors, the Lagrangian density should be a function of $Q_{\alpha}(\mathbf{x},t)$, $\dot{Q}_{\alpha}(\mathbf{x},t)$, and $\partial Q_{\alpha}(\mathbf{x},t)/\partial x_k$; in four-vector notation, we may write these functions as $Q_{\alpha}(x^{\mu})$ and $\partial_{\mu}Q_{\alpha}$ where $\mu = 0, 1, 2, 3$. By use of appropriate boundary conditions, the variation in Eq.(11.21) leads to the following set of equations of motion

$$\frac{\partial \mathcal{L}}{\partial Q_{\alpha}} - \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} Q_{\alpha})} \right) = 0 \qquad \mu = 0, 1, 2, 3.$$
(11.22)

The equations in Eq.(11.22) are the Lagrange's equations for classical fields.

11.6 Transitions to Quantum Mechanics

11.6.1 Introduction

The laws of classical mechanics are not in general valid for the microworld, and new laws (quantum theory) that are appropriate for the microworld were developed during the period 1900–1927. In this Section, the transition from classical mechanics to quantum mechanics (a) in the Heisenberg picture, (b) in the Schrödinger picture, and (c) by use of the action functional (path integral) approach due to Dirac and Feynman will be made. For convenience of notations, the discussion is restricted to the case of one non-relativistic particle. The starting point in both the Heisenberg and Schrödinger pictures is Hamiltonian mechanics while the Feynman approach (Dirac-Feynman approach) begins with Lagrangian mechanics.

The postulates of quantum mechanics may be stated as follows.

- 1. Each state of a physical system corresponds to a normalized vector in Hilbert space called the state vector, Ψ or $|\Psi\rangle$.
- 2. Physical quantities are represented by linear Hermitian operators in Hilbert space.
- 3. If a system is in a state $|\Psi\rangle$, then the probability that a measurement (consistent with quantum theory) of the quantity corresponding to \hat{A} will yield one of the eigenvalues a_k (where $\hat{A} |\Psi\rangle = a_k |\Psi\rangle$) is given by $|\langle a_k |\Psi\rangle|^2$. The system will change from state $|\Psi\rangle$ to $|a_k\rangle$ as a result of the measurement. The quantity $\langle a_k |\Psi\rangle$ is the amplitude.

11.6.2 The Heisenberg Picture

In the Heisenberg¹ approach, a system is quantized by

- 1. letting q_k and p_k be Hermitian operators in a Hilbert space such that $q_k \to \hat{q}_k$ (in quantum theory, \hat{q}_k normally as q_k) and $p_k \to -i\hbar\partial/\partial q_k$ and
- 2. replacing Poisson brackets with commutators, $\{A, B\} \rightarrow [A, B]/i\hbar$ where [A, B] = AB BA; in the commutator, A and B are understood to be operators. If $[f, g] = i\hbar$, the operators f and g are said to be **canonically conjugate**. The resulting Heisenberg equations of motion for a quantum mechanical system are

$$i\hbar\dot{p}_k = [p_k, H]$$
 and $i\hbar\dot{q}_k = [q_k, H]$. (11.23)

The equations in Eq.(11.23) are basic for Heisenberg matrix mechanics.

11.6.3 The Schrödinger Picture

From a classical mechanical point of view, the Hamiltonian of a particle subject to conservative forces equals the total energy of the particle, and one may write

$$H = E = \frac{\mathbf{p}^2}{2m} + V(x, y, z).$$
(11.24)

The transition to quantum mechanics is the Schrödinger picture is achieved by use of the following replacements:

¹Werner Karl Heisenberg (1901–1976), German physicist who is known for his invention of matrix mechanics (the first version of quantum mechanics) and for the discovery of the uncertainty principle. He was awarded the 1932 Nobel Prize in physics for his work on matrix mechanics.

1. $E \to i\hbar\partial/\partial t$ and

2. $\mathbf{p} \to i\hbar \nabla$.

By use of these replacements, Eq.(11.24) is transformed into an operator equation. Operating on some function $\Psi(x, y, z, t)$ or $|\Psi\rangle$ in Hilbert space yields

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi \quad \text{or} \quad i\hbar\frac{\partial|\Psi\rangle}{\partial t} = H|\Psi\rangle.$$
 (11.25)

Schrödinger's wave equation, Eq.(11.25), is the basic equation of motion of a particle in quantum mechanics in the Schrödinger picture.

11.6.4 The Feynman Path Integral

The special case of one particle with one degree of freedom is consider here to simplify the notation and make the explanations clear. Feynman's² formulation of quantum mechanics was stimulated by some work of Dirac (1933) and is based on the following two postulates:

- 1. The amplitude $\langle q(t'') | q(t') \rangle$ for a particle to be found at q(t'') at time t'' if its initial position is q(t') at time t' equals a sum of complex contributions (amplitudes) for each space-time path starting at q(t') and ending at q(t'').
- 2. All paths connecting q(t') and q(t'') contribute equally in magnitude, but the phase (weight) of their contribution is $\exp(iS/\hbar)$ where S is the classical action integral for the corresponding paths.

The measure on the functional space of paths is q(t) denoted by $\mathcal{D}[q(t)]$, and appropriate normalization factors for the amplitude are contained in $\mathcal{D}[q(t)]$. Feynman's interpretation of the indicated functional integration is as follows:

- 1. Divide the time interval t'' t' into N equal parts, each with duration $\epsilon = t_{k+1} t_k$.
- 2. In the limit $N \to \infty$, it is assumed that the sequence of points $q(t_0), \ldots, q(t_n)$ approximates the path q(t).

The action functional associated with the classical path joining $q(t_k) = q_k$ and $q(t_{k+1}) = q_{k+1}$ is

$$S[q_{k+1}, q_k] = \int_{t_k}^{t_{k+1}} L(q, \dot{q}) dt.$$

²Richard Feynman (1918–1988), USA physicist who is known for his development of a new approach to quantum mechanics using the principle of least action. In his approach to quantum mechanics, the wave model was replaced with a model based on particle interactions mapped into space-time; in this latter context, he introduced diagrams (now called Feynman diagrams) that are graphic analogs of mathematical expressions needed to describe the behavior of systems of interacting particles. He shared the 1965 Nobel Prize in physics with Schwinger and Tomonoga.



Figure 11.4

Feynman's postulates thus assert that the amplitude $\langle q(t') | q(t') \rangle$ is a sum of all amplitudes for all paths connecting q(t'') and q(t'), and it may be written as (see Fig. 11.4)

$$\langle q(t'') | q(t') \rangle = \lim_{\substack{\epsilon \to 0 \\ N \to \infty}} \int \cdots \int \prod_{k=0}^{N} \exp\left[\frac{i}{\hbar} S(q_{k+1}, q_k)\right] \frac{dq_k}{A_k}$$

=
$$\int \cdots \int \exp\left[\frac{i}{\hbar} \int_{t'}^{t''} L(q, \dot{q}) dt\right] \mathcal{D}[q(t)].$$
(11.26)

The normalization factors A_k in Eq.(11.26) are independent of the path from q_k to q_{k+1} but depend on the mass of the particle and on the time interval ϵ . Equation (11.26) is a mathematical statement that the amplitude for a particle at q(t') at time t' to move to q(t'') at time t'' equals the sum of all possible paths between the two points times $\exp(iS/\hbar)$; the corresponding probability is the absolute square of the amplitude.

The path integral approach to quantum mechanics can be extended to include formulations of (a) quantum field theory (a combination of quantum mechanics and special relativity), (b) the partition function in statistical mechanics, and (c) systems obeying Bose-Einstein and Fermi-Dirac statistics. The path integral method is the foundation for Feynman diagrams.

11.7 Problems

11.1 In Example 103, use $f(x, y) = x^2 + y^2$ and $\varphi(x, y) = y + x^2 - 1 = 0$ to eliminate y and find points where f(x) has an extremum by use of elementary calculus. 11.2 A particle is constrained to move along the path $\varphi(x, y) = x^2 - y^2 - 1 = 0$. By use of the Lagrange multiplier method, find the shortest distance from the origin to this particle. 11.3 Show that Euler's equations

$$\frac{\partial F}{\partial u} - \frac{d}{dx} \left(\frac{\partial F}{\partial u'} \right) = 0 \qquad \text{(Form)}$$

1)

can be written in the following two forms:

(Form 2)
$$\frac{\partial F}{\partial x} - \frac{d}{dx} \left(F - y'_i \frac{\partial F}{\partial y'_i} \right) = 0$$
 where $F = F(y_i, y'_i, x)$
(Form 3) $F - y' \frac{\partial F}{\partial y} = \text{constant}$ where $F = F(y, y')$.

11.4 Consider

$$J(\alpha) = \int_{x_1}^{x_2} F[y(x,\alpha), y'(x,\alpha), x] dx.$$

Derive Euler's equation by expanding the integrand in a Taylor series in two variables about α and setting $\alpha = 0$.

11.5 Prove that the path of shortest distance between two points (r_1, θ_1) and (r_2, θ_2) is a straight line. (Work in polar coordinates.)

11.6 The kinetic energy of a particle of mass m in Cartesian coordinates is given by $T = m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)/2$. Show that this kinetic energy is (a) $T = m(\dot{r}^2 + r^2\dot{\theta}^2)/2$ in plane polar coordinates, (b) $T = m \left(\dot{\rho}^2 + \dot{\phi}^2 + \dot{z}^2\right)/2$ in right circular cylindrical coordinates, and (c) $T = m \left(\dot{r}^2 + r^2 \dot{\phi}^2 + r^2 \dot{\phi}^2 \sin \theta \right)$ in spherical polar coordinates. 11.7 Show that (Euler's theorem)

$$\sum_{i=1}^{n} q_i \frac{\partial T}{\partial \dot{q}_i} = 2T \qquad \text{(Euler's theorem)}.$$

11.8 For conservative systems, show that the Hamiltonian reduces to the total energy of the system, H = T + V.

11.9 Develop the equation of motion of a simple pendulum by use of (a) Newtonian mechanics, (b) Lagrangian mechanics, and (c) Hamiltonian mechanics.

11.10 Given functions f, g, h, and constant c, show that

- $\begin{array}{ll} \text{(a)} & \{f,g\} = \, \{g,f\} & \text{(b)} & \{f,c\} = 0 \\ \text{(c)} & \{f+g,h\} = \{f,h\} + \{g,h\} & \text{(d)} & \{f,g+h\} = \{f,g\} + \{f,h\} \end{array} \end{array}$
- (e) $\{fg,h\} = f\{g,h\} + \{f,h\}g$ (Leibniz identity)
- (f) $\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0$ (Jacobi identity).

11.11 Show that

(a)
$$\{f, g_k\} = -\frac{\partial f}{\partial p_k}$$
 and (b) $\{f, p_k\} = \frac{\partial f}{\partial q_k}$

11.12 By use of the direct application of δ on the phase space variables, show that

$$\delta \int_{t_1}^{t_2} \left(\sum_{i=1}^n \dot{q}_i p_i - H \right) dt = 0$$

leads to Hamilton's canonical equations.

11.13 For L' = L + df/dt, show that Hamilton's variational principle yields the same equation of motion for L and L'.

Chapter 12

Geometrical Methods in Physics

12.1 Introduction

A review of the Section on topological spaces (see page 76) may be useful for this chapter. Here we consider the manifold point of view of geometry by use of concepts of differential geometry. **Differential geometry** is the branch of mathematics in which differential and integral calculus are applied to geometry. Problems in differential geometry are classified as local and global. The derivative of a function is viewed as the tangent line or slope of a curve, and the integral of a function is interpreted as the area under a curve. The tangent space at a point and curvature are local problems. The validity of certain local properties may impose restrictions on the manifold (space) as a whole, and the determination of these restrictions is a global problem. **Topology** (more specifically, differential topology) is the main tool for the study of global properties of manifolds. In general, differential geometry is the study of a class of spaces called manifolds, defined below.

A set of points is a differentiable manifold if the following properties are valid.

- 1. M is a topological space;
- 2. *M* is provided with a family of pairs $\{(M_{\alpha}, \phi_{\alpha})\}$;
- 3. M_{α} are a family of open sets with cover $M, \cup_{\alpha} M_{\alpha} = M$; The ϕ_{α} are homeomorphisms from M_{α} to an open subset of O_{α} of $\mathbb{R}^{n}, M_{\alpha} : M_{\alpha} \to O_{\alpha}$.
- 4. Given M_{α} and M_{β} such that $M_{\alpha} \cap M_{\beta} \neq \emptyset$; the composite map $\phi_{\beta} \circ \phi_{\alpha}^{-1}$ from the subset $\phi_{\alpha} (M_{\alpha} \cap M_{\beta})$ of \mathbb{R}^{n} is infinitely differentiable, C^{∞} .

The family $\{(M_{\alpha}, \phi_{\alpha})\}$ satisfying properties 2, 3, and 4 is called an **atlas** and the individual members $(M_{\alpha}, \phi_{\alpha})$ are called **charts** (see Figs.12.1 and 12.2). Properties 1, 2, and 3 mean M that is a space which is locally Euclidean. Property 4 asserts that when two patches overlap, the overlap region $M_{\alpha} \cap M_{\beta}$ has two sets of coordinates in \mathbb{R}^n , $x^1, x^2, \ldots, x^n \equiv \{x^i\}$ for $\phi_{\alpha}(M_{\alpha} \cap M_{\beta})$ and $\bar{x}^1, \bar{x}^2, \ldots, \bar{x}^n \equiv \{\bar{x}^i\}$ for $\phi_{\beta}(M_{\alpha} \cap M_{\beta})$ respectively. Also, it asserts that the change from one set of coordinates to the other is done in C^{∞} manner. We may therefore write $\bar{x}^i = \phi^i(\{x^i\})$. These local coordinates have



Figure 12.1

no geometrical meaning, and the mathematical tool for the study of manifolds must be furnished by concepts (objects) that behave in a simple manner under a change of coordinates; tensors (tensor fields) are the most important of these concepts.

In developing differential geometry, Gauss, Riemann, and Christoffel¹ introduced the concept of a tensor. The subject of tensor analysis (absolute differential calculus) was introduced and developed by Ricci² and his student Levi-Civita. Tensor analysis is a technique for making calculations with indexed quantities, introduced by Ricci. Einstein³ introduced the term "tensor" and made extensive use of tensor calculus in his 1916 formulation of the general theory of relativity. A **tensor** consists of a set of quantities called components whose properties are independent of the coordinate system used to describe them. The components of a tensor in two different coordinate systems are related by the characteristic transformation laws discussed below.

12.2 Transformation of Coordinates in Linear Spaces

In equation form, we may write the relation between the two coordinate systems mentioned in the previous Section as

$$\bar{x}^i = \phi^i \left(x^1, x^2, \dots, x^n \right); \quad i = 1, 2, \dots, n.$$
 (12.1)

The ϕ^i are assumed to be single-valued real functions of the coordinates and possess continuous partial derivatives. These assumptions are characteristic properties of differentiable

 $^{^{1}}$ Elwin Bruno Christoffel (1829–1900), German mathematician noted for his work in mathematical analysis and tensor calculus.

 $^{^{2}}$ Georgorio Ricci-Curbastro (1853–1925), Italian mathematician and scientist who invented absolute differential calculus (i.e., tensor calculus).

³Albert Einstein (1879–1955), German physicist who contributed more than any other scientist to the modern view of physical reality. He is best known for his theories of special and general relativity. He was awarded the Nobel Prize for physics in 1921 for his theory of the photoelectric effect.



Figure 12.2

manifolds. The total differential of \bar{x}^i may be written as

$$d\bar{x}^{i} = \sum_{j=1}^{n} \frac{\partial \bar{x}^{i}}{\partial x^{j}} dx^{j} = \frac{\partial \bar{x}^{i}}{\partial x^{j}} dx^{j}.$$
(12.2)

The Einstein summation convention (when the same index appears once as a superscript and once as a subscript, it is understood that a summation is to occur on that index) is used in the last step of Eq.(12.2). Note that the j index in the denominator of Eq.(12.2) is considered to be a subscript; in addition, the index j is called a dummy index since the letter used for such an index in immaterial. To avoid confusion in notations, an index must not appear more than twice in any single term or product. Equation (12.2) will serve as the foundation for the characteristic transformation law for the components of tensors. On considering Eq.(12.2) in the matrix form $\bar{X} = AX$, the solution has the form $X = A^{-1}\bar{X}$ where $A^{-1} = A^{CT}/\det |A|$. Hence, the inverse transformation exists if

$$\det \left| \frac{\partial \bar{x}^{i}}{\partial x^{j}} \right| = \left| \begin{array}{ccc} \frac{\partial \bar{x}^{1}}{\partial x^{1}} & \cdots & \frac{\partial \bar{x}^{1}}{\partial x^{n}} \\ \vdots & \cdots & \vdots \\ \frac{\partial \bar{x}n}{\partial x^{1}} & \cdots & \frac{\partial \bar{x}^{n}}{\partial x^{n}} \end{array} \right| \neq 0.$$
(12.3)

The determinant in Eq.(12.3) is called the **Jacobian** of the transformation.

Example 109 Find the Jacobian of the transformation for a rotation in two dimensions (see Section 2.2.5).
Solution : In this case, we have

$$\bar{x}^1 = x^1 \cos \theta + x^2 \sin \theta$$
 and $\bar{x}^2 = -x^1 \sin \theta + x^2 \cos \theta$.

In matrix form, we write

$$\begin{pmatrix} \bar{x}^1\\ \bar{x}^2 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta\\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x^1\\ x^2 \end{pmatrix}$$

Here, the Jacobian is the determinant of the rotation matrix and is given by

$$\det \left| \frac{\partial \bar{x}^{i}}{\partial x^{j}} \right| = \left| \begin{array}{c} \frac{\partial \bar{x}^{1}}{\partial x^{1}} & \frac{\partial \bar{x}^{1}}{\partial x^{2}} \\ \frac{\partial \bar{x}^{2}}{\partial x^{1}} & \frac{\partial \bar{x}^{2}}{\partial x^{2}} \end{array} \right| = \left| \begin{array}{c} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{array} \right| = 1.$$

12.3 Contravariant and Covariant Tensors

The characteristic transformation laws for tensors will now be discussed. In 1889, Ricci introduced the use of superscripts and subscripts to distinguish between the contravariant and covariant tensors; also, these indices make the mathematical development of tensor analysis compact. The superscripts, contravariant indices, are used to denote the contravariant components of a tensor, $T^{ij\dots}$. The subscripts, covariant indices, are used to represent the covariant components of a tensor, $T_{ij\dots}$. The components of a mixed tensor are specified by indicating both subscripts and superscripts, $T^{ij\dots}_{\ell mn\dots}$. Throughout this chapter, this notation (letters and indices) will be used to denote the components of a tensor or the tensor itself. The **rank** (order or degree) of a tensor is the number (without counting an index which appears once as a subscript and once as a superscript) of indices in the symbol representing a tensor (or the components of a tensor). For example,

The components of tensors of ranks less than three can be put into matrix form. In an *n*-dimensional space, the number of components of a tensor of rank r is n^r . For example, $G_{\mu\nu}$ has sixteen components in a four-dimensional space, $4^2 = 16$.

12.3.1 Tensors of Rank One

A set of quantities A^i associated with a point P having coordinates x^i is said to be the components of a contravariant tensor of rank one (a vector) if they transform $(x^i \to \bar{x}^i)$ according to Eq.(2.2); for example, the components $A^j(x^j)$ and $\bar{A}^i(\bar{x}^i)$ are connected by

$$\bar{A}^{i} = \frac{\partial \bar{x}^{i}}{\partial x^{j}} A^{j}.$$
(12.4)

To obtain the inverse transformation in Eq.(12.4), multiply both sides by $\partial x^k / \partial \bar{x}^i$ and sum over *i*; we obtain

$$\frac{\partial x^{k}}{\partial \bar{x}^{i}} \bar{A}^{i} = \frac{\partial x^{k}}{\partial \bar{x}^{i}} \frac{\partial \bar{x}^{i}}{\partial x^{j}} A^{j} = \delta^{k}_{j} A^{j} = A^{k} \quad \text{or} \\
A^{j} = \frac{\partial x^{j}}{\partial \bar{x}^{i}} \bar{A}^{i}.$$
(12.5)

The Kronecker delta function is given by

$$\delta_j^k = \begin{cases} 1 & \text{for } j = k \\ 0 & \text{for } j \neq k. \end{cases}$$
(12.6)

A shortcut for obtaining Eq.(12.5) from Eq.(12.4) is to remove the bars from originally barred symbols and place bars on originally unbarred symbols.

If A^k are the components of an arbitrary tensor, then the quantities B_k are the components of a covariant tensor of rank provided the following condition holds.

$$A^{k}B_{k} \text{ is invariant (i.e., a scalar)}$$
$$A^{k}B_{k} = \bar{A}^{k}\bar{B}_{k}. \tag{12.7}$$

If A^k from Eq.(12.5) is substituted into Eq.(12.7), the result is

$$\bar{A}^k \bar{B}_k = \frac{\partial x^k}{\partial \bar{x}^i} \bar{A}^i B_k = \frac{\partial x^\alpha}{\partial \bar{x}^k} \bar{A}^k B_\alpha$$

or

$$\bar{A}^{k}\left[\bar{B}_{k}-\frac{\partial x^{\alpha}}{\partial \bar{x}^{k}}B_{\alpha}\right]=0.$$

Since components A^k are arbitrary, the above equation leads to

$$\bar{B}_k = \frac{\partial x^{\alpha}}{\partial \bar{x}^k} B_{\alpha}.$$
(12.8)

Equation (12.8) is the basic transformation law for the components of a covariant tensor of rank one.

In matrix form, we write

$$A^{k} = (a_{11} \cdots) \quad \text{and} \quad A_{k} = \left(\begin{array}{c} a_{11}^{*} \\ \vdots \end{array}
ight).$$

Note that A_k is the adjoint of A^k .

12.3.2 Higher-Rank Tensors

If the n^2 quantities $A^{k\alpha}$ transform according to

$$\bar{A}^{ij} = \frac{\partial \bar{x}^i}{\partial x^k} \frac{\partial \bar{x}^j}{\partial x^\alpha} A^{k\alpha}, \qquad (12.9)$$

then $A^{k\alpha}$ are the components of a second-rank contravariant tensor. If the n^2 quantities $A_{k\alpha}$ transform according to

$$\bar{A}_{ij} = \frac{\partial x^k}{\partial \bar{x}^i} \frac{\partial x^\alpha}{\partial \bar{x}^j} A_{k\alpha}, \qquad (12.10)$$

then the $A_{k\alpha}$ are the components of a second-rank covariant tensor. Similarly,

$$\bar{A}^{i}_{j} = \frac{\partial \bar{x}^{i}}{\partial x^{k}} \frac{\partial x^{\alpha}}{\partial \bar{x}^{j}} A^{k}_{\alpha}, \qquad (12.11)$$

means that A^k_{α} are the components of a second-rank mixed tensor. For a general tensor of rank s + p with n^{s+p} components, we have

$$\bar{A}_{r_1\cdots r_p}^{u_1\cdots u_s} = \frac{\partial \bar{x}^{u_1}}{\partial x^{t_1}} \cdots \frac{\partial \bar{x}^{u_s}}{\partial x^{t_s}} \frac{\partial x^{g_1}}{\partial \bar{x}^{r_1}} \cdots \frac{\partial x^{g_p}}{\partial \bar{x}^{r_p}} A_{g_1\cdots g_p}^{t_1\cdots t_s}.$$
(12.12)

Equation (12.12) is referred to as the characteristic transformation law for the components of tensors. Note that by use of the transformation law we find that: If all the components of a tensor are zero in one coordinate system, they are zero in all coordinate systems. This property is extremely important when discussing physical quantities.

12.3.3 Symmetric and Antisymmetric Tensors

Tensors A_{rs}^k and B_{rs}^k are said to be symmetric and antisymmetric (skew symmetric), respectively, in the indices r and s if

$$A_{rs}^{k} = A_{sr}^{k} \quad \text{or} \quad A_{k}^{rs} = A_{k}^{sr} \quad (\text{symmetric})$$

$$B_{rs}^{k} = -B_{sr}^{k} \quad \text{or} \quad B_{k}^{rs} = -B_{k}^{sr} \quad (\text{antisymmetric}) \quad (12.13)$$

The definition of symmetric and antisymmetric tensors can of course be extended, in a straight forward manner, to higher rank tensors. By use of the characteristic transformation law in Eq.(12.12), we find that the symmetric (or antisymmetric) property is conserved under a transformation of coordinates. From a given tensor, one can construct a symmetric and an antisymmetric tensor in any pair of subscripts or any pair of superscripts; for example consider the tensor C_{kj} with symmetric S_{kj} and antisymmetric A_{kj} tensors given by

$$S_{kj} = \frac{1}{2} \left(C_{kj} + C_{jk} \right)$$
 and $A_{kj} = \frac{1}{2} \left(C_{kj} - C_{jk} \right)$.

A tensor, for example C_{kj} , can be written as a sum of constructed symmetric and antisymmetric parts as follows:

$$C_{kj} = \frac{1}{2} \left(C_{kj} + C_{jk} \right) + \frac{1}{2} \left(C_{kj} - C_{jk} \right).$$

12.3.4 Polar and Axial Vectors

In Chapter 1, the components of vectors referred to the projections of vectors on the three coordinate axes in a right-hand Cartesian system. For clarity, we will call such components ordinary components of vectors. By contrast, contravariant and covariant components of vectors as developed in this chapter are not restricted to a specific coordinate system. It is shown below Eq.(12.26) that components of contravariant and covariant vectors are identical in Cartesian coordinates. In general, vectors whose components transform according to the following equations are called **polar** (true or proper) vectors.

$$\bar{A}^i = \frac{\partial \bar{x}^i}{\partial x^j} A^j$$
 or $\bar{A}_i = \frac{\partial x^j}{\partial \bar{x}^i} A_j$

Polar vectors are used to represent quantities such as displacements and forces. In Cartesian coordinates, the cross product written in terms of components is

$$\mathbf{T} = \mathbf{A} \times \mathbf{B} \Longrightarrow T_{ij} = A_i B_j - A_j B_i = -T_{ji}.$$

We see that the components of a cross product of two polar vectors transform like the components of a second-rank antisymmetric tensor. Vectors like T are called **axial** vectors (or pseudovectors) and are used to represent rotational quantities such as angular momentum and torque (moment of a force). Geometrically, axial vectors correspond to areas.

12.4 Tensor Algebra

12.4.1 Addition (Subtraction)

As is clear from the characteristic transformation law in Eq.(12.12), two tensors of the same type (each having the same number of covariant and the same number of contravariant indices) can be added (or subtracted) to produce a single tensor. In equation form, we write

$$C_{i_1\cdots i_p}^{t_1\cdots t_s} = A_{i_1\cdots i_p}^{t_1\cdots t_s} + B_{i_1\cdots i_p}^{t_1\cdots t_s}.$$
(12.14)

For example, $C_{ij}^k = A_{ij}^k + B_{ij}^k$.

12.4.2 Multiplication (Outer Product)

The outer (tensor) product of two tensors with components $A_{i_1\cdots i_p}^{i_1\cdots i_p}$ and $B_{j_1\cdots j_m}^{i_1\cdots i_n}$ is defined by

$$C_{i_{1}\cdots i_{p}}^{t_{1}\cdots t_{s}}{}_{j_{1}\cdots j_{m}}^{i_{1}\cdots i_{n}} = A_{i_{1}\cdots i_{p}}^{t_{1}\cdots t_{s}} B_{j_{1}\cdots j_{m}}^{j_{1}\cdots j_{n}}.$$
(12.15)

For example, $C_{nps}^{kj} = A_{np}^k B_s^j$.

The division of a tensor of rank greater than zero by another tensor of rank greater than zero is not uniquely defined.

12.4.3 Contraction

The operation of **contraction** is the process by which the number of covariant and contravariant indices of a mixed tensor is reduced by one; that is to say, a contravariant index is equated to a covariant index (thus a summation over the index results). For example, consider the contraction of a mixed tensor with components A_{kmn}^{ij} ,

$$B_{kn}^{j} = A_{kin}^{ij}.$$
 (12.16)

In Eq.(12.16), the components B_{kn}^{j} are obtained from the components A_{kmn}^{ij} by contracting the indices i and m (i = m); by use of the Einstein summation convention, a summation on i is then understood. In general, the contraction operation enables a tensor of rank r-2 to be obtained from a mixed tensor of rank r. Any index of the contravariant set and any index of the covariant set may be used to form the components of the new tensor.

12.4.4 Inner Product

Inner multiplication is the process of combining outer multiplication and contraction; the resulting tensor is called the **inner product** of the two tensors involved. For example, the inner product of A_s^{ij} and B_{mnt}^k is

$$A_{s}^{ij}B_{mnt}^{k} = C_{smnt}^{ijk} = D_{mnt}^{ij} \quad \text{(for } k = s\text{)}.$$
 (12.17)

12.4.5 The Quotient Law

The quotient law is a simple indirect test for determining if a set of quantities forms the components of a tensor. The direct test is, of course, to determine if the set of quantities satisfies the characteristic transformation law in Eq.(12.12).

Quotient Law If the product (outer or inner) of a set of quantities $A_{j_1\cdots j_p}^{i_1\cdots i_p}$ with the components of an arbitrary tensor $B_{m_1\cdots m_q}^{i_1\cdots i_k}$ yields a nonzero tensor, then the quantities $A_{j_1\cdots j_p}^{i_1\cdots i_p}$ are the components of a tensor. To illustrate the quotient law, consider the specific inner product of an arbitrary tensor with components B_i and quantities A^{ik} that yield a nonzero tensor C^k ; in equation form, we write

$$C^k = A^{ik} B_i. (12.18)$$

According to the quotient law, A^{ik} are the components of a tensor since the B_i are the components of an arbitrary tensor and C^k are the components of a nonzero tensor. In the \bar{x}^i coordinate system, Eq.(12.18) becomes

$$\bar{C}^k = \bar{A}^{ik} \bar{B}_i. \tag{12.19}$$

By use of the transformation law for contravariant and for covariant tensors of rank one (see Eqs. 12.5 and 12.8), Eq.(12.18) becomes

$$\frac{\partial \bar{x}^k}{\partial x^j} C^j = \bar{A}^{ik} \frac{\partial x^\alpha}{\partial \bar{x}^i} B_\alpha.$$
(12.20)

On substituting Eq.(12.18) into Eq.(12.20), we obtain

$$\frac{\partial \bar{x}^k}{\partial x^j} A^{\alpha j} B_{\alpha} = \bar{A}^{ik} \frac{\partial x^{\alpha}}{\partial \bar{x}^i} B_{\alpha}.$$
(12.21)

Since B_{α} is an arbitrary tensor, we obtain the following from Eq.(12.21).

$$\bar{A}^{ik} = \frac{\partial \bar{x}^i}{\partial x^{\alpha}} \frac{\partial \bar{x}^k}{\partial x^j} A^{\alpha j}.$$
(12.22)

We see that the components $A^{\alpha j}$ are the components tensor since Eq.(12.22) is the basic transformation for a second-rank contravariant tensor.

For an arbitrary nonzero tensor with components A_i , we may form the inner product

$$A_j = \delta^i_j A_i. \tag{12.23}$$

In Eq.(12.23), $\delta_i^i = \partial x^i / \partial x^j$. In terms of the \bar{x}^i coordinates, we write Eq.(12.23) as

$$\bar{A}_j = \bar{\delta}^i_j \bar{A}_i = \frac{\partial \bar{x}^i}{\partial \bar{x}^j} \left(\frac{\partial x^k}{\partial \bar{x}^i} A_k \right) = \frac{\partial x^k}{\partial \bar{x}^j} A_k.$$
(12.24)

Equation (12.24) is just the fundamental transformation law for a covariant tensor of rank one, and it demonstrates that A_j are the components of a tensor. By use of the quotient law, δ_j^i are the components of a second rank mixed tensor. Moreover, it can be shown that $\delta_j^i = \bar{\delta}_j^i$ which means that the components of δ_j^i have the same value in all coordinate systems.

12.5 The Line Element

12.5.1 The Fundamental Metric Tensor

The generalized form of the square of the invariant distance ds^2 (a scalar, tensor of rank zero) between two points with coordinates x^i and $x^i + dx^i$ as defined by Riemann is given by the following quadratic differential form:

$$ds^2 = g_{ij}dx^i dx^j. aga{12.25}$$

By use of the quotient law, g_{ij} are the components of the tensor since ds and dx^i are tensors; g_{ij} are called the components of the fundamental metric tensor (or metric tensor). In Eq.(12.25), it is assumed that (a) the $g_{ij} = g_{ij}(x^i)$ are functions of the x^i , (b) $g_{ij} = g_{ji}$ (symmetric), and (c) det $|g_{ij}| \neq 0$. In this case, the space is called a **Riemannian** space and the quadratic form $g_{ij}dx^i dx^j$ is called the metric. If rectangular Cartesian coordinates are introduced in a Euclidean space, we have $g_{ij} = \delta_{ij}$, and the square of the element of length reduces to the familiar form

$$ds^{2} = (dx^{1})^{2} + (dx^{2})^{2} + (dx^{3})^{2}.$$

12.5.2 Associate Tensors

The tensor associate to A^{j} is the result of the inner product of A^{j} and the fundamental metric tensor; in equation form, we write

$$A_i = g_{ij} A^j. \tag{12.26}$$

The process in Eq.(12.26) is called lowering the superscript, and A_i is the tensor associate to A^j . For Cartesian coordinates in Euclidean space, $g_{ij} = \delta_{ij}$ and the contravariant components of a tensor of rank one (vector) are identical to the covariant components as can be seen from Eq.(12.26).

Treating the components in Eq.(12.26) as matrices and solving for A^{j} , we obtain

$$A^j = g^{ij} A_i. \tag{12.27}$$

In Eq.(12.27), the components g^{ij} are defined by

$$g^{ij} = \frac{(g_{ij})^{CT}}{\det|g_{ij}|}.$$
(12.28)

The right-hand side of Eq.(12.28) is the inverse of the matrix g_{ij} where $(g_{ij})^{CT}$ (means the cofactor transpose of the matrix g_{ij} . On applying the quotient law in Eq.(12.27), we determine that g^{ij} is a tensor (the inverse of g_{ij}); it is called the **reciprocal tensor** to g_{ij} . The process in Eq.(12.27) is known as raising the subscript. The process of lowering or raising indices may be performed on tensors of ranks higher than one. For example,

$$A_{rpmn}^{\cdot jk} = g_{ri} A_{pmn}^{ijk}.$$
(12.29)

The dot notation is introduced to indicate which index has been lowered (or raised).

12.6 Tensor Calculus

12.6.1 Introduction

Consider the invariant (a scalar) $\bar{\phi}(\bar{x}^i) = \phi(x^i)$; on differentiating both sides of this equation with respect to \bar{x}^i , we obtain

$$\frac{\partial \phi}{\partial \bar{x}^i} = \frac{\partial x^j}{\partial \bar{x}^i} \frac{\partial \phi}{\partial x^j}.$$
(12.30)

Note that Eq.(12.30) is the transformation equation for the components of a covariant tensor of rank one, $\partial \phi / \partial x^j$. We have, therefore, generated a tensor of rank one from a tensor of rank zero, ϕ , by use of ordinary differentiation. If we try to extend this process to obtain a tensor of rank two by differentiating a tensor of rank one

$$A^j = \frac{\partial x^j}{\partial \bar{x}^n} \bar{A}^n,$$

we find that

$$\frac{\partial A^{j}}{\partial x^{p}} = \frac{\partial x^{j}}{\partial \bar{x}^{n}} \frac{\partial \bar{x}^{m}}{\partial x^{p}} \frac{\partial \bar{A}^{n}}{\partial \bar{x}^{m}} + \frac{\partial^{2} x^{j}}{\partial \bar{x}^{n} \partial x^{p}} \bar{A}^{n}.$$
(12.31)

The right-hand side of Eq.(12.31) is not a tensor because of the presence of the second term. Hence, the ordinary derivative of a tensor of rank one results in a quantity that is not a tensor.

The plan now is to develop a scheme for a new kind of derivative, the covariant derivative, which enables us to always obtain a tensor when we differentiate a tensor of any rank. Since covariant derivatives make use of the two Christoffel symbols, we begin with the definitions and a discussion of these two Christoffel symbols.

12.6.2 Christoffel Symbols

The Christoffel symbols of the first and second kinds are defined, respectively, by

$$[ij,k] \equiv \frac{1}{2} \left(\frac{\partial g_{ik}}{\partial x^j} + \frac{\partial g_{jk}}{\partial x^i} - \frac{\partial g_{ij}}{\partial x^k} \right)$$
(12.32)

and

$$\begin{cases} p\\ij \end{cases} \equiv g^{pk} \left[ij,k \right]. \tag{12.33}$$

In the two Christoffel symbols, i, j, and k are subscripts and p is a superscript. The summation convention is implied in Eq.(12.33) for the Christoffel symbol of the second kind. The symbol Γ_{ij}^{p} is often used for the Christoffel symbol of the second kind; it, however, is important of note that the Christoffel symbol of the second kind is not always a tensor as suggested by the notation, Γ_{ij}^{p} .

By use of the definition in Eq.(12.32), we note that the Christoffel symbol of the first kind is symmetric respect to the i and j indices. Hence we may write

$$[ij,k] = [ji,k]$$

The symbol [ij, k] will be used to represent the Christoffel symbol of the first kind in terms of \bar{x}^i coordinates; we obtain

$$\overline{[pm,n]} = \frac{\partial x^i}{\partial \bar{x}^p} \frac{\partial x^j}{\partial \bar{x}^m} \frac{\partial x^k}{\partial \bar{x}^n} [ij,k] + \frac{\partial x^i}{\partial \bar{x}^n} \frac{\partial^2 x^j}{\partial \bar{x}^p \partial \bar{x}^m} g_{ij}.$$
(12.34)

Equation (12.34) shows that [ij, k] transforms like a tensor only if the second term vanishes; when the second term in Eq.(12.34) vanishes, the transformation is said to be **affine**.

By use of the definition in Eq.(12.33), it is clear that the Christoffel symbol of the second kind is symmetric in the i and j indices, and we may write

$$\left\{ {p\atop{ij}} \right\} = \left\{ {p\atop{ji}} \right\}.$$

By use of the inner product, we may write

$$g_{pm}\left\{\substack{p\\ij}\right\} = g_{pm}g^{pk}\left[ij,k\right] = \delta_m^k\left[ij,k\right] = \left[ij,m\right].$$

The Christoffel symbol of the second kind in terms of the \bar{x}^i coordinates may be written as

$$\overline{\{{}^{k}_{pm}\}} = \frac{\partial \bar{x}^{k}}{\partial x^{n}} \frac{\partial x^{i}}{\partial \bar{x}^{p}} \frac{\partial x^{j}}{\partial \bar{x}^{m}} \{{}^{n}_{ij}\} + \frac{\partial \bar{x}^{k}}{\partial x^{j}} \frac{\partial^{2} x^{j}}{\partial \bar{x}^{p} \partial \bar{x}^{m}}.$$
(12.35)

Note that the Christoffel symbol of the second kind is not, in general, a tensor because of the presence of the second term on the right-hand side of Eq.(12.35). Inner multiplication of Eq.(12.35) with $\partial x^r / \partial \bar{x}^q$ yields

$$\frac{\partial^2 xr}{\partial \bar{x}^p \partial \bar{x}^m} = \frac{\partial x^r}{\partial \bar{x}^q} \overline{\{}^q_{pm} \overline{\}} - \{ ^r_{ij} \} \frac{\partial x^i}{\partial \bar{x}^p} \frac{\partial x^j}{\partial \bar{x}^m}.$$
(12.36)

Equation (12.36) is an extremely useful relation for the second partial derivative of x^r in terms of the first derivative and the Christoffel symbol of the second kind.

12.6.3 Covariant Differentiation of Tensors

Returning to Eq. (12.31) and substituting Eq. (12.36) for the second term on the right-hand side of Eq. (12.31), we obtain

$$\frac{\partial A^{j}}{\partial x^{p}} + {j \atop pk} A^{k} = \left(\frac{\partial \bar{A}^{n}}{\partial \bar{x}^{m}} + \overline{{n \atop mq}} \bar{A}^{q}\right) \frac{\partial x^{j}}{\partial \bar{x}^{n}} \frac{\partial \bar{x}^{m}}{\partial x^{p}}.$$
(12.37)

To obtain Eq. (12.37), the fundamental transformation equation for tensors was used. Equation (12.37) is normally written in the following compact form.

$$A^{j}_{,p} = \frac{\partial x^{j}}{\partial \bar{x}^{n}} \frac{\partial \bar{x}^{m}}{\partial x^{p}} \bar{A}^{n}_{,m}.$$
(12.38)

Equation (12.38) is just the characteristic transformation equation for the second-rank mixed tensor which is referred to as the **covariant derivative** of A^{j} with respect to x^{p} ; it is given by

$$A_{,p}^{j} = \frac{\partial A^{j}}{\partial x^{p}} + {j \atop pk} A^{k}.$$
(12.39)

By use of a similar procedure, we find that the covariant derivative of B_j with respect to x^p is given by

$$B_{j,p} = \frac{\partial \bar{x}^i}{\partial x^j} \frac{\partial \bar{x}^k}{\partial x^p} \bar{B}_{i,k}.$$
(12.40)

To obtain Eq.(12.40), we use the notation

$$B_{j,p} = \frac{\partial B_j}{\partial x^p} - \left\{\substack{i\\jp}\right\} B_i.$$
(12.41)

The above relations for the covariant derivatives of a tensor may be extended in a natural way to the case of a general mixed tensor $T_{i_1\cdots i_p}^{j_1\cdots j_p}$; we obtain

$$T_{i_{1}\cdots i_{p},k}^{j_{1}\cdots j_{s}} = \frac{\partial T_{i_{1}\cdots i_{p}}^{j_{1}\cdots j_{s}}}{\partial x^{n}} - \left\{ {}^{q}_{i_{1}k} \right\} T_{qi_{2}\cdots i_{p}}^{j_{1}\cdots j_{s}} - \left\{ {}^{q}_{i_{2}k} \right\} T_{i_{1}qi_{3}\cdots i_{p}}^{j_{1}\cdots j_{s}} - \cdots - \left\{ {}^{q}_{i_{p}} \right\} T_{i_{1}\cdots i_{p}}^{j_{1}\cdots j_{s}} + \left\{ {}^{i_{1}}_{qk} \right\} T_{i_{1}\cdots i_{p}}^{j_{1}\cdots j_{s}} + \left\{ {}^{j_{2}}_{qk} \right\} T_{i_{1}\cdots i_{p}}^{j_{1}qi_{3}\cdots j_{s}} + \cdots + \left\{ {}^{j_{s}}_{qk} \right\} T_{i_{1}\cdots i_{p}}^{j_{1}\cdots j_{s}}.$$
(2.42)

The covariant derivative of a tensor of rank zero (a scalar) is defined to be the same as the ordinary derivative; that is to say,

$$A_{,j} = \frac{\partial A}{\partial x^j}.$$

We have discussed (a) basic tensor notations; (b) the fundamental transformation equation for the components of tensors; and (c) the algebra and calculus of tensors. These concepts will now be used in some examples.

Example 110 By use of the electromagnetic field tensor $F_{\mu\nu}$, develop the tensor form of Maxwell's equations.

Solution : Maxwell's equation in differential form are

 $\begin{array}{ll} 1. \quad \nabla \cdot \mathbf{E} = \rho & (\text{Gauss's law}) & 2. \quad \nabla \cdot \mathbf{B} = 0 & (\text{no free magnetic poles}) \\ 3. \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} & (\text{Faraday's law}) & 4. \quad \nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} & (\text{Ampère's law}) \end{array}$

We have set $c = \epsilon_0 = \mu_0 = 1$ throughout this Example.

The components of the four-vectors (four-dimensional orthogonal coordinate system Minkowski⁴ space) for position, current density, and vector potential are

$$\begin{aligned} x^{\nu} &= \left(x^{0}, x^{1}, x^{2}, x^{3}\right) = \left(t, x, y, z\right) \\ J_{\lambda} &= \left(\rho, J_{1}, J_{2}, J_{3}\right) = \left(\rho, J_{x}, J_{y}, J_{z}\right) \\ A_{\mu} &= \left(A_{0}, A_{1}, A_{2}, A_{3}\right) = \left(A_{0}, A_{x}, A_{y}, A_{z}\right). \end{aligned}$$

Also, note that

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \text{and} \quad \mathbf{E} = \nabla A_0 - \frac{\partial \mathbf{A}}{\partial t}$$

(In this Example, the range of Greek indices is 0, 1, 2, 3 and the range for Latin indices is 1, 2, 3.)

The electromagnetic field tensor is an antisymmetric tensor and is defined by

$$F_{\mu\nu} = \frac{\partial A_{\nu}}{\partial x^{\mu}} - \frac{\partial A_{\mu}}{\partial x^{\nu}}$$
$$= \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} \quad (\mu, \nu = 0, 1, 2, 3).$$

In terms of the components of the electric and magnetic fields, the electromagnetic field tensor reduces to

$$F_{\mu\nu} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_z \\ E_z & B_y & -B_x & 0 \end{pmatrix}.$$

⁴Hermann Minkowski (1864–1909), Russian-born German mathematician who developed a new view of space and time that provided the mathematical foundation for the theory of relativity.

Consider the following equation involving the electromagnetic field tensor (which is valid for an arbitrary antisymmetric tensor)

$$\frac{\partial F_{\alpha\beta}}{\partial x^{\mu}} + \frac{\partial F_{\beta\mu}}{\partial x^{\alpha}} + \frac{\partial F_{\mu\alpha}}{\partial x^{\beta}} = 0 \qquad (\alpha, \beta, \mu = 0, 1, 2, 3).$$

Since $F_{\mu\nu}$ is an antisymmetric tensor, it can be shown that only four independent equations result from the sixty-four possible equation that are indicated by the above tensor equation. Typical values for, α , β , and μ are

Set 1:
$$1, 2, 3$$
; Set 2: $0, 2, 3$; Set 3: $0, 3, 1$; and Set 4: $0, 1, 2$.

The resulting equation for Set 1 is Maxwell's second equation, $\nabla \cdot \mathbf{B} = 0$. On combining the results for Sets 2, 3, and 4, one obtains Maxwell's third equation, $\nabla \times \mathbf{E} + \partial \mathbf{B}/\partial t = 0$. The remaining two Maxwell's equations may be obtained from the following tensor equation:

$$\sum_{\nu=0}^{3} \frac{\partial F_{\mu\nu}}{\partial x^{\nu}} = J_{\mu}.$$

12.7 The Equation of the Geodesic Line

In three-dimensional Euclidean space, a straight line is the shortest distance between two points (see the Example on page 280). In this section, we generalize this fundamental concept to Riemannian space.

If the curve $x^{i} = x^{i}(u)$ joins two fixed points $P_{1}(u_{1})$ and $P_{2}(u_{2})$, then the distance along this curve between the two points is given by

$$s = \int_{P_1}^{P_2} ds = \int_{u_1}^{u_2} \left[F\left(x^i, \dot{x}^i, u\right)
ight]^{1/2} du$$

where $F = g_{ij} rac{dx^i}{du} rac{dx^j}{du}$ and $\dot{x}^i = rac{dx^i}{du}$.

The solution of Euler's equation yields the shortest distance between P_1 and P_2 , geodesic; Euler's equation for this case becomes

$$0 = \frac{\partial F^{1/2}}{\partial x^{i}} - \frac{d}{du} \left(\frac{\partial F^{1/2}}{\partial \dot{x}^{i}} \right)$$

$$= \frac{d}{du} \left(\frac{1}{F^{1/2}} \frac{\partial F}{\partial \dot{x}^{i}} \right) - \frac{1}{2F^{1/2}} \frac{\partial F}{\partial x^{i}}$$

$$= \frac{d}{du} \left(\frac{1}{F^{1/2}} \right) \frac{\partial F}{\partial \dot{x}^{i}} + \frac{1}{F^{1/2}} \frac{d}{du} \left(\frac{\partial F}{\partial \dot{x}^{i}} \right) - \frac{1}{F^{1/2}} \frac{\partial F}{\partial x^{i}}$$

$$= \frac{d}{du} \left(\frac{\partial F}{\partial \dot{x}^{i}} \right) - \frac{\partial F}{\partial x^{i}} - \frac{1}{2F} \frac{\partial F}{\partial \dot{x}^{i}} \frac{dF}{du}.$$
 (12.43)

If u equals the distance s along the curve in question, then dF/ds = 0 since it is an arbitrary parameter. In this case, we have

$$\dot{x}^{i} = \frac{dx^{i}}{ds}; \quad F = g_{ij}\frac{dx^{i}}{ds}\frac{dx^{j}}{ds}; \quad \frac{\partial F}{\partial \dot{x}^{i}} = 2g_{ij}\dot{x}^{j}; \quad \text{and} \quad \frac{\partial F}{\partial x^{i}} = \dot{x}^{\mu}\dot{x}^{\nu}\frac{\partial g_{\mu\nu}}{\partial x^{i}}$$

Equation (12.43) now becomes

$$0 = \frac{d}{ds} \left(\frac{\partial F}{\partial \dot{x}^{i}} \right) - \frac{\partial F}{\partial x^{i}} = \frac{d \left(2g_{ij} \dot{x}^{j} \right)}{ds} - \dot{x}^{\mu} \dot{x}^{\nu} \frac{\partial g_{\mu\nu}}{\partial x^{i}}$$
$$= g_{ij} \frac{d^{2} x^{j}}{ds^{2}} + \frac{\partial g_{ij}}{\partial x^{k}} \frac{dx^{k}}{ds} \frac{dx^{j}}{ds} - \frac{1}{2} \frac{\partial g_{\mu\nu}}{\partial x^{i}} \frac{dx^{\mu}}{ds} \frac{dx^{\nu}}{ds}.$$

By use of the Christoffel symbol of the first kind, we may write the above equation in the form

$$0 = g_{ij}\frac{d^2x^j}{ds^2} + [\mu\nu, i]\frac{dx^{\mu}}{ds}\frac{dx^{\nu}}{ds}.$$

= $g^{i\alpha}g_{ij}\frac{d^2x^j}{ds^2} + g^{i\alpha}[\mu\nu, i]\frac{dx^{\mu}}{ds}\frac{dx^{\nu}}{ds}.$ (12.44)

Inner product with respect to α in Eq.(12.44) leads to

$$\frac{d^2 x^{\alpha}}{ds^2} + \left\{^{\alpha}_{\mu\nu}\right\} \frac{dx^{\mu}}{ds} \frac{dx^{\nu}}{ds} = 0.$$
(12.45)

Equation (12.45) is the differential equation of the geodesic line in Riemannian space.

Example 111 Find the equation of the geodesic line for a three-dimensional Cartesian coordinate system.

Solution : For Cartesian coordinate in a three-dimensional Euclidean space, we have

$$g_{\mu\nu} = \begin{cases} 1 & \text{for } \mu = \nu \\ 0 & \text{for } \mu \neq \nu, \end{cases} \qquad \begin{cases} \alpha \\ \mu\nu \end{cases} = 0 & \text{for } \mu, \nu = 1, 2, 3. \end{cases}$$

The equation of the geodesic line in this special case becomes

$$\frac{d^2x^{\alpha}}{ds^2} = 0 \quad (\alpha = 1, 2, 3).$$

If we consider an observer traveling with an object that is moving from P_1 to P_2 (the object is at rest with respect to the observer), ds = dt where dt is called the **proper** time. Since $dv^{\alpha}/dt = A$, we obtain $x^{\alpha} = At + B$ where A and B are arbitrary constants. This is the required equation for the geodesic line; it is the equation for a straight line.

12.8 Special Equations Involving the Metric Tensor

In 1854, Riemann assumed that the quadratic form $ds^2 = g_{\mu\nu}dx^{\mu}dx^{\nu}$ defines the metrical properties of space and that this form should be regarded as a physical reality. It, however, was Einstein, in his theory of general relativity, who attached physical significance to $g_{\mu\nu}$ by showing that the gravitational potential is proportional to the fourth component of this fundamental metric tensor. Einstein thus asserted that gravitational phenomena are intimately connected with the metrical properties of space-time. Space-time in special relativity is a four-dimensional flat manifold, Minkowskian space, with constant metric $\eta_{\mu\nu}$, the Lorentzian metric. In the normal convention, the values for the indices are $\mu, \nu = 0, 1, 2, 3$. This Lorentzian metric with +2 signature is given by

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
 (12.46)

In general relativity, space-time is a four-dimensional curve manifold. That is to say, the components of $g_{\mu\nu}$ are not constant.

It is important to note that the gravitational potential according to general relativity has an invariant quadratic differential form (a 2-form). Electromagnetic phenomena are governed by a potential, A_{μ} , which has an invariant linear differential form (a 1-form) given by $A_{\mu}dx^{\mu}$. The existence of these two separate invariant forms is the source of the difficulty involved in developing a theory which unifies gravitational and electromagnetic phenomena.

12.8.1 The Riemann-Christoffel Tensor

Here, the main purpose is to obtain a tensor that contains $g_{\mu\nu}$ only by means of differentiation. The covariant derivatives of A_{α} and $A_{\alpha,\beta}$ are respectively given by

$$A_{\alpha,\beta} = \frac{\partial A_{\alpha}}{\partial x^{\beta}} - \left\{ {}^{\mu}_{\alpha\beta} \right\} A_{\mu}$$
(12.47)

and

$$A_{\alpha,\beta\gamma} = \frac{\partial A_{\alpha,\beta}}{\partial x^{\gamma}} - \left\{ {}^{\mu}_{\gamma\alpha} \right\} A_{\alpha,\beta} - \left\{ {}^{\mu}_{\gamma\beta} \right\} A_{\alpha\mu}.$$
(12.48)

On substituting $A_{\alpha,\beta}$ (with the appropriate change of indices) from Eq.(12.47) into Eq.(12.48), we obtain

$$A_{\alpha,\beta\gamma} = \frac{\partial}{\partial x^{\gamma}} \left(\frac{\partial A_{\alpha}}{\partial x^{\beta}} - \left\{ {}^{\mu}_{\alpha\beta} \right\} A_{\mu} \right) - \left\{ {}^{\lambda}_{\gamma\alpha} \right\} \left(\frac{\partial A_{\lambda}}{\partial x^{\beta}} - \left\{ {}^{\mu}_{\lambda\beta} \right\} A_{\mu} \right) - \left\{ {}^{\lambda}_{\gamma\beta} \right\} \left(\frac{\partial A_{\alpha}}{\partial x^{\lambda}} - \left\{ {}^{\mu}_{\alpha\lambda} \right\} A_{\mu} \right).$$
(12.49)

Interchanging the indices β and γ ($\beta \rightarrow \gamma$ and $\gamma \rightarrow \beta$) in Eq.(12.49) yields

$$A_{\alpha,\gamma\beta} = \frac{\partial}{\partial x^{\beta}} \left(\frac{\partial A_{\alpha}}{\partial x^{\gamma}} - \left\{ {}^{\mu}_{\alpha\gamma} \right\} A_{\mu} \right) - \left\{ {}^{\lambda}_{\alpha\beta} \right\} \left(\frac{\partial A_{\lambda}}{\partial x^{\gamma}} - \left\{ {}^{\mu}_{\lambda\gamma} \right\} A_{\mu} \right) - \left\{ {}^{\lambda}_{\beta\gamma} \right\} \left(\frac{\partial A_{\alpha}}{\partial x^{\lambda}} - \left\{ {}^{\mu}_{\alpha\lambda} \right\} A_{\mu} \right).$$
(12.50)

Subtracting Eq.(12.50) from Eq.(12.49) yields

$$A_{\alpha,\beta\gamma} - A_{\alpha,\gamma\beta} = R^{\mu}_{\gamma,\alpha\beta} A_{\mu}$$

where

$$R^{\mu}_{\gamma,\alpha\beta} = \frac{\partial}{\partial x^{\beta}} \left\{ {}^{\mu}_{\alpha\gamma} \right\} - \frac{\partial}{\partial x^{\gamma}} \left\{ {}^{\mu}_{\alpha\beta} \right\} + \left\{ {}^{\lambda}_{\gamma\alpha} \right\} \left\{ {}^{\mu}_{\lambda\beta} \right\} - \left\{ {}^{\lambda}_{\beta\alpha} \right\} \left\{ {}^{\mu}_{\lambda\gamma} \right\}.$$
(12.51)

Since $A_{\alpha,\beta\gamma} - A_{\alpha,\gamma\beta}$ is a tensor and A_{μ} is an arbitrary tensor, $R^{\mu}_{\gamma,\alpha\beta}$ is a fourth-rank mixed tensor by use of the quotient law; this fourth-rank mixed tensor in Eq.(12.51) is called the **Riemann-Christoffel tensor**. Note that the Riemann-Christoffel tensor is composed exclusively from derivatives of the fundamental metric tensor, $g_{\mu\nu}$. If a coordinate system is selected such that the components of $g_{\mu\nu}$ are constants (e.g., Minkowski space), then all components of the Riemann-Christoffel tensor vanish in that system (and in all other systems).

12.8.2 The Curvature Tensor

The curvature tensor, $R_{\lambda\gamma\alpha\beta}$, is obtained by use of the inner product of the fundamental metric tensor and the Riemann-Christoffel tensor; we may write

$$R_{\lambda\gamma\alpha\beta} = g_{\lambda\mu} R^{\mu}_{\gamma\alpha\beta}. \tag{12.52}$$

12.8.3 The Ricci Tensor

Contracting the Riemann-Christoffel tensor, Eq.(12.51), with respect to the μ and β indices, we obtain the **Ricci tensor**

$$R_{\gamma\alpha} = \frac{\partial}{\partial x^{\beta}} \left\{ {}^{\beta}_{\alpha\gamma} \right\} - \frac{\partial}{\partial x^{\gamma}} \left\{ {}^{\beta}_{\alpha\beta} \right\} + \left\{ {}^{\lambda}_{\gamma\alpha} \right\} \left\{ {}^{\beta}_{\lambda\beta} \right\} - \left\{ {}^{\lambda}_{\beta\alpha} \right\} \left\{ {}^{\beta}_{\lambda\gamma} \right\}.$$
(12.53)

12.8.4 The Einstein Tensor and Equations of General Relativity

The Einstein tensor, $G_{\mu\nu}$, is defined as

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R.$$
 (12.54)

The curvature scalar, in Eq.(12.54) is given by

$$R = g^{\mu\nu} R_{\mu\nu}.$$

Einstein's equations of general relativity are

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi T_{\mu\nu} \qquad (\mu,\nu=0,1,2,3).$$
(12.55)

In Eq.(12.55), the energy-momentum tensor which describes the distribution of mass and energy (except gravitational energy) is given by

$$T_{\mu\nu} = (\rho + P) u_{\mu}u_{\nu} - g_{\mu\nu}P + T^{EM}_{\mu\nu}.$$
(12.56)

In Eq.(12.56), u_{μ} and u_{ν} are four velocities, ρ is density, and P is pressure. In a vacuum, $T_{\mu\nu} = 0$.

The basic equations of general relativity are (a) Einstein's equations, Eq.(12.55), which relate the curvature structure of space-time (the left-hand side) to the mass-energy (through the energy-momentum tensor, except gravitational fields) contents of space-time and (b) the geodesic equations, Eq.(12.45), whose solution determines the path of a particle through

space-time. In the Einstein's equations, note that the last two terms of the Ricci tensor, $R_{\mu\nu}$, in Eq.(12.53) involve products of derivatives of the fundamental metric tensor; hence the presence of these two terms in the Einstein tensor, $G_{\mu\nu}$, means that Einstein's equations are nonlinear differential equations. As is well known, there exists no general method for solving nonlinear differential equations. The twistor theory due to Penrose⁵ is an attempt to transform the Einstein equations into a twistor space (a complex manifold of three complex dimensions) with the hope of then finding a solution in this twistor space. The inverse transform would then provide the required solution in four-dimensional curve spacetime. The successes of Einstein's theory of general relativity include (a) explanation of the precession of the perihelion of planets, (b) prediction of the deflection of light rays passing near a body of large mass, (c) prediction of the gravitational red shift of spectral lines, and (d) a general theory of cosmology.

12.9 Exterior Differential Forms

12.9.1 Introduction

It was explained at the beginning of this Chapter that the local coordinates $\{x^n\}$ and $\{\bar{x}^n\}$ in the overlap region $M_{\alpha} \cap M_{\beta}$ of the manifold M have no intrinsic geometrical or physical meaning. In this Section, we introduce a coordinate free development of the tensor concept.

The idea of a physical vector (in \mathbb{R}^3 ; see Chapter 1) as a directed straight-line segment does not directly extend to a manifold. For a manifold, vectors at a point can be introduced by use of the notion of tangents to curves passing through the point. Let S be a curve through the point P of the differentiable manifold M. Local coordinates $\{x^n\}$ can be used to specify S in the following parametric form: $x^i = x^i(t)$ for $i = 1, 2, \ldots, n$. The quantities dx^i/dt are components of the tangent vector to S at P. Tangent vectors to all possible curves in M through P generate a vector space (with the same dimensions as M) called the **tangent space** TM_p (also, the notation T_pM is used). The union of tangent spaces to M at all its points is called the **tangent bundle** of M and is denoted as TM. If we consider an arbitrary differentiable function f which assigns a real number to every point t on S, then

$$\frac{df}{dt} = \sum_{i=1}^{n} \frac{dx^{i}}{dt} \partial_{i} f \Longrightarrow \frac{d}{dt} = \sum_{i=1}^{n} \frac{dx^{i}}{dt} \partial_{i}.$$
(12.57)

In Eq.(12.57), df/dt is the derivative of f along S (the directional derivative) and $\partial_i f = \partial f/\partial x^i$. Here d/dt acting on the space of real functions on M contains all the components of the tangent vector; each component of the tangent vector is associated with a corresponding partial derivative, ∂_i . By use of the second equation in Eq.(12.57), we may say that the tangent vector at P is the directional derivative operator d/dt with $\{\partial_i\}$ being the natural coordinate basis of vectors for the vector space; an arbitrary vector V

 $^{^{5}}$ Roger Penrose (* 1931), English mathematical physicist is known for his contributions to the theory of relativity and for his study of celestial objects.

can be expanded in this basis as

$$V = \sum_{i=1}^{n} V^i \partial_i. \tag{12.58}$$

In Eq.(12.58), the V^i are said to be the components of a contravariant vector. The tangent space is the natural space in Lagrangian mechanics where the Lagrangian has the following functional form: $L[q^i(t), \dot{q}^i(t)]$.

The coordinate free definition of a tangent vector is as follows. If F(M) is the space of all differentiable real functions on a manifold M, then a tangent vector at P is defined as V acting on elements of F(M) to produce real numbers: $V: F(M) \to \mathbb{R}$ such that

1.
$$V(af + bg) = aV(f) + bf(g);$$
 and

2. V(fg) = g(P)V(f) + f(P)V(g) where $f, g \in F(M)$ and $a, b \in \mathbb{R}$.

The dual space of $TM_p, \omega: TM_p \to \mathbb{R}$, is called the cotangent space at P and is denoted as T^*M_p . The function ω is referred to as an exterior differential one-form (or simply a 1-form). That is to say, a 1-form on the tangent space to M, TM_p , is a cotangent vector to M at the point P. The union of cotangent spaces to the manifold at all its points is called the **cotangent bundle** of M and is written as T^*M . A simple example of a one-form is total differential df of a function $f \in F(M)$; it is defined as the element of T^*M_p satisfying $\langle df, V \rangle = Vf$ for any $V \in TM_p$. On setting $f = x^i$ and $V = \partial_i$, one finds that the set $\{dx^i\}$ of total differentials of the coordinates constitutes the natural coordinate basis for the dual space (cotangent space, T^*M_p) since $\langle dx^i, \partial_i \rangle = \partial_j x^i = \delta_j^i$. An arbitrary one-form ω expanded in the dual basis becomes

$$\omega = \sum_{i=1}^{n} \omega_i dx^i. \tag{12.59}$$

The quantities ω_i are the components of a covariant tensor. In general, tensors are elements of the tangent and cotangent spaces of the (underlying) manifold M.

Differential forms provide a means of generalizing the basic operations of vector calculus in \mathbb{R}^3 (gradient, divergence, curl, and the integral theorems of Gauss, Green, and Stokes) to manifolds of arbitrary finite dimensions.

Consider the set of totally antisymmetric covariant tensors of type (0, p) at point P of an n-dimensional manifold M. These tensors are called exterior differential forms of degree p (or simply p-forms); they span a vector space denoted by $\Lambda^p T^* M_p$ (or simply $\Lambda^p T^*$). If p = 0, then $\Lambda^0 T^*$ is the space of real smooth functions on M, normally written as F(M). Note that $p \leq n$ because a form where p > n is identically zero since the only nonzero components of totally antisymmetric p-tensors are the ones with different indices; hence, all differential forms of degree higher than the dimension of the underlying space are zero. The dimension of the vector space $\Lambda^p T^*$ is the number of ways of choosing p elements from n distinct elements without regard to order and is determined by use of the binomial coefficient formula

$$\binom{n}{p} = \frac{n!}{p! (n-p)!}.$$

In terms of dimensions, we have the following relations:

$$\begin{split} &\dim \Lambda^0 T^* = 1 \\ &\dim \Lambda^1 T^* = n \\ &\dim \Lambda^2 T^* = n(n-1)/2 \\ &\vdots \\ &\dim \Lambda^{(n-1)} T^* = n \\ &\dim \Lambda^n T^* = 1. \end{split}$$

Note that $\dim \Lambda^p T^* = 0$ for p > n and that $\dim \Lambda^p T^* = \dim \Lambda^{(n-p)} T^*$. The **Hodge**⁶ star operator for the spaces of *p*-forms and (p-1)-forms, $*: \Lambda^p T^* \mapsto \Lambda^{(n-p)} T^*$, is defined for manifolds M that have a metric g, and it may be used to construct a relation between these two spaces. The Hodge star operator is denoted by * in the exponent.

12.9.2 Exterior Product

In 1862, Grassmann⁷ introduced an algebra of vectors based on a definition of the cross product of vectors in Euclidean space. E. Cartan⁸ (a) made use of Grassmann algebra in geometry and in mechanics and (b) discovered that Grassmann algebra applied to differential forms as elements of the algebra could be combined with a special differentiation process, exterior differentiation, to produce a very compact notation that is useful in geometry and in mathematical physics. A *p*-form is a covariant antisymmetric tensor field of rank (or degree) p, and exterior differentiation of a *p*-form is an operation that produces a (p+1)-form.

The sum (or difference) of two *p*-forms is a *p*-form, and the product of a *p*-form and a function f (a 0-form) is a *p*-form. Cartan's exterior differential product (wedge product \wedge) of a *p*-form and a *q*-form is the mapping

$$\wedge : \Lambda^{p}T^{*} \times \Lambda^{q}T^{*} \mapsto \Lambda^{p+q}T^{*}.$$
(12.60)

The above definition for two 1-forms α_1 and α_2 reduces to

$$\alpha_1 \wedge \alpha_2 = \frac{1}{2} \left(\alpha_1 \otimes \alpha_2 - \alpha_2 \otimes \alpha_1 \right) = -\alpha_2 \wedge \alpha_1. \tag{12.61}$$

Note that the wedge product is a rule for constructing 2-forms from 1-forms since the righthand side of Eq.(12.61) is a 2-form. In general, the wedge product of a p-form (an element of $\Lambda^p T^*$) and a q-form (an element of $\Lambda^q T^*$) produces a (p+q)-form such that

$$\delta \wedge \omega = (-1)^{pq} \omega \wedge \delta. \tag{12.62}$$

⁶William Vallance Douglas Hodge (1903–1975), English mathematician who is known for his work in algebraic geometry and differential geometry.

⁷Hermann Günter Grassmann (1809–1877), German mathematician best known for his development of a general calculus for vectors and the invention of what is now called exterior algebra.

⁸Elie Joseph Cartan (1869–1951), French mathematician who is noted for his work on continuous groups, Lie algebras, differential equations, and differential geometry.

The larger vector space ΛT^* consisting of the direct sum of all the vector spaces $\Lambda^p T^*$ has dimension given by

$$\sum_{p=1}^n \binom{n}{p} = 2^n.$$

The space ΛT^* together with the exterior (wedge) product is called the Cartan exterior algebra of T^*M_p (Grassmann algebra where the objects are differential forms).

12.9.3 Exterior Derivative

The exterior derivative operation maps a *p*-form into a (p+1)-form,

$$d: \Lambda^p T^* \mapsto \Lambda^{(p+1)} T^*, \tag{12.63}$$

such that for p-forms $\omega, \omega_1 \in \Lambda^p T^*$ and q-form $\omega_2 \in \Lambda^q T^*$ the following are satisfied.

- 1. $d(\omega_1 + \omega_2) = d\omega_1 + d\omega_2$
- 2. $d(\omega_1 \wedge \omega_2) = (d\omega_1 \wedge \omega_2) + (-1)^p (\omega_1 \wedge d\omega_2)$

3.
$$d(d\omega) = 0$$

Let f and g be functions (0-forms) and let α and β be 1-forms; the following properties of the exterior derivative are valid.

- 4. df is the ordinary total differential of f
- 5. d(fg) = (df)g + fdg
- 6. $d(f\alpha) = df \wedge \alpha + f d\alpha$
- 7. $d(\alpha \wedge \beta) = da \wedge \beta \alpha \wedge \beta$.

If the derivative of the *p*-form φ equals zero $(d\varphi = 0)$, then φ is said to be closed. If the form φ equals $d\omega (\varphi = d\omega)$ or $\varphi = 0$, then φ is said to be exact.

12.9.4 The Exterior Product and Exterior Derivative in \mathbb{R}^3

Exterior differential forms in \mathbb{R}^3 with Cartesian coordinates are the integrands of three of the integrals on page 31. The one-, two-, and three-forms are respectively given by

$$\int \alpha$$
 (line integral); $\int \beta$ (surface integral); $\int \gamma$ (volume integral)

In the above integrands, we have

$$\begin{aligned} \alpha &= a_1 dx + a_2 dy + a_3 dz \quad (1\text{-form}) \\ \beta &= b_1 dy dz + b_2 dz dx + b_3 dx dy \\ &= b_1 dy \wedge dz + b_2 dz \wedge dx + b_3 dx \wedge dy \quad (2\text{-form}) \\ \gamma &= f dx dy dz = f dx \wedge dy \wedge dz \quad (3\text{-form}). \end{aligned}$$

In the above equations f, a_i , and b_i are 0-forms (functions). The Hodge star operator takes *p*-forms to (3 - p)-forms in \mathbb{R}^3 . For example, we have

- 1. $1^{\star} = dx \wedge dy \wedge dz$
- 2. $(dx \wedge dy \wedge dz)^* = 1$
- 3. $dx^{\star} = dy \wedge dz; \ dy^{\star} = dz \wedge dx; \ dz^{\star} = dx \wedge dy$
- 4. $(dy \wedge dz)^{\star} = dx; \quad (dz \wedge dx)^{\star} dy; \quad (dx \wedge dy)^{\star} = dz.$

Consider the two 1-forms $\alpha = a_1 dx + a_2 dy + a_3 dz$ and $\beta = b_1 dx + b_2 dy + b_3 dz$. The exterior product $\alpha \wedge \beta$ is given by

$$\begin{aligned} \alpha \wedge \beta &= (a_1 dx + a_2 dy + a_3 dz) \wedge (b_1 dx + b_2 dy + b_3 dz) \\ &= (a_2 b_3 - a_3 b_2) \, dy \wedge dz - (a_1 b_3 - a_3 b_1) \, dz \wedge dx + (a_1 b_2 - a_2 b_1) \, dx \wedge dy. \end{aligned}$$

The correspondence to $\alpha \wedge \beta$ in vector calculus is the cross product. Note that the cross product of $\mathbf{A} = a_1 \mathbf{i} + a_2 \mathbf{j} + a_3 \mathbf{k}$ and $\mathbf{B} = b_1 \mathbf{i} + b_2 \mathbf{j} + b_3 \mathbf{k}$ equals

$$\mathbf{A} \times \mathbf{B} = (a_2b_3 - a_3b_2)\mathbf{i} - (a_1b_3 - a_3b_1)\mathbf{j} + (a_1b_2 - a_2b_1)\mathbf{k}.$$

In making this correspondence, note the following: $\mathbf{i} = \mathbf{j} \times \mathbf{k}$ (is like $dy \wedge dz$), $\mathbf{j} = \mathbf{k} \times \mathbf{i}$ (is like $dz \wedge dx$), and $\mathbf{k} = \mathbf{i} \times \mathbf{j}$ (is like $dx \wedge dy$). The wedge product of a 1-form and a 2-form corresponds to the dot product; for example, $\alpha \wedge \beta^*$ corresponds to $\mathbf{A} \cdot \mathbf{B}$. The exterior derivative of the 0-form is

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz.$$

The above equation corresponds to grad f. The exterior derivative of a 1-form α is

$$dlpha = \left(rac{\partial a_3}{\partial y} - rac{\partial a_2}{\partial z}
ight) dy \wedge dz + \left(rac{\partial a_1}{\partial z} - rac{\partial a_3}{\partial x}
ight) dz \wedge dx + \left(rac{\partial a_2}{\partial x} - rac{\partial a_1}{\partial y}
ight) dx \wedge dy.$$

The above equation corresponds to curl **A**. The exterior derivative of the 2-form represented by $\beta = Ady \wedge dz + Bdz \wedge dx + Cdx \wedge dy$ where A, B, and C are 0-forms reduces to

$$d\beta = \left(rac{\partial A}{\partial x} + rac{\partial B}{\partial y} + rac{\partial C}{\partial z}
ight) dx \wedge dy \wedge dz.$$

The above equation corresponds to div V times an element of volume. The above results are summarized below.

0-Form		2-Form	
df	$\operatorname{grad} f$	$d\beta$	divergence
1-Forms		1-and 2-Form	
$lpha_1 \wedge lpha_2$	cross product	$\alpha \wedge \alpha^{\star}$	dot product
dlpha	curl		

By use of $d^2 = dd = 0$, we obtain ddf = d(1-form) = curl grad f = 0.

Here we note that the cross product, dot product, grad, curl, and div are just special cases of the wedge product and exterior derivative of exterior differential forms. It, however, should be clearly understood that our purpose for introducing exterior calculus is considerably more important than the demonstration of this correspondence for \mathbb{R}^3 . Moreover, we find that this correspondence with vector calculus will not be possible for \mathbb{R}^n where n > 3; for example, there is nothing that corresponds to a 2-form in \mathbb{R}^4 . That is to say, vector calculus for spaces with dimensions greater than three is not valid, but the calculus of differential forms is valid for n arbitrary.

12.9.5 The Generalized Stokes Theorem

We conclude the discussion of exterior calculus by writing down the generalized Stokes theorem. Let M be a compact oriented smooth k-manifold with boundary ∂M and let φ be a (k-1)-form on M. In equation form, the generalized Stokes theorem is

$$\int_{M} d\varphi = \int_{\partial M} \varphi. \tag{12.64}$$

In the above equation, φ is a (k-1)-form and $d\varphi$ is a k-form. Note that M is a onedimensional connected manifold when k = 1. If M is contained in \mathbb{R}^1 , then M is just an interval [a, b]; the boundary ∂M has dimension zero and is the pair of points a, b. The function f(x) is a 0-form on [a, b], and we have

$$df = \frac{\partial f}{\partial x} dx = f'(x) \, dx.$$

For this case (k = 1), the generalized Stokes theorem reduces to

$$\int_{a}^{b} df = \int_{a}^{b} f'(x) \, dx = f(a) - f(b) \, .$$

The above equation is referred to as the fundamental theorem of calculus.

The generalized Stokes theorem is one of the most useful tools of the calculus of exterior differential forms, and it contains, as special cases, all of the integral theorems of vector calculus and the fundamental theorem of calculus.

12.10 Problems

12.1 By use of the summation convention, rewrite

$$d\phi = rac{\partial \phi}{\partial x} dx + rac{\partial \phi}{\partial y} dy + rac{\partial \phi}{\partial z} dz.$$

12.2 Determine the number of equations in a four-dimensional space that are represented by $R^{\eta}_{\alpha\beta\delta} = 0.$

12.3 Show that the symmetric (or antisymmetric) property of a tensor is conserved under a transformation of coordinates.

12.4 Show that $g_{ij} = 0$ for $i \neq j$ is required for orthogonal coordinate systems.

12.5 By use of the Riemannian metric, show that $g_{ij} = g_{ji}$.

12.6 Determine the conditions that must exist for the Christoffel symbols to be tensors.

12.7 Show that the covariant derivative of g_{ij} equals zero (**Ricci's theorem**).

12.8 By use of the definition of the components of the four-vector current density, write the continuity equation.

12.9 Compute Γ_{ik}^{i} in (a) Cartesian and (b) cylindrical coordinates.

12.10 For the surface of a sphere (a two-dimensional Riemannian space), compute (a) the components of the fundamental metric tensor and (b) the two Christoffel symbols.

12.11 Compute the components of the fundamental metric tensor and ds^2 for the new coordinate system when the transformation from Cartesian coordinates (x, y, z) to spherical coordinates (r, θ, ϕ) is made.

12.12 By use of the definition of the Christoffel symbol of the first kind, show that

$$rac{\partial g_{ik}}{\partial x^j} = [ij,k] + [kj,i]$$
 .

12.13 By use of the definition of the Christoffel symbol of the second kind, show that

$$\frac{\partial g^{mk}}{\partial x^p} = -g^{ik} \left\{ {}^m_{ip} \right\} - g^{jm} \left\{ {}^k_{jp} \right\}.$$

12.14 By use of the fundamental transformation law for the components of a tensor, show that the quantities $\delta^{\nu}_{\mu}A_{\nu}$ transform like the components of a tensor.

12.15 In Example 110, show that (a) the components of $F_{\mu\nu}$ are those given in the matrix form, (b) Set 1 leads to $\nabla \cdot \mathbf{B} = 0$ (c) Sets 2, 3, and 4 lead to Maxwell's third equation, and (d) the equations

$$\sum_{\nu=0}^{3} \frac{\partial F_{\mu\nu}}{\partial x^{\nu}} = J_{\mu}$$

lead to Maxwell's first and fourth equations.

12.16 By contracting the Einstein field equations with $g^{\mu\nu}$, show that these field equations may be written as

$$R_{\mu\nu} = 8\pi \left(T_{\mu\nu} - \frac{1}{2} g_{\mu\nu} T \right).$$

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