Friedel theorem for two-dimensional relativistic spin-$\frac{1}{2}$ systems

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The Friedel sum rule is generalized to relativistic systems of spin-$\frac{1}{2}$ particles in two dimensions. The change in energy due to the presence of an impurity is studied. The relation of the sum rule with the relativistic Levinson theorem is presented. Density oscillations in such systems are discussed. Since the Friedel theorem has been of major importance in understanding the impurity scattering in materials, the present results would be helpful to explain some phenomena in two-dimensional fermionic many body systems.

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I. INTRODUCTION

It was pointed out by Friedel [1] that the change of the number of states ΔN around an impurity in solid can be in terms of a sum, well-known as the Friedel sum rule (FSR) [2,3], which sets up the relation between ΔN and the phase shifts at the Fermi surface. In three-dimensional (3D) systems, the theorem can be described by

$$\Delta N = \frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\delta_l(E_F), \tag{1}$$

where $\delta_l(E_F)$ denotes the phase shift of scattered state in the angular-momentum channel l with energy at the Fermi surface. The result is one of the most interesting results in the theory of impurity. It provides a powerful method in calculating some important properties of electron structures [2–4]. The subject was then studied by many authors and generalized to include the internal degree of freedom of particles [5,6]. Recently, based on the Dirac equation, the FSR for relativistic spin-$\frac{1}{2}$ particles in 3D systems is proved to be

$$\Delta N = \frac{1}{\pi}\sum_{\kappa=-\infty,\kappa\neq 0}^{\infty} 2|\kappa|\Bigg\{[\delta_\kappa(E_F)-\delta_\kappa(\mu)+\delta_\kappa(-E_F')-\delta_\kappa(-\mu)] + \epsilon_\kappa\frac{\pi(-1)^{|\kappa|}}{2}[\sin^2\delta_\kappa(\mu)-\sin^2\delta_\kappa(-\mu)]\Bigg\}, \tag{2}$$

where $\delta_\kappa(\pm E_\lambda)$ and $\delta_\kappa(\pm\mu)$, classified by the angular momentum $\kappa=\pm(j+1/2)$ and $\epsilon_\kappa\equiv 1(-1)$ for $\kappa>0$ $(\kappa<0)$, are the phase shifts of scattering states at Fermi energies ($E_\lambda=E_F$ and $-E_F'$) and zero-momentum ($E_\lambda=\pm\mu$) [7]. The result provides a basis to explore the effect of an impurity by the FSR for 3D relativistic systems.

Over the past 2 decades, a number of interesting physical systems have been expected to be described by the two-dimensional (2D) Dirac equation [8–11] rather than the Schrödinger equation. The anticipation has been confirmed by experiments in the perfect graphene recently [10,11], which pose new questions on the nature of the electronic properties in such systems and shows a possibility of studying relativistic phenomena in a table-top experiment. To my knowledge, the FSR for 2D Dirac fermions is still lacking. It is the aim of the report to extend the FSR for 3D relativistic systems to 2D ones.

The report is organized as follows. In Sec. II, the 2D FRS for the relativistic spin-$\frac{1}{2}$ particles moving in a short range potential $|V(r)|$ when $r<a$ and $V(r)=0$ when $r\geqslant a$ caused by an impurity is established. ΔN is shown to relate to the phase shifts $\delta_j(E_\lambda)$ of scattering states at Fermi energies ($E_\lambda=E_F$ and $-E_F'$) and zero-momentum ($E_\lambda=\pm\mu$) as follows:

$$\Delta N = \frac{1}{\pi}\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(E_F)-\delta_j(\mu)+\delta_j(-E_F')-\delta_j(-\mu)], \tag{3}$$

where j $(j=\pm 1/2,\pm 3/2,\ldots)$ is the total angular momentum. The FSR for massless Dirac fermions is discussed. Section III is used to discuss the change in energy of a relativistic spin-$\frac{1}{2}$ system in the presence of an impurity. In Sec. IV, the relation between the FSR and the 2D relativistic Levinson theorem [12–15] is presented. Density oscillation is discussed. Our conclusions are summarized in Sec. V.

II. FRIEDEL SUM RULE FOR RELATIVISTIC SPIN-$\frac{1}{2}$ SYSTEMS IN TWO DIMENSIONS

We consider the 2D model. The Dirac equation of a spin-$\frac{1}{2}$ particle with effective mass μ moving in a symmetric potential $V(r)$ specified in the above is

$$[\vec{\alpha}\cdot\hat{\mathbf{p}}+\gamma^0\mu+V(r)]\Psi_\lambda(\mathbf{r}) = E_\lambda\Psi_\lambda(\mathbf{r}), \tag{4}$$

where $\alpha^i=\gamma^0\gamma^i (i=1,2)$ are Dirac matrices. As usual, they are chosen as the Pauli matrices $\gamma^0=\sigma^3, \gamma^1=i\sigma^1$, and $\gamma^2=i\sigma^2$. For our purposes it is very convenient to write the spin wave function in a form

$$\Psi_\lambda(\mathbf{r}) = \sum_{j=\pm 1/2,\pm 3/2,\ldots} c_j\Psi_{\lambda j}(\mathbf{r}) = \sum_{j=\pm 1/2,\pm 3/2,\ldots} c_j\begin{bmatrix} f_{\lambda j}(r)\dfrac{e^{i(j-1/2)\varphi}}{\sqrt{2\pi}} \\ g_{\lambda j}(r)\dfrac{e^{i(j+1/2)\varphi}}{\sqrt{2\pi}}\end{bmatrix}. \tag{5}$$

Here c_j's are coefficients dependent on the particular form required for Ψ_λ and $j=\pm 1/2,\pm 3/2,\ldots$ denote the quantum number of the total angular momentum $\hat{J}=\hat{L}+\hat{S}$ with

$\hat{S}=(i\epsilon^{ij}\gamma^i\gamma^j)/4$. Using (5), we can show that the radial equations for spinors $f_{\lambda j}(r)$ and $g_{\lambda j}(r)$ are given by

$$\left(\frac{d}{dr}-\frac{j-1/2}{r}\right)f_{\lambda j}(r)+[E_\lambda+\mu-V(r)]g_{\lambda j}(r)=0, \quad (6)$$

$$\left(\frac{d}{dr}+\frac{j+1/2}{r}\right)g_{\lambda j}(r)-[E_\lambda-\mu-V(r)]f_{\lambda j}(r)=0. \quad (7)$$

Thus, at regions of $V(r)=0$, the asymptotic solutions for particle (positive energy) and antiparticle (negative energy) can be found as

$$f_{\lambda j}(r)\to\sqrt{\frac{(|E_\lambda|\pm\mu)}{\pi kr}}\sin\left[kr-\frac{\kappa\pi}{2}-\frac{\pi}{4}+\delta_j\right], \quad (8)$$

and

$$g_{\lambda j}(r)\to\mp\sqrt{\frac{(|E_\lambda|\mp\mu)}{\pi kr}}\cos\left[kr-\frac{\kappa\pi}{2}-\frac{\pi}{4}+\delta_j\right], \quad (9)$$

where $k\equiv\sqrt{E_\lambda^2-\mu^2}\geqslant 0$, $\kappa\equiv|j-1/2|$, δ_j is the phase shift caused by the potential barrier, and the upper and lower signs indicate the scattering states of particle (positive-energy $E_\lambda>\mu$) and antiparticle (negative-energy $E_\lambda<-\mu$), respectively. To approach the FSR, we note that the change of the number of states ΔN around the barrier $V(r)$ is obtained by integrating up to the Fermi energy E_F $(-E_F')$,

$$\Delta N=\lim_{R\to\infty}\lim_{E_{\lambda'}\to E_\lambda}\left(\int_{-E_F'}^{-\mu}+\int_{\mu}^{E_F}\right)dE_\lambda \times\int d^2r[\Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r})-\Psi_\lambda^{(0)\dagger}(\mathbf{r})\Psi_{\lambda'}^{(0)}(\mathbf{r})], \quad (10)$$

which can be simplified by the equalities

$$(E_{\lambda'}-E_\lambda)\Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r})=-i\,\boldsymbol{\nabla}\cdot[\Psi_\lambda^\dagger(\mathbf{r})\vec{\alpha}\Psi_{\lambda'}(\mathbf{r})], \quad (11)$$

and

$$\int d^2r\Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r})=\frac{R}{(E_{\lambda'}-E_\lambda)}\sum_j[f_{\lambda j}^*(R)g_{\lambda' j}(R) - g_{\lambda j}^*(R)f_{\lambda' j}(R)], \quad (12)$$

where R is the radius of a large 2D circular area, and one take $c_j=1$, for since we are only interested in the difference of states its complex nature is of no interest. For free Dirac particles, the integral can be expanded as

$$\int d^2r\Psi_\lambda^{(0)\dagger}(\mathbf{r})\Psi_{\lambda'}^{(0)}(\mathbf{r})=\frac{R}{(E_{\lambda'}-E_\lambda)}\sum_j[f_{\lambda j}^{(0)*}(R)g_{\lambda' j}^{(0)}(R) - g_{\lambda j}^{(0)*}(R)f_{\lambda' j}^{(0)}(R)] \quad (13)$$

with $f_{\lambda j}^{(0)}=f_{\lambda j}(\delta_j=0)$, and $g_{\lambda j}^{(0)}=g_{\lambda j}(\delta_j=0)$. Making use of (8) and (9), and noting that in 2D space $\delta_j(k=0)/\pi$ always take integers [13,14], ΔN finally can be in terms of the phase shifts at Fermi surfaces and the critical points $\pm\mu$ of zero-momentum as follows:

$$\Delta N=\frac{1}{\pi}\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(E_F)-\delta_j(\mu)+\delta_j(-E_F')-\delta_j(-\mu)]. \quad (14)$$

This is the FSR for 2D relativistic fermionic systems. Antiparticles turn out to be significant. The variance of states is the effect of two kinds of particles together. Moreover, the zero-momentum behavior is quite different from that in Eq. (2) for 3D systems where half bound states [13] with phase shifts $\pi/2$ are significant. It is interesting to point out that the Lorentz group often occurs as an approximate symmetry for low energy excitation for 2D fermions in semimetals [8–11], relativistic spectra appear naturally for massless conduction electrons in such systems. It is worthy to discuss the FSR in the condition of the fermion mass tends to zero. With (14), one can see that as the effective mass μ tends to zero, ΔN becomes

$$\Delta N=\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(E_F)+\delta_j(-E_F')-2\delta_j(0)], \quad (15)$$

which indicates the phase shifts of particle and antiparticle at zero-momentum merge to become twice. For systems containing single carrier types, Friedel sums become

$$\Delta N_{\text{particle}}=\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(E_F)-\delta_j(0)] \quad (16)$$

for particle and

$$\Delta N_{\text{antiparticle}}=\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(-E_F')-\delta_j(0)] \quad (17)$$

for antiparticle. This is the extreme case of the graphene where the carrier type can be controlled by the external gate voltage [10,11].

III. THE CHANGE IN ENERGY DUE TO AN IMPURITY IN RELATIVISTIC 2D SYSTEMS

Equations (8) and (9) show that the wave functions undergo phase shifts. This fact entails a change of the kinetic energy of particles. It can be quantified by the reasonable requirements $\Psi_{\lambda j}^{(0)}(\mathbf{r})|_{\text{BC}}=0$ and $\Psi_{\lambda j}(\mathbf{r})|_{\text{BC}}=0$ on boundary of the Dirichlet condition, and give

$$kR-\frac{\kappa\pi}{2}-\frac{\pi}{4}=n\pi, \quad n=1,2,\ldots \quad (18)$$

for spinor $f_{\lambda j}^{(0)}$, and

$$kR-\frac{\kappa\pi}{2}-\frac{\pi}{4}+\delta_j(k)=n\pi, \quad n=1,2,\ldots \quad (19)$$

for spinor $f_{\lambda j}$. Here R is on boundary. The spinors $g_{\lambda j}^{(0)}$ and $g_{\lambda j}$ are treated similarly. The number dn of allowed states between k and $k+dk$ is given by differentiating both members of (18), which yields $Rdk=\pi dn$. Thus the unperturbed density of states for a definite j reads

$$D(k) = \frac{dn}{dk} = \frac{R}{\pi}. \tag{20}$$

Equations (18) and (19), and the similar conditions for spinors $g_{\lambda j}^{(0)}$ and $g_{\lambda j}$, tell us that the change of the wave number Δk of a particle with angular momentum j is proved to be $\Delta kR = -\delta_j(k)$, and the change in energy is

$$\Delta E|_{e^-} = \frac{k\Delta k}{E_\lambda} = \frac{-k\delta_j(k)|_{e^-}}{R\sqrt{k^2+\mu^2}}. \tag{21}$$

Similarly, the change in energy for an antiparticle is given by

$$\Delta E|_{e^+} = \frac{k\Delta k}{E_\lambda} = \frac{k\delta_j(k)|_{e^+}}{R\sqrt{k^2+\mu^2}}. \tag{22}$$

Here e^- (e^+) is used to denote the particle (antiparticle). Thus the change in energy due to the presence of an impurity in 2D relativistic systems is

$$\begin{aligned}\Delta E &= \sum_{j=\pm1/2,\pm3/2,\ldots}\left(\int_0^{k_F}\Delta E|_{e^-}\frac{R}{\pi}dk - \int_0^{k_F'}\Delta E|_{e^+}\frac{R}{\pi}dk\right)\\ &= -\sum_{j=\pm1/2,\pm3/2,\ldots}\left[\int_0^{k_F}\frac{k\delta_j(k)|_{e^-}}{R\sqrt{k^2+\mu^2}}\frac{R}{\pi}dk\right.\\ &\quad\left.+\int_0^{k_F'}\frac{k\delta_j(k)|_{e^+}}{R\sqrt{k^2+\mu^2}}\frac{R}{\pi}dk\right],\end{aligned} \tag{23}$$

where R/π is the density of states for j particles and antiparticles. The result is a 2D relativistic generalization of Fermi theorem [16] where the change of the kinetic energy due to the impurity for nonrelativistic systems was studied. It is worthy to note that in the massless limit, the change in energy becomes a more compact representation

$$\Delta E = -\frac{1}{\pi}\sum_{j=\pm1/2,\pm3/2,\ldots}\left[\int_0^{k_F}\delta_j(k)|_{e^-}dk + \int_0^{k_F'}\delta_j(k)|_{e^+}dk\right]. \tag{24}$$

It states that the variance of system's energy due to an impurity can be completely ascertained as soon as the phase shift is decided.

IV. DISCUSSIONS

A. The relation with the relativistic Levinson theorem

The Levinson theorem (LT) is one of the most interesting and beautiful results in nonrelativistic quantum theory [12,13]. For 2D relativistic many-body systems, an interesting relation between the LT and the FSR can be established by the relationship of completeness of relativistic states

$$\begin{aligned}&\sum_{\text{discrete}}\psi_{\lambda j}(\mathbf{r})\psi_{\lambda j}^\dagger(\mathbf{r}') + \sum_j\left(\int_{-E_F'}^{-\mu} + \int_\mu^{E_F}\right)dE_\lambda\Psi_{\lambda j}(\mathbf{r})\Psi_{\lambda j}^\dagger(\mathbf{r}')\\ &\quad= \delta(\mathbf{r}-\mathbf{r}').\end{aligned} \tag{25}$$

Here $\psi_{\lambda j}(\mathbf{r})$ denotes a discrete bound state with a definite angular momentum j and energy E_λ allowed by the short range potential. Subtracting the relation from the ones of free states $\Psi_{\lambda j}^{(0)}(\mathbf{r})$, setting $\mathbf{r}=\mathbf{r}'$, taking trace, and integrating over the 2D plane, one finds the relation between the total number of bound states N (LT) and the difference of scattering states ΔN (FSR) as follows:

$$N = \sum_j N_j = -\Delta N. \tag{26}$$

The total number of bound states is then given by

$$N = \frac{1}{\pi}\sum_{j=\pm1/2,\pm3/2,\ldots}[\delta_j(\mu) - \delta_j(E_F) + \delta_j(-\mu) - \delta_j(-E_F')]. \tag{27}$$

The equality implies the bound-state number for a definite angular-momentum channel j is

$$N_j = \frac{1}{\pi}[\delta_j(\mu) - \delta_j(E_F) + \delta_j(-\mu) - \delta_j(-E_F')]. \tag{28}$$

The result is the Levinson theorem for relativistic spin-$\frac{1}{2}$ particles in 2D many-body systems. Different from the single particle case [14,15]

$$N_j = \frac{1}{\pi}[\delta_j(\mu) + \delta_j(-\mu)], \tag{29}$$

where the upper bound of the phase is ruled out by the relation $\delta_j(\infty)+\delta_j(-\infty)=0$. The phase shifts at Fermi energy play an important role here. The relation (26) reflects the completeness of the whole set of states. The total number of states is not altered by an external field, except that some scattering states are pulled down into the bound state region if the external potential is attractive. On the other hand, (26) implies that there is an upper bound on ΔN which depends on the potential $V(r)$. A finite deep potential may have a finite bound state such that the change of the number of scattering states is finite.

B. Density oscillation in relativistic systems

Another way to express the change of the number of states ΔN which enables us to indicate the variance of the density of states may be expressed as

$$\Delta N = 2\pi\int_0^\infty rdr[\rho(r) - \rho_0(r)], \tag{30}$$

where $(\rho-\rho_0)\equiv\delta\rho$ is the difference of the density of states given as

$$\delta\rho = \int_{k<k_F}\frac{d^2k}{(2\pi)^2}[|\Psi_\lambda(\mathbf{r})|^2 - |\Psi_\lambda^{(0)}(\mathbf{r})|^2]. \tag{31}$$

At large distances, with (8) and (9), it is shown that

$$\begin{aligned}\delta\rho &= \frac{1}{(2\pi)^2}\sum_j\int_{k<k_F}kdk\\ &\quad\times\left[(-1)^{\kappa+1}\epsilon_E\frac{2\mu}{\pi kr}\cos(2kr+\delta_j)\sin\delta_j\right],\end{aligned} \tag{32}$$

where $\epsilon_E\equiv1(-1)$ for $E_\lambda\geqslant\mu$ ($E_\lambda\leqslant-\mu$). The integration about the wave vector is difficult because the phase shifts depend on k. But we can obtain an approximate answer by expending it around the Fermi wave vector as $\delta_j = \delta_j(k_F) + (k - k_F)(d\delta_j/dk)$ such that

$$\lim_{r\to\infty} \delta\rho = \frac{1}{(2\pi)^2} \sum_j (-1)^{\kappa+1} \frac{\epsilon_E \mu}{\pi} \frac{1}{r^2} \times \sin[2k_F r + \delta_j(k_F)] \sin \delta_j(k_F) + O\left(\frac{1}{r^3}\right). \quad (33)$$

The density oscillates with a period of $2k_F$ and decreases in amplitude as r^{-2} which describes density oscillation in 2D systems decay less rapidly than r^{-3} of 3D ones. Equation (33) shows that two branches of energy have the opposite oscillating phases. Thus the antiparticle will tend to suppress the oscillation for the same phase shifts. Another interesting result about massless fermions can be observed from (32): As the effective mass tends to zero the difference of the density of states at far regions turns into a constant, and independent of the details of the system. The argument probably enables us to decide the magnitude of effective mass in a nonideal effective relativistic 2D system via Friedel oscillation at far zones.

C. The control of the change of the total number of states

Since a specified number of bound states in quantum dot can be realized in the present-day nanotechniques, it seems to us we can control the number of states around an impurity. This is due to the fact that quantum dots can be carved out of a 2D electron gas (2DEG) [17] such that the change of the number of states around them can be counted according to (26). The fact may be very useful in controlling spin bus (a controllable coupler of many qubits) via Friedel oscillation of spin systems [17].

V. CONCLUSIONS

In this report, the 2D Friedel sum rule for the relativistic spin-$\frac{1}{2}$ systems is established. The change in energy of the spin-$\frac{1}{2}$ system due to the presence of an impurity is studied. The relation of the rule with the 2D relativistic Levinson theorem is presented. Density oscillation is discussed. Since in 2D semimetals the low energy effective theory for conduction electrons is described by the Dirac's relativistic theory [8–11] the result would be helpful in studying the effects of impurities in the corresponding nanostructures.

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