Eur. Phys. J. D **38**, 307–313 (2006)
DOI: 10.1140/epjd/e2006-00053-y

THE EUROPEAN PHYSICAL JOURNAL D

Friedel theorem for one dimensional relativistic spin-1/2 systems

D.-H. Lin[a]

Department of Physics, National Sun Yat-sen University, 804 Kaohsiung, Taiwan

Received 10 August 2005 / Received in final form 29 September 2005
Published online 14 March 2006 –

Abstract. The Friedel sum rule is generalized to relativistic systems of spin-1/2 particles in one dimension. The change of the total 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 may be useful to explain some phenomena in one dimensional atomic chain, quantum wire, and fermionic many body systems.

PACS. 34.10.+x General theories and models of atomic and molecular collisions and interactions (including statistical theories, transition state, stochastic and trajectory models, etc.) – 11.80.Et Partial-wave analysis – 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 73.21.Hb Quantum wires

1 Introduction

The Friedel sum rule (FSR) [1–3] is an important theorem in studying effects of an impurity on the electron structure in solids, which sets up the relation between the change of the number of states ΔN around the impurity and the phase shift at 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 states that the change of the number of states caused by the potential of the impurity can be quantified in terms of the scattering phase shift at Fermi surface. The subject was then studied by many authors and generalized to include the internal degree of freedom of particles [4,5], which provides a powerful method in calculating the residual resistance, diamagnetic susceptibility [2,3], spectral properties of spin-1/2 fermions in the presence of an impurity [6,7], and so forth. Recently, based on the Dirac equation, the FSR for relativistic spin-1/2 particles in 3D systems is proved to be

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

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 ($E_\lambda = \pm\mu$) [8]. The result may provide a basis for exploring the effect of an impurity by the FSR for 3D relativistic systems.

Over the past twenty years, remarkable phenomena have been observed in 1D nanostructures such as the quantized conductance [9,10], reduced temperature dependence of threshold current in quantum wires [11], end states in 1D atom chains [12], and so forth. On the other hand, from the viewpoint of applications many nanostructures have been designed to take advantage of the spin degree of freedom in 1D electron gas (1DEG) [13–17]. A deeper understanding of the effect of impurities on fermions of spin-1/2 in 1D systems [18] is clearly important for the development of 1D spin-dependent nanostructures. Furthermore, since the relativistic spectra appear naturally as a low energy effective spectra for massless electrons in 1D metals [19], it is beneficial to establish the FSR for 1D relativistic spin-1/2 systems. In one dimension, the non-relativistic FSR can be proved to be (see Appendix)

$$\Delta N = \frac{2}{\pi}\sum_{p=e,o}\left[\delta_p(E_f) - \delta_p(0) + \epsilon_p\frac{\pi}{2}\sin^2\delta_p(0)\right], \tag{3}$$

where $\delta_p(0)$ is the phase shift at zero-momentum, and the phase shifts $\delta_p(E_\lambda)$ ($p = e, o$) are classified by even parity (e) and odd parity (o) of wave functions. In this paper we will study the FSR for relativistic spin-1/2 particles in one dimension. From which the change in energy due to the presence of an impurity, and the relation between the FSR and the Levinson theorem [20–22] are discussed.

[a] e-mail: dhlin@mail.nsysu.edu.tw

This paper is organized as follows. In Section 2, the 1D FRS is generalized to the relativistic spin-1/2 particles moving in a symmetric potential $|V(x)|$ when $|x| \le a$ and $V(x) = 0$ when $|x| \ge a$. The total change of the number of states ΔN around the potential is shown to relate to the phase shifts $\delta_p(E_\lambda)$ of scattering states at Fermi energies ($E_\lambda = E_f$ and $-E'_f$) and zero-momentum ($E_\lambda = \pm\mu$) as follows:

$$\Delta N = \frac{1}{\pi} \sum_{p=e,o} \left\{ \left[\delta_p(E_f) - \delta_p(\mu) + \delta_p(-E'_f) - \delta_p(-\mu)\right] - \epsilon_p \frac{\pi}{2}\left[\sin^2\delta_p(\mu) - \sin^2\delta_p(-\mu)\right] \right\}, \quad (4)$$

where $\epsilon_p = 1(-1)$ for even parity (odd parity). Section 3 is used to discussed the change in energy of a relativistic spin-1/2 system in the presence of an impurity. In Section 4, the relation between the FSR and the 1D relativistic Levinson theorem is presented. Density oscillations are discussed. The FSR for the massless relativistic spin-1/2 particles is also presented here. Our conclusions are summarized in Section 5.

2 Friedel theorem for relativistic spin-1/2 systems in one dimension

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

$$\left[\alpha\hat{p} + \gamma^0\mu + V(x)\right]\Psi_{\lambda p}(x) = E_\lambda \Psi_{\lambda p}(x), \quad (5)$$

where $\hat{p} = -i\partial_x$, and $\alpha = \gamma^0\gamma^1$ is Dirac matrix. In one dimension, they are chosen as the Pauli matrices $\gamma^0 = \sigma^3$, $\gamma^1 = i\sigma^1$. The explicit form of two-component spinor $\Psi_{\lambda p}(x)$ is expressed as

$$\Psi_{\lambda p}(x) = \begin{pmatrix} f_{\lambda p}(x) \\ g_{\lambda p}(x) \end{pmatrix}. \quad (6)$$

Here the second subscript p indicates the parity of the spinor. With this, Dirac equation is written as a system of first-order differential equations for $f_{\lambda p}(x)$ and $g_{\lambda p}(x)$

$$\frac{d}{dx} f_{\lambda p} + \left[E_\lambda + \mu - V(x)\right] g_{\lambda p} = 0, \quad (7)$$

and

$$\frac{d}{dx} g_{\lambda p} - \left[E_\lambda - \mu - V(x)\right] f_{\lambda p} = 0. \quad (8)$$

Since $V(x)$ is even function of x, one can show that $(f_{\lambda p}(-x), -g_{\lambda p}(-x))^T$ is also a solution of (5) if $(f_{\lambda p}(x), g_{\lambda p}(x))^T$ is its solution, where the superscript T denotes matrix transposition. Therefore the components of the even-parity solution

$$\Psi_{\lambda e}(x) = \begin{pmatrix} f_{\lambda e}(x) \\ g_{\lambda e}(x) \end{pmatrix} \quad (9)$$

at region $x < 0$ have the reflections

$$f_{\lambda e}(x) = f_{\lambda e}(-x), \quad g_{\lambda e}(x) = -g_{\lambda e}(-x). \quad (10)$$

Similarly, the components of odd-parity solution at region $x < 0$ have the reflections

$$f_{\lambda o}(x) = -f_{\lambda o}(-x), \quad g_{\lambda o}(x) = g_{\lambda o}(-x). \quad (11)$$

These equalities provides a convenient method to obtain solutions at $x < 0$ for a definite parity. The differential equations at regions of $V(x) = 0$ can be decoupled into

$$\frac{d^2}{dx^2} f_{\lambda p} + k^2 f_{\lambda p} = 0, \quad (12)$$

and

$$\frac{d^2}{dx^2} g_{\lambda p} + k^2 g_{\lambda p} = 0 \quad (13)$$

with $k = \sqrt{E_\lambda^2 - \mu^2} \ge 0$. Thus the asymptotic solutions of scattering state of f for positive-energy ($E_\lambda > \mu$) are

$$f_{\lambda e}(x) \stackrel{|x|\to\infty}{\longrightarrow} \sqrt{\frac{E_\lambda + \mu}{2\pi k}} \cos\left(k|x| + \delta_e\right), \quad (14)$$

$$f_{\lambda o}(x) \stackrel{|x|\to\infty}{\longrightarrow} \epsilon_x \sqrt{\frac{E_\lambda + \mu}{2\pi k}} \sin\left(k|x| + \delta_o\right), \quad (15)$$

where $\epsilon_x = 1(-1)$ for positive (negative) x, δ_e (δ_o) is the phase shift of even-(odd-)parity solution, and the normalization constant $\sqrt{(E_\lambda + \mu)/2\pi k}$ is determined by the normalization condition of $\delta(E_\lambda - E_{\lambda'})$ for free particles. Substituting (14) and (15) into (7), one obtains for $E_\lambda > \mu$

$$g_{\lambda e}(x) \stackrel{|x|\to\infty}{\longrightarrow} \epsilon_x \sqrt{\frac{E_\lambda - \mu}{2\pi k}} \sin\left(k|x| + \delta_e\right), \quad (16)$$

$$g_{\lambda o}(x) \stackrel{|x|\to\infty}{\longrightarrow} -\sqrt{\frac{E_\lambda - \mu}{2\pi k}} \cos\left(k|x| + \delta_o\right). \quad (17)$$

Similar procedures give the entire asymptotic solutions

$$f_{\lambda e}(x) \stackrel{|x|\to\infty}{\longrightarrow} \sqrt{\frac{|E_\lambda| \pm \mu}{2\pi k}} \cos\left(k|x| + \delta_e\right), \quad (18)$$

$$f_{\lambda o}(x) \stackrel{|x|\to\infty}{\longrightarrow} \epsilon_x \sqrt{\frac{|E_\lambda| \pm \mu}{2\pi k}} \sin\left(k|x| + \delta_o\right), \quad (19)$$

and

$$g_{\lambda e}(x) \stackrel{|x|\to\infty}{\longrightarrow} \pm\epsilon_x \sqrt{\frac{|E_\lambda| \mp \mu}{2\pi k}} \sin\left(k|x| + \delta_e\right), \quad (20)$$

$$g_{\lambda o}(x) \stackrel{|x|\to\infty}{\longrightarrow} \mp\sqrt{\frac{|E_\lambda| \mp \mu}{2\pi k}} \cos\left(k|x| + \delta_o\right). \quad (21)$$

Here the upper (lower) sign denotes the solutions of the positive-energy (negative-energy) branch $E_\lambda \ge \mu$ ($E_\lambda \le -\mu$). These asymptotic solutions will be used to evaluate the change of the number of states around the potential

$V(x)$. For our purposes it is very convenient to write the spin wave function in a form

$$\Psi_\lambda(x) = \sum_{p=e,o} c_p \Psi_{\lambda p}(x) = \sum_{p=e,o} c_p \begin{pmatrix} f_{\lambda p}(x) \\ g_{\lambda p}(x) \end{pmatrix} \quad (22)$$

which include solutions of different parities and is the general solution of the Dirac equation (5). Here c_p's are coefficients dependent on the particular form required for Ψ_λ. Now we consider a large distance $|R|$, centred on the origin. By multiplying equation (5) through by $\Psi^\dagger_\lambda(x)$ and the corresponding equation for $\Psi^\dagger_\lambda(x)$ by $\Psi_\lambda(x)$, it follows after subtraction of the two equations

$$(E_{\lambda'} - E_\lambda)\Psi^\dagger_\lambda(x)\Psi_{\lambda'}(x) = -i\partial_x \left\{ \Psi^\dagger_\lambda(x)\alpha\Psi_{\lambda'}(x) \right\}. \quad (23)$$

Integrating over the whole x-axis, and using the divergence theorem, we find

$$\int_{-R}^{R} dx \Psi^\dagger_\lambda(x)\Psi_{\lambda'}(x) = \frac{1}{(E_{\lambda'} - E_\lambda)} \sum_{p=e,o} \left[f^*_{\lambda p}(x) g_{\lambda' p}(x) - g^*_{\lambda p}(x) f_{\lambda' p}(x) \right]_{-R}^{R}, \quad (24)$$

where one take $c_p = 1$, 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

$$\int_{-R}^{R} dx \Psi^{(0)\dagger}_\lambda(x)\Psi^{(0)}_{\lambda'}(x) = \frac{1}{(E_{\lambda'} - E_\lambda)} \sum_{p=e,o} \left[f^{(0)*}_{\lambda p}(x) g^{(0)}_{\lambda' p}(x) - g^{(0)*}_{\lambda p}(x) f^{(0)}_{\lambda' p}(x) \right]_{-R}^{R} \quad (25)$$

with $f^{(0)}_{\lambda p} = f_{\lambda p}(\delta_p = 0)$, and $g^{(0)}_{\lambda p} = g_{\lambda p}(\delta_p = 0)$. In solids, the electron (hole) states are occupied up to the Fermi energy E_f $(-E'_f)$. So the total change of the number of states ΔN around the potential $V(x)$ is obtained by integrating up to the Fermi energy E_f $(-E'_f)$

$$\Delta N = \lim_{R\to\infty} \lim_{E_{\lambda'}\to E_\lambda} \left(\int_{-E'_f}^{-\mu} + \int_{\mu}^{E_f} \right) dE_\lambda \times \int_{-R}^{R} dx \left[\Psi^\dagger_\lambda(x)\Psi_{\lambda'}(x) - \Psi^{(0)\dagger}_\lambda(x)\Psi^{(0)}_{\lambda'}(x) \right], \quad (26)$$

where the lower bound of the Fermi surface for negative-energy is denoted by $-E'_f$ for accounting of different levels generally. Since at large distances the wave function $\Psi_\lambda(x)$ must be unchanged except for the phase shifts in different parities, the wave functions f and g in (22) can be replaced by the asymptotic representations of (18–21). It follows that

$$\begin{aligned}
&\int_{-R}^{R} dx \left[\Psi^\dagger_\lambda(x)\Psi_{\lambda'}(x) - \Psi^{(0)\dagger}_\lambda(x)\Psi^{(0)}_{\lambda'}(x) \right] = \\
&\frac{1}{(E_{\lambda'} - E_\lambda)} \sum_{p=e,o} \left\{ \left[f^*_{\lambda p}(x) g_{\lambda' p}(x) - g^*_{\lambda p}(x) f_{\lambda' p}(x) \right]_{-R}^{R} \right. \\
&\qquad \left. - \left[f^{(0)*}_{\lambda p}(x) g^{(0)}_{\lambda' p}(x) - g^{(0)*}_{\lambda p}(x) f^{(0)}_{\lambda' p}(x) \right]_{-R}^{R} \right\} \\
&= \frac{-\epsilon_E C}{(E_{\lambda'} - E_\lambda)} \sum_{p=e,o} 2\cos\left[(k-k')R + \frac{1}{2}(\delta_p - \delta_{p'}) \right] \\
&\qquad \times \sin\left[\frac{1}{2}(\delta_p - \delta_{p'}) \right] \\
&+ \frac{D}{(E_{\lambda'} - E_\lambda)} \sum_{p=e,o} \epsilon_p \left\{ -2\sin\left[(k+k')R\right] \sin^2\left[\frac{1}{2}(\delta_p + \delta_{p'}) \right] \right. \\
&\qquad \left. + \cos\left[(k+k')R\right] \sin(\delta_p + \delta_{p'}) \right\}, \quad (27)
\end{aligned}$$

where

$$\begin{aligned}
C &= \frac{1}{2\pi\sqrt{kk'}} \left\{ \left[(|E_\lambda| + \mu)(|E_{\lambda'}| - \mu) \right]^{1/2} \right. \\
&\quad \left. + \left[(|E_\lambda| - \mu)(|E_{\lambda'}| + \mu) \right]^{1/2} \right\}, \quad (28) \\
D &= \frac{1}{2\pi\sqrt{kk'}} \left\{ \left[(|E_\lambda| + \mu)(|E_{\lambda'}| - \mu) \right]^{1/2} \right. \\
&\quad \left. - \left[(|E_\lambda| - \mu)(|E_{\lambda'}| + \mu) \right]^{1/2} \right\} \quad (29)
\end{aligned}$$

with $\epsilon_E \equiv 1(-1)$ for $E_\lambda \geq \mu$ $(E_\lambda \leq -\mu)$. Taking the limit $E_{\lambda'} \to E_\lambda$, equations (28) and (29) yield $C \to 1/\pi$ and $D/(E_{\lambda'} - E_\lambda) \to \epsilon_E(\mu/2\pi k^2)$ such that

$$\lim_{E_{\lambda'}\to E_\lambda} \frac{-\epsilon_E C}{(E_{\lambda'} - E_\lambda)} 2\cos\left[(k-k')R + \frac{1}{2}(\delta_p - \delta_{p'}) \right] \times \sin\left[\frac{1}{2}(\delta_p - \delta_{p'}) \right] \longrightarrow \frac{\epsilon_E}{\pi}\frac{d\delta_p}{dE_\lambda} \quad (30)$$

and

$$\begin{aligned}
&\lim_{E_{\lambda'}\to E_\lambda} \frac{\epsilon_p D}{(E_{\lambda'} - E_\lambda)} \left\{ -2\sin\left[(k+k')R\right] \sin^2\left[\frac{1}{2}(\delta_p + \delta_{p'}) \right] \right. \\
&\qquad \left. + \cos\left[(k+k')R\right] \sin(\delta_p + \delta_{p'}) \right\} \\
&\longrightarrow \epsilon_E \epsilon_p \frac{\mu}{2\pi k^2} \left[-2\sin(2kR)\sin^2\delta_p + \cos(2kR)\sin(2\delta_p) \right]. \quad (31)
\end{aligned}$$

Since $\delta_p(k = 0)/\pi$ always take integers or half integers in 1D space [20], $E_\lambda dE_\lambda = kdk$, and $\lim_{R\to\infty}\cos(2kR)$ oscillates, the integration of the second term in (31) $\lim_{R\to\infty} \int dE_\lambda \left[\cos(2kR)\sin 2\delta_p \right]/k^2 \to 0$. Moreover, due to $\lim_{R\to\infty}\sin(2kR)/\pi k=\delta(k)$, the integration of the first term in (31)

$$\lim_{R\to\infty}\left(\int_{-E_f'}^{-\mu}+\int_{\mu}^{E_f}\right)dE_\lambda\frac{-\epsilon_E\epsilon_p\mu\sin(2kR)\sin^2\delta_p}{\pi k^2}=\left(\int_{-E_f'}^{-\mu}+\int_{\mu}^{E_f}\right)dE_\lambda\epsilon_E\epsilon_p\mu\frac{-\delta(k)\sin^2\delta_p}{k}=-\frac{\epsilon_p}{2}\left[\sin^2\delta_p(\mu)-\sin^2\delta_p(-\mu)\right]. \quad (32)$$

Thus the difference of the number of states is found to be

$$\Delta N=\frac{1}{\pi}\sum_{p=e,o}\left\{\left[\delta_p(E_f)-\delta_p(\mu)+\delta_p(-E_f')-\delta_p(-\mu)\right]-\epsilon_p\frac{\pi}{2}\left[\sin^2\delta_p(\mu)-\sin^2\delta_p(-\mu)\right]\right\}. \quad (33)$$

The sine functions at the zero-momentum is important and used to count the marginal (half) bound states with the phase shift $\pi/2$ at $E_\lambda=\pm\mu$ [20,22]. Comparing with the nonrelativistic FT (3), we see that the negative-energy branch turns out to be significant. Positive (negative) ion will attract (repulse) electrons (holes), and repulse (attract) holes such that the variance of states is together the effect of two kinds of particles.

3 The change in energy due to an impurity in relativistic 1D systems

We discuss the change in energy in the presence of an impurity here. By equations (18–21), one see that the wave functions undergo phase shifts. This fact entails a change of the kinetic energy of particles. To quantify the change, we first consider the solutions of even parity and notice that the reasonable requirement $\Psi_{\lambda e}^{(0)}(x)\Big|_{\text{B.C.}}=0$ for a Dirichlet boundary condition in an 1D system gives

$$k\,|L|=\frac{(2n+1)\pi}{2},\quad n=0,1,2,\cdots \quad (34)$$

for function $f_{\lambda e}^{(0)}$, and

$$k\,|L|=n\pi,\quad n=1,2,\cdots \quad (35)$$

for function $g_{\lambda e}^{(0)}$. Here $|L|$ is used to denote the boundary of 1D system. The number dn of allowed states between k and $k+dk$ is given by differentiating both members of (34) and (35) which yield $|L|\,dk=\pi dn$. Thus the unperturbed density of states for even parity reads

$$D(k)=\frac{dn}{dk}=\frac{|L|}{\pi}. \quad (36)$$

On the other hand, the boundary condition for perturbed wave functions vanish at $x=|L|$ yield

$$k\,|L|+\delta_e(k)=\frac{(2n+1)\pi}{2},\quad n=0,1,2,\cdots \quad (37)$$

for function $f_{\lambda e}$, and

$$k\,|L|+\delta_e(k)=n\pi,\quad n=1,2,\cdots \quad (38)$$

for function $g_{\lambda e}$. From equations (34), (37) and (35), (38), we find that the change Δk of the wave number of an even-parity spin-1/2 particle (antiparticle) is $\Delta k\,|L|=-\delta_e(k)$ ($\delta_e(k)$) and the change in energy are

$$\Delta E|_{e^-}=\frac{k\Delta k}{E_\lambda}=\frac{-k\;\delta_e(k)|_{e^-}}{|L|\sqrt{k^2+\mu^2}} \quad (39)$$

and

$$\Delta E|_{e^+}=\frac{k\Delta k}{E_\lambda}=\frac{k\;\delta_e(k)|_{e^+}}{|L|\sqrt{k^2+\mu^2}}, \quad (40)$$

where we used e^- (e^+) to denote the particle (antiparticle). Similarly, an odd-parity spin-1/2 particle (antiparticle) gives the variation of energy as follows:

$$\Delta E|_{e^-}=\frac{k\Delta k}{E_\lambda}=\frac{-k\;\delta_o(k)|_{e^-}}{|L|\sqrt{k^2+\mu^2}} \quad (41)$$

and

$$\Delta E|_{e^+}=\frac{k\Delta k}{E_\lambda}=\frac{k\;\delta_o(k)|_{e^+}}{|L|\sqrt{k^2+\mu^2}}. \quad (42)$$

The total change in energy in the presence of the impurity in 1D relativistic spin-1/2 systems is then given by

$$\Delta E=\sum_{p=e,o}\left(\int_0^{k_f}\Delta E|_{e^-}\frac{|L|}{\pi}dk-\int_0^{k_f'}\Delta E|_{e^+}\frac{|L|}{\pi}dk\right)=-\sum_{p=e,o}\left(\int_0^{k_f}\frac{k\;\delta_p(k)|_{e^-}}{|L|\sqrt{k^2+\mu^2}}\frac{|L|}{\pi}dk+\int_0^{k_f'}\frac{k\;\delta_p(k)|_{e^+}}{|L|\sqrt{k^2+\mu^2}}\frac{|L|}{\pi}dk\right), \quad (43)$$

where $|L|/\pi$ is the density of states of particles and antiparticles. This result is an 1D relativistic generalization of Fumi theorem [23] where the change of the kinetic energy due to the impurity for non-relativistic systems was studied. It is worthy to note that in the massless limit, the change in energy becomes a more compact representation

$$\Delta E=-\frac{1}{\pi}\sum_{p=e,o}\left(\int_0^{k_f}\delta_p(k)|_{e^-}\,dk+\int_0^{k_f'}\delta_p(k)|_{e^+}\,dk\right), \quad (44)$$

which states the variance of system energy due to the impurity can be completely ascertained as soon as the phase shifts is decided.

4 Discussions

4.1 The relation with the relativistic Levinson theorem

In 1949, Levinson established a theorem in non-relativistic quantum mechanics [21]. Well-known as the Levinson theorem, it clarifies the relation between the phase shifts of a quantum particle scattered by a short range potential and the number of bound states therein. In 3D systems, the theorem can be described as

$$\delta_l(0) = n_l\pi, \quad l = 0, 1, 2, \cdots \tag{45}$$

where $\delta_l(0)$ denotes the phase shift of scattered state with a momentum k at the threshold ($k = 0$) in the angular momentum channel l, and n_l is the total number of bound states in the angular momentum channel l allowed by the short range potential. When the angular momentum $l = 0$, the theorem must be modified to

$$\delta_0(0) = (n_0 + 1/2)\pi, \tag{46}$$

due to the existence of a zero-energy resonance (a half-bound state) [22]. The theorem is one of the most interesting and beautiful results in non-relativistic quantum theory. The subject was then studied and generalized by many authors (e.g. [22] and reference therein). In [20], the 1D Levinson theorem is generalized to Dirac particles moving in a cutoff potential $V(x) = 0$ for $x \geq a$, and obtain relation between the number of bound states with even (odd) parity, n_e (n_o), and the phase shifts $\delta_e(\pm E_\lambda)$ $[\delta_o(\pm E_\lambda)]$ of scattering states with the same parity at zero-momentum as follows:

$$[\delta_e(\mu) + \delta_e(-\mu)] + \frac{\pi}{2}\left[\sin^2\delta_e(\mu) - \sin^2\delta_e(-\mu)\right] = n_e\pi, \tag{47}$$

and

$$[\delta_o(\mu) + \delta_o(-\mu)] - \frac{\pi}{2}\left[\sin^2\delta_o(\mu) - \sin^2\delta_o(-\mu)\right] = n_o\pi. \tag{48}$$

Since the potential is set up in the free space, the phase shifts at the upper and lower bounds of energy can be ruled out by a relation $\delta_p(\infty) + \delta_p(-\infty) = 0$ ($p = e, o$). However, in the 1D fermionic many body systems, the equality does not hold due to restrictions of Fermi surfaces. The Levinson theorem must be modified by

$$\left[\delta_e(\mu) - \delta_e(E_f) - \delta_e(-E_f') + \delta_e(-\mu)\right] + \frac{\pi}{2}\left[\sin^2\delta_e(\mu) - \sin^2\delta_e(-\mu)\right] = n_e\pi, \tag{49}$$

and

$$\left[\delta_o(\mu) - \delta_o(E_f) - \delta_o(-E_f') + \delta_o(-\mu)\right] - \frac{\pi}{2}\left[\sin^2\delta_o(\mu) - \sin^2\delta_o(-\mu)\right] = n_o\pi. \tag{50}$$

Comparing (33) with these two equalities, one find the relation between the difference of scattering states and the Levinson theorem of the specified potential

$$\Delta N + \sum_{p=e,o} n_p = 0. \tag{51}$$

The relation 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, equation (51) expresses that there is an upper bound on ΔN which depends on the potential $V(x)$. A finite deep potential may have finite bound states such that the change of the number of states is finite. The necessary and sufficient condition to be satisfied by the potential in the relativistic Levinson theorem is still an open problem.

4.2 Density oscillation in one dimensional relativistic systems

There is another way to express the change of the number of states, which enables us to indicate the variance of the density of states. It may be expressed as

$$\Delta N = \int_{-\infty}^{\infty} dx\,[\rho(x) - \rho_0(x)]\,, \tag{52}$$

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

$$\delta\rho = \int_{k<k_f} \frac{dk}{2\pi}\left[\left|\Psi_\lambda(x)\right|^2 - \left|\Psi_\lambda^{(0)}(x)\right|^2\right]. \tag{53}$$

At large distances, with equations (18–21), it is found to be

$$\delta\rho = \frac{1}{2\pi}\sum_{p=e,o}\int_{k<k_f} dk\left[-\epsilon_p\epsilon_E\frac{\mu}{\pi k}\sin(2kx + \delta_p)\sin\delta_p\right]. \tag{54}$$

The wave vector integral 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 $\delta_p = \delta_p(k_f) + (k - k_f)(d\delta_p/dk)$, which yields

$$\lim_{|x|\to\infty}\delta\rho = -\frac{1}{2\pi}\sum_{p=e,o}\epsilon_p\epsilon_E\frac{\mu}{\pi}\,\mathrm{Si}(2k_f x)\sin\delta_p(k_f). \tag{55}$$

Here $\mathrm{Si}(z) = \int_0^z(\sin t/t)dt$ is sine integral [24] which is a regular oscillatory function but gradually decays to zero as $|x| \to \infty$. The Fermi wave number k_f must be replaced by k_f' (corresponding to $-E_f'$) when the negative-energy branch is written out. By comparing with the 2D and 3D systems, where the density oscillates with a period of $2k_f$ and decreases in amplitude as r^{-2} (2D) and r^{-3} (3D), here it tends to zero only as $1/x$, thus it is a more significant effect, and the power is consistent with that in [18]. Another remarkable result is that two branches of energy have the opposite oscillating phases. The negative-energy branch will tend to suppress the oscillation for the same phase shifts.

4.3 The 1D FSR for massless Dirac fermions

Since the Lorentz group often occurs as an approximate symmetry for low energy excitation for 1D fermions in metals and antiferromagnets [19], relativistic spectra appear naturally for massless conduction electrons in such systems. It is interesting to discuss the FSR in the condition of the fermion mass tends to zero. From (33), one see that as the effective mass tends to zero, the contribution of the final term to ΔN at zero-momentum vanishes, and ΔN becomes

$$\Delta N = \frac{1}{\pi} \sum_{p=e,o} \left[\delta_p(E_f) + \delta_p(-E_f') - 2\delta_p(0)\right], \qquad (56)$$

which indicates the phase shifts of particle and anti-particle at zero-momentum merge to become twice. Another interesting result about massless fermions comes from (54). 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. This argument probably enables us to decide the magnitude of effective mass in a non-ideal effective relativistic 1D system via Friedel oscillation at far zones.

4.4 Extension the potential to more general case

Although in the procedure of our proof we assume the potential must be short range, we do not specify the radius a beyond which $V(x) = 0$. Hence we expect that the FT given in the article should be valid for a very general potential as long as the potential decrease rapidly enough when $|x| \to \infty$.

4.5 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 modern microelectronic technique, it seems to us that we can control the number of states around an impurity. The reason is that today quantum dots can be carved out of a 1D electron gas such that the change of the number of states around them can be counted according to (51). This may be useful in controlling spin bus (a controllable coupler of many qubits) via nonlocal spin interaction [25].

5 Conclusions

In this paper, the 1D Friedel sum rule is generalized to the relativistic spin-1/2 systems. The change in energy of the spin-1/2 system in the presence of an impurity is studied. The relation of the rule with the 1D relativistic Levinson theorem is presented. Density oscillations of relativistic spin-1/2 systems are discussed. Since in 1D metals the low energy effective theory for conduction electrons is described by the Dirac's relativistic theory [19] we hope the result is useful in studying the properties of 1D nanostrutures.

Appendix

Here we prove the Friedel sum rule for non-relativistic particles in 1D systems. Consider the 1D Schrödinger equation

$$\frac{\partial^2}{\partial x^2}\varphi(x) + \left[k^2 - 2mV(x)\right]\varphi(x) = 0 \qquad (57)$$

with $k = \sqrt{2mE} \geq 0$. For a symmetric potential $V(x) = V(-x)$ when $|x| \leq a$ and $V(x) = 0$ when $|x| \geq a$, two linearly independent scattering solutions $\varphi_1(x)$ and $\varphi_2(x)$ are given by

$$\varphi_1(x) = \begin{cases} T(k)e^{ikx}, & x \geq a \\ e^{ikx} + R(k)e^{-ikx}, & x \leq -a \end{cases} \qquad (58)$$

and

$$\varphi_2(x) = \begin{cases} e^{-ikx} + R(k)e^{ikx}, & x \geq a \\ T(k)e^{-ikx}, & x \leq -a \end{cases}, \qquad (59)$$

where $\varphi_1(x)$ and $\varphi_2(x)$ represent the incident direction is from left and right, and $R(k)$ and $T(k)$ denote the transmission and reflection coefficients. For our purposes, the solutions of definite parities can be obtained by linear combinations of equations (58) and (59), which yield

$$\varphi_e(x) = \begin{cases} (1/\sqrt{\pi})e^{i\delta_e}\cos(kx + \delta_e), & x \geq a \\ (1/\sqrt{\pi})e^{i\delta_e}\cos(kx - \delta_e), & x \leq -a \end{cases} \qquad (60)$$

and

$$\varphi_o(x) = \begin{cases} (i/\sqrt{\pi})e^{i\delta_o}\sin(kx + \delta_o), & x \geq a \\ (i/\sqrt{\pi})e^{i\delta_o}\sin(kx - \delta_o), & x \leq -a \end{cases}. \qquad (61)$$

Here the phase shifts are defined as

$$e^{2i\delta_{e,o}} \equiv T \pm R, \qquad (62)$$

and the normalization constants are chosen as the wave functions for the free particle, i.e. the case $\delta_e = 0 = \delta_o$, are normalized to $(1/2)[\delta(x - x') \pm \delta(x + x')]$. The total change of the number of states ΔN around the potential $V(x)$ is obtained by integrating from $-L$ to L and up to the Fermi surface k_f

$$\Delta N = \lim_{L\to\infty} \sum_{p=e,o} \int_0^{k_f} dk \int_{-L}^{L} dx \left[|\varphi_p(x)|^2 - \left|\varphi_p^{(0)}(x)\right|^2\right], \qquad (63)$$

where $\varphi_p^{(0)}(x)$ denotes the state of a free particle with a definite parity. The integral on x can be evaluated by the following procedures. By multiplying (57) through by φ_p^* and the corresponding equation for φ_p^* by φ_p, it follows that

$$\frac{\partial}{\partial x}\left[\varphi_p^*(k', x)\frac{\partial}{\partial x}\varphi_p(k, x) - \varphi_p(k, x)\frac{\partial}{\partial x}\varphi_p^*(k', x)\right] = \left(k'^2 - k^2\right)\varphi_p^*(k', x)\varphi_p(k, x), \qquad (64)$$

where the dependence of φ_p on the variables k, x is expressed explicitly. By taking the limit $k' \to k$, it can be shown that

$$|\varphi_p(x)|^2 = \frac{1}{2k}\frac{\partial}{\partial x}\left[\frac{\partial \varphi_p}{\partial x}\frac{\partial \varphi_p^*}{\partial k} - \varphi_p\frac{\partial^2 \varphi_p^*}{\partial x \partial k}\right]. \qquad (65)$$

Thus, for large L, using equations (60) and (61), one find

$$\sum_{p=e,o}\int_{-L}^{L}dx\left[\left|\varphi_p(x)\right|^2-\left|\varphi_p^{(0)}(x)\right|^2\right]=$$
$$\frac{1}{\pi}\sum_{p=e,o}\left\{\frac{d\delta_p}{dk}+\epsilon_p\frac{1}{2k}\left[\sin\left(2kL+2\delta_p\right)-\sin(2kL)\right]\right\}$$
$$=\frac{1}{\pi}\sum_{p=e,o}\left\{\frac{d\delta_p}{dk}-\epsilon_p\pi\sin^2\delta_p\frac{\sin(2kL)}{\pi k}+\epsilon_p\frac{1}{2k}\sin(2\delta_p)\cos(2kL)\right\}. \quad (66)$$

Since $\lim_{L\to\infty}\sin(2kL)/\pi k=\delta(k)$ and $\lim_{L\to\infty}\cos(2kL)$ oscillates, the integration over k in (63) can be carried out, which yields the 1D Friedel sum rule

$$\Delta N=\frac{2}{\pi}\sum_{p=e,o}\left[\delta_p(E_f)-\delta_p(0)-\epsilon_p\frac{\pi}{2}\sin^2\delta_p(0)\right], \quad (67)$$

where the factor of 2 is spin degeneracy and we have used the fact $\delta_p(0)/\pi$ always take half-integers [22] such that the integration in the final term in (66)

$$\lim_{L\to\infty}\int_0^{k_f}dk\frac{1}{k}\sin(2\delta_p)\cos(2kL)\longrightarrow 0. \quad (68)$$

As usual, $\sin^2\delta_p(0)$ accounts for the half bound state which has the phase shift $\pi/2$ at the critical energy $E=0$. The interesting relation between the number of bound states and the change in the scattering states ΔN can be established by the completeness relationship

$$\sum_{p=e,o}\sum_{i=1}^{N_p}\Psi^*_{p,E_i}(x)\Psi_{p,E_i}(x')+\sum_{p=e,o}\int_0^{k_f}dk\varphi_p^*(k,x)\varphi_p(k,x')=\delta(x-x'). \quad (69)$$

Here N_p and $\Psi_{p,E_i}(x)$ are the bound-state number and eigenfunction with a definite parity. Subtracting the relation from the free particles solutions $\varphi_p^{(0)}(k,x)$, setting $x=x'$ and integrating from $-L$ to L, we obtains the equality

$$N=N_e+N_o=-\Delta N \quad (70)$$

which implies the number of the bound states

$$N=\frac{2}{\pi}\sum_{p=e,o}\left[\delta_p(0)-\delta_p(E_f)+\epsilon_p\frac{\pi}{2}\sin^2\delta_p(0)\right]. \quad (71)$$

This is the Levinson theorem for non-relativistic particles in 1D systems. Different from the single particle case [26], the phase shifts at Fermi energy play an important role.

References

1. J. Friedel, J. Philos. Mag. **43**, 153 (1952); J. Friedel, Adv. Phys. **3**, 446 (1953); J. Friedel, Nuovo Cim. Supl. **7**, 287 (1958)
2. J.M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, New York, 1972), p. 159
3. G.D. Mahan, *Many-Particle Physics* (Plenum Press, New York, 2000), p. 195
4. J.S. Langer, V. Ambegaokar, Phys. Rev. **121**, 1090 (1961)
5. D.C. Langreth, Phys. Rev. **150**, 516 (1966)
6. H. Johannesson, N. Andrei, C.J. Bolech, Phys. Rev. B **68**, 075112 (2003)
7. H. Johannesson, C.J. Bolech, N. Andrei, Phys. Rev. B **71**, 195107 (2005)
8. D.H. Lin, Phys. Rev. A **72**, 012701 (2005)
9. B.J. van Wees, H. van Houten, C.W.J. Beenakker, J.G. Williamson, L.P. Kouwenhoven, D. van der Marel, C.T. Foxon, Phys. Rev. Lett. **60**, 848 (1988)
10. D.A. Wharam, T.J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J.E.F. Frost, D.C. Hasko, D.C. Peacock, D.A. Ritchie, G.A.C. Jones, J. Phys. C **21**, L209 (1988)
11. Z.I. Alferov, Rev. Mod. Phys. **73**, 767 (2001)
12. J.N. Crain, D.T. Pierce, Science **307**, 703 (2005)
13. G. Rubio, N. Agrait, S. Vieira, Phys. Rev. Lett. **76**, 2302 (1996)
14. A. Rosch, N. Andrei, Phys. Rev. Lett. **85**, 1092 (2000)
15. *Semiconductor Spintronics and Quantum Computation*, edited by D.D. Awschalom, N. Samarth, D. Loss (Springer-Verlag, Berlin, 2002)
16. A.V. Moroz, C.H.W. Barnes, Phys. Rev. B **60**, 14272 (1999); F. Mireles, G. Kirczenow, Phys. Rev. B **64**, 024426 (2001); J.C. Egues, G. Burkard, D. Loss, Phys. Rev. Lett. **89**, 176401 (2002)
17. M. Governale, U. Zülicke, Phys. Rev. B **66**, 073311 (2002)
18. R. Egger, H. Grabert, Phys. Rev. Lett. **75**, 3505 (1995)
19. A.M. Tsvelik, *Quantum Field Theory in Condensed Matter Physics* (Cambridge, 2003), Ch. 14
20. Q.G. Lin, Eur. Phys. J. D **7**, 515 (1999)
21. N. Levinson, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **25**, No. 9 (1949)
22. R.G. Newton, J. Math. Phys. **1**, 319 (1960); R.G. Newton, J. Math. Phys. **18**, 1348 (1977); R.G. Newton, J. Math. Phys. **18**, 1582 (1977); R.G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, New York, 1982)
23. F.G. Fumi, Phil. Mag. **46**, 1007 (1955)
24. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970), p. 231
25. N.J. Craig, J.M. Taylor, E.A. Lester, C.M. Marcus, M.P. Hanson, A.C. Gossard, Science **304**, 565 (2004); L.I. Glazman, R.C. Ashoori, Science **304**, 524 (2004)
26. M. Sassoli de Bianchi, J. Math. Phys. **35**, 2719 (1994)