Violation of general Friedel sum rule in mesoscopic systems

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In the wake of a new kind of phase generally occurring in mesoscopic transport phenomena, we discuss the validity of Friedel sum rule in the presence of this phase. We find that the general Friedel sum rule may be violated.

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With large scale research in Mesoscopic Physics over the last few decades, many of the well established notions of Condensed Matter Physics has been found to be violated in mesoscopic samples. Breakdown of Onsager reciprocity relation [1], violation of Ohms law [2], absence of material specific quantities like resistivity [3], violation of Hund’s rule [4] etc., are a few such examples. The purpose of this work is to show the violation of Friedel sum rule in mesoscopic systems.

Friedel sum rule relates the density of states inside a fixed potential scatterer to the scattering phase shifts [5]. A deduction of the sum rule can be found in many text books [6,7] and intuitively it can be understood as follows. Consider for example a fixed spherically symmetric impurity. Now we enclose it in a larger spherically symmetric volume. In an energy interval dE, the number of states depend on the number of times the specific boundary conditions can be fulfilled by the wave function of the electron. So when the energy is changed, it introduces a phase shift of the electron wave function and so changes the number of times the specific boundary condition can be satisfied. Hence as defined in Eq. 2

\[
\frac{\partial \theta}{\partial E} = \pi \rho',
\]

This can be extended to the partial wave analysis of scattering states and many important issues can be understood in terms of the Friedel sum rule [8]. In case of a non-spherical scatterer or non-spherical Fermi surface, the scattering matrix is in general an NxN matrix. For any such general NxN scattering matrix \( S \), the Friedel sum rule can be written as

\[
\theta = \sum_{\xi} \xi \exp(2i\xi) \text{ being the eigenvalues of the scattering matrix } S. \text{ This can be further written in a compact form as}
\]

\[
\frac{1}{2i} \frac{\partial}{\partial E} \ln(\det[S]) = \pi \rho'.
\]

For one-dimensional systems where the scattering matrix is 2x2, the Friedel sum rule was thought to be further simplified to give

\[
\frac{\partial \arg(t)}{\partial E} = \pi \rho',
\]

where \( t \) is the transmission amplitude but this is not true. Recently a new phase has been discussed in Ref. [10] for scattering by a stub where the scattering matrix is 2x2, and it is believed [11] that this phase is also observed in mesoscopic systems experimentally [12]. This phase is a general feature of transmission zeroes that always occur in Fano resonances in Quantum Wires and Dots, the stub structure being the simplest example [13]. It was shown in Ref. [11] that the phase slips is a new phase associated with the violation of parity effect because it is different from Aharonov-Bohm phase, statistical phase and phase due to wave-like motion of electrons depending on their wave vector or energy. Had it not been different from the other three phases, parity effect would not have been violated [10]. The specialty of this phase is that it is discontinuous as a function of energy, i.e., the phase of the wavefunction changes by \( \pi \) although its energy does not change. To be more precise this phase does not originate from change in wave-vector due to change in energy. Hence in view of the discussions before Eq. 1 one can question the validity of Friedel sum rule in the presence of this phase [13]. We shall give a pictorial description of this phase later (short-dashed and long-dashed curves in Fig. 1).

The scattering matrix for the stub is

\[
S = \begin{pmatrix} r & t \\ t & r \end{pmatrix}
\]

where \( r \) and \( t \) are reflection and transmission amplitudes across the stub and are

\[
r = \frac{\cos[kL]}{-\cos[kL] + 2i\sin[kL]}
\]

(6)

and

\[
t = \frac{(2i\sin[kL])/(\cos[kL] - 2i\sin[kL])}. \quad \text{ (7)}
\]

The eigenvalues of the S matrix are

\[
(\cos[kL] + 2i\sin[kL])/(\cos[kL] + 2i\sin[kL]) \quad \text{ and } \quad -1
\]

(8)

Hence as defined in Eq. 2

\[
\theta = \frac{1}{2} \text{ArcTan}[\frac{-4\cos[kL]\sin[kL]}{(-\cos[kL]^2 + 4\sin[kL]^2)}]
\]

(9)
In Fig. 1 we plot $\theta$ (solid curve), $\arg(t)$ (short-dashed curve) and $\arg(r)$ (long-dashed curve) (given in Eqs. 6, 7 and 9) versus $kL$. It can be seen that $\arg(t)$ and $\arg(r)$ show discontinuous jumps and drops by $\pi$, but they cancel in such a way that $\theta$ is continuous and monotonously increasing. Hence one finds that the Friedel sum rule (Eqs. 2 and 3) is not violated although because of the discontinuous slips in $\arg(t)$ Eq. 4 is obviously violated because density of states can never be infinite while the LHS of Eq. 4 can be infinite. And hence one can say that so far no one has found a violation of Friedel sum rule (Eqs. 2 and 3). We shall show the violation of the Friedel sum rule in the presence of this new phase.

Transport across the stub structure has acquired a lot of importance recently\(^\text{1,3-4}\). All analysis so far are based on calculations with a hard wall boundary condition (an infinite step barrier potential or an infinite step well potential) at the dead end of the stub (we refer to it as the hard walled stub and for which Eqs. 6, 7, 8 and 9 are derived). An infinite potential well at the dead end of the stub reflects an incident electron with unit probability. Now a small perturbation from this would be a finite but very deep potential well at the dead end of the stub (soft walled stub). Electrons are almost entirely reflected from the end of the stub and a negligible fraction escapes. Dephasing can also give similar escape probability. The scattering problem in this case is depicted in Fig. 2 and also explained in the figure caption. It is solved using the mode matching technique or Griffith’s boundary conditions\(^\text{5}\), that give the continuity of wavefunction and the conservation of currents at the junctions. In this case the transmission zero in x-direction is replaced by a minimum\(^\text{6}\). We first intend to understand what happens to the discontinuous phase change that occur due to transmission zeroes in this case. So in Fig. 3 we plot transmission coefficient $T = |t|^2$ (solid curve) and the argument of the transmission amplitude $t$ (short-dashed curve) in x direction, versus $kL$ for an almost hard walled stub. The transmission coefficient shows very deep minima and at the same points $\arg(t)$ show very sharp but continuous drops. For the completely hard walled stub there is an exact zero and associated with it a discontinuous slip by $\pi$ as shown in Fig. 1. In the same figure (Fig. 3) we also plot transmission coefficient in the x-direction (dash-dotted curve) and the corresponding argument of the transmission amplitude (long-dashed curve) versus $kL$ for a very soft walled stub. At the points where the solid curve show very deep minima, dash-dotted curve show shallow minima. Also the fast phase drops change over to a slower decrease.

Having understood the phase slips further we move on to the three prong scatterer (Fig. 4) that is often encountered in mesoscopic systems\(^\text{7}\) including the experimental set up of Ref.\(^\text{8}\) and many such similar experiments. The scattering problem in this case is described in the figure caption. From the continuity of wavefunctions (first Griffith’s boundary condition) we get the following equations (variables and parameters are defined in Fig. 4 and it’s caption).

\[
1 + r = a \exp[-iqL_1] + b \exp[iqL_1]; \quad a + b = c + d; \\
a + b = f + g, \quad c \exp[iqL_2] + d \exp[-iqL_2] = e; \\
f \exp[iqL_3] + g \exp[-iqL_3] = h. \quad (10)
\]

And from the second Griffith’s boundary condition which is the conservation of currents at the junctions ($\Sigma \frac{\partial \rho}{\partial x} = 0$, that can be derived from current conservation, here $\psi_i$ is a wavefunction at a junction, $x_i$ is coordinate at that junction, and the sum over $i$ stands for all such wavefunctions incoming or outgoing at a junction, the convention followed is that currents flowing into the junction is positive while currents flowing out of the junction is negative) we get the following equations.

\[
k - kr - qa \exp[-iqL_1] + qb \exp[iqL_1] = 0; \\
a - b - c + d - f + g = 0; \\
qc \exp[iqL_2] - qd \exp[-iqL_2] - ke = 0; \\
qf \exp[iqL_3] - qg \exp[-iqL_3] - kh = 0. \quad (11)
\]

Thus we have 9 equations and exactly 9 unknown quantities ($a, b, c, d, e, f, g, h$ and $r$) and so the problem is completely defined. Once the unknowns are solved, the wavefunction is known at all points exactly and so the density of states as well as the scattering matrix can be calculated exactly. The scattering matrix in this case is

\[
S = \begin{pmatrix}
t_{11} & t_{12} & t_{13} \\
t_{21} & t_{22} & t_{23} \\
t_{31} & t_{32} & t_{33}
\end{pmatrix}.
\quad (12)
\]

Here $t_{11}=r=\text{transmission amplitude to the first prong}$ when the incident beam is from the first prong. $t_{12} = e$ is the transmission amplitude to the second prong when the incident beam is from the first prong. $t_{13} = h$ is the transmission amplitude to the third prong when the incident beam is from the first prong. The other matrix elements are to be calculated when similar incident beam of unit flux is from the other two directions in Fig. 4. For the case of Fig. 4, the partial density of states is given by the following expression

\[
\rho_1 = \pi \rho_1' = \frac{\pi}{h} \left[ \int_{-L_1}^{0} |a \exp[iqx] + b \exp[-iqx]|^2 dx + \right. \\
\left. \int_{0}^{L_2} |c \exp[iqy] + d \exp[-iqy]|^2 dy + \int_{0}^{L_3} |f \exp[iqz] + g \exp[-iqz]|^2 dz \right],
\quad (13)
\]
where \( v = \hbar k / m \). \( a, b, c, d, f \) and \( g \) are determined from Eqs. 10 and 11. \( \rho_2 \) and \( \rho_3 \) are to be evaluated similarly when the incident beam is from the other two directions in Fig. 4, and \( \rho = \rho_1 + \rho_2 + \rho_3 \). For the symmetric three prong scatterer \((L_1 = L_2 = L_3 = L)\), the antiresonances are almost cancelled by the resonances but still a violation of Eq. 2 or 3 can be seen at low energy. This cancelling effect of resonance and antiresonance can be avoided by choosing incommensurate values of \((L_1 + L_2)\) and \(L_2\), i.e., for asymmetric configurations. We will now go to the asymmetric configuration and demonstrate a large difference between \( \tau = \partial \theta / \partial E = \frac{1}{2} \frac{\partial}{\partial E} \ln [\text{Det}[S]] \) and \( \rho = \pi \rho' \) at large energies \((E \approx V)\). This is shown in Fig. 5. We want to emphasize that at very high energy, compared to the energy scale \( V \) in the system, when multiple scattering and the new phase becomes insignificant, we recover Friedel sum rule perfectly. But when this new phase is present at energies \((E < V)\), there is a large difference between \( \tau \) and \( \rho \) and hence a complete violation of Friedel sum rule. In Fig. 5, \( \tau \) or \( \partial \theta / \partial E \), can become substantially negative, i.e., \( \theta \) can undergo a drop like \( \arg(t) \) in Fig. 3. The new phase need not always appear as a drop but can also appear as a rise and then the LHS of Eq. 3 can remain positive all the time while deviating from the RHS of Eq. 3. This is shown in Fig 6.

Thus our exact calculation of density of states and scattering matrix elements show the deviation of \( \frac{1}{2} \frac{\partial}{\partial E} \ln [\text{Det}[S]] \) from \( \pi \rho' \) in the presence of phase slips. The phase slips are a general feature of Quantum wires with defects \([12]\) and Quantum Dots and these phase slips are at the origin of drops in \( \theta \) and hence deviation or violation of Friedel sum rule. Only 2x2 S-matrix is a special case where as shown in Fig. 1 some scattering matrix elements undergo a phase jump and some undergo a phase drop in such a manner that they cancel and the phase slips do not affect \( \ln [\text{Det}[S]] \) or \( \theta \). The general feature is that they do not cancel and Friedel sum rule gets violated. The attractive potential in the three prong scatterer offsets the symmetry between the phase jumps and the phase drops so that they do not cancel each other.

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[5] For charge neutral systems there is a one to one correspondence between density of states and accumulated charge in the field of a scatterer. In that case Friedel sum rule also relates scattering phase shifts to the displaced charge (see Ref. 8). There can be situations when charge neutrality is violated as in the case of R. Egger and H. Grabert, Phys. Rev. Lett. 79, 3463 (1997). However we will show a violation of Friedel sum rule at a more fundamental level i.e., density of states itself starts deviating from that predicted by Friedel sum rule.

Figure captions

**Fig. 1** \( \arg(r) \) (long-dashed curve), \( \arg(t) \) (short-dashed curve) and \( \theta \) (solid curve) for the hard wall stub. Length of the stub is \( L \) and it is taken to be the unit of length. We choose \( h = 2m = 1 \).

**Fig. 2** A scattering problem with conventional notations is depicted here. \( k = \sqrt{E} \) is the wave vector in the thin regions where the Quantum Mechanical potential is 0. \( q = \sqrt{E + V} \) is the wave vector in the thick regions where the Quantum Mechanical potential is \(-V\). \( x \) and \( y \) are coordinates and the origin of coordinates is also depicted in the figure. \( t \) and \( c \) are transmission amplitudes in \( x \) and \( y \) directions, respectively, while \( r \) is the reflection amplitude. Distance between points \( P \) and \( Q \) is \( L \).

**Fig. 3** The solid curve is transmission coefficient \( T = |t|^2 \) across the soft walled stub described in Fig. 2. The short-dashed curve is the phase of the transmission amplitude \( t \) across the stub. We choose \( V L^2 = -100 \) and plot the transmission coefficient \( T \) in dash-dotted curve. The phase of the transmission amplitude \( t \) is given by long-dashed curve.
Fig. 4 A scattering problem with conventional notations is depicted here. \( k = \sqrt{E} \) is the wave vector in the thin regions where the Quantum Mechanical potential is 0. \( q = \sqrt{E + V} \) is the wave vector in the thick regions where the Quantum Mechanical potential is \(-V\). \( x,y,z,u,v \) and \( w \) are coordinates and the origin of coordinates is also depicted in the figure. \( e \) and \( h \) are transmission amplitudes in respective directions, while \( r \) is the reflection amplitude. Distance between \((u=0)\) and \((x=0,y=0,z=0)\) is \( L_1 \). Distance between \((v=0)\) and \((x=0,y=0,z=0)\) is \( L_2 \). Distance between \((w=0)\) and \((x=0,y=0,z=0)\) is \( L_3 \).

Fig. 5 \( \rho \) (solid curve) and \( \tau = \frac{d\theta}{dE} = \text{LHS of Eq. 3} \) (dotted curve) versus \( kL \) for the scattering problem described in Fig. 4. We choose \( VL_2^2 = -100 \), \( L_1 = L_3 = L \), \( L_2=4L \) and \( h = 2m = 1 \).

Fig. 6 \( \rho \) (solid curve) and \( \tau = \frac{d\theta}{dE} = \text{LHS of Eq. 3} \) (dotted curve) versus \( kL \) for the scattering problem described in Fig. 4. We choose \( VL_2^2 = -100 \), \( L_1 = L_3 = L \), \( L_2=2.4L \) and \( h = 2m = 1 \).
arg(r), arg(t)
