Friedel Sum Rule for single channel quantum wire

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(Dated: October 30, 2018)

Elastic scattering in a quantum wire has several novel features not seen in 1D, 2D or 3D. In this work we consider a single channel quantum wire as its application is inevitable in making devices based on quantum interference effects. We consider a point defect or a single delta function impurity in such a wire and show how some of these novel features affect Friedel-sum-rule (FSR) in a way, that is quite unlike in 1D, 2D and 3D.

PACS numbers: PACS: 73.23.-b, 72.10.-d, 72.10.Bg

The density of states in a mesoscopic sample is very important to understand mesoscopic transport phenomena and also thermodynamic properties. It is believed that the properties of a mesoscopic sample, connected to leads, can be formalized in terms of the scattering matrix. The Friedel-sum-rule (FSR) relates the density of states (DOS) to the scattering matrix and can be stated as $\theta_f(E_2) - \theta_f(E_1) = \pi N(E_2, E_1)$ \[3\]. In 1D, 2D and 3D, the equality being approximate is almost exact in the WKB regime where generally transport occurs. Here $N(E_2, E_1)$ is the variation in the number of states in the energy interval $[E_1, E_2]$ due to the scatterer and $\theta_f(E) = \frac{1}{2} \sum_j \xi_j = \frac{1}{2i} \ln(\det[S])$. $S$ is the scattering matrix and $e^{i \xi_j}$, $j=1,2,\ldots,n$ are the $n$ eigenvalues of the unitary matrix $S$. In differential form the FSR can also be stated as

$$\frac{\partial}{\partial E} \theta_f(E) = \frac{1}{2i} \frac{\partial}{\partial E} \ln(\det[S]) \approx \pi [\rho(E) - \rho_0(E)], \quad (1)$$

where $[\rho(E) - \rho_0(E)]$ is the variation of the DOS or the difference in the DOS due to the presence of the scatterer. $\rho(E)$ and $\rho_0(E)$ can be found by integrating the local DOS (LDOS) $\rho(x,y,z,E)$ and $\rho_0(x,y,z,E)$.

In 1994, Ref. \[1\] explored a relation between LDOS and the scattering matrix. We refer to it as the Böttiker-Thomas-Pretre (BTP) sum rule which could be exact but is of limited practical value as far as the global DOS is concerned, because of the following reasons. First of all if one wants to integrate the LDOS to find the DOS, then it is very cumbersome and may not be at all possible for complicated potentials. Secondly, in this local formalism, one has to take the derivatives of the $S$ matrix elements with respect to the local potential and in some cases one encounters problems in including the non-local effects and non-local disturbances in the LDOS. Thirdly, if one wants to find the change in the $S$ matrix due to an infinitesimal change in the local potential, then one has to know the change in the local wave-function due to that infinitesimal change in the local potential and then use the transfer matrix multiplication method or any other equivalent method to find the change in the $S$ matrix. So then integrating the LDOS to find the DOS is just equivalent to integrating the wavefunction to find the DOS. Another such relation between the LDOS and the scattering matrix is given by Titov and Schomerus. Whereas, the power of the FSR lies in the fact that it gives this integrated quantity straightaway, without having to tamper the internal structure of the potential, but just by infinitesimally changing the energy of an external probing particle. Although, the BTP sum rule is of use in certain cases, it is definitely not a competitor of or a substitute for the FSR. No doubt, even the authors of Refs. \[1\], much after the proposition of the BTP sum rule in 1994, refers to Eq. 1 as the FSR, and are worried about to what extent it is valid.

The scattering matrix of an impurity in a quantum wire have very unusual features that were not realized until very recently. In a single channel quantum wire, in the presence of a single attractive impurity, taken as a negative delta-function potential, the transmission probability can go to zero for some finite energy of the incident electron. At the corresponding energy, the scattering phase-shift shows a discontinuous jump(slip) by $\pi$. It was shown that in the single channel case the Friedel phase $\theta_f$ is not affected by the discontinuous phase drops.

In the multichannel case, when the unitarity of a particular channel is not present and the electron can escape to a different channel, the transmission zeroes are replaced by minima and the discontinuous phase slip by $\pi$ are replaced by continuous and less than $\pi$ phase drops. It was also shown that in the multichannel case too the Friedel phase $\theta_f$ is not affected by these continuous phase drops. However, $\partial E \theta_f$ may not bear any resemblance to $\pi [\rho(E) - \rho_0(E)]$.

In this work we intend to study the FSR (Eq. 1) for a single channel quantum wire with a delta-function impurity. The single channel case being the most important because it is in this regime that one can really control the quantum interference effects and use them to build mesoscopic devices and point impurities like the delta function potential are always present. Besides, to study the transport across a quantum dot connected to two ideal leads on two sides, most theoretical works model the dot by a single bound state at the site of the dot as the Coulomb blockade makes the other levels of the dot to be very far away. As an attractive delta potential is capable of creating such a single bound state, it was used in Ref. \[3\] to explain the Fano resonances in
quantum dots and the unusual features of the scattering phase shift observed across the quantum dot. Besides, the present study provides general understandings, and we also understand the system and the results of Ref. [6] better.

Scattering due to a spherical defect leads to asymptotic wave-functions that are plane waves and whose radial part is of the form $\psi_{k,l}(r) \sim \frac{1}{r} \sin(\kappa r - \frac{\eta}{r} + \eta l)$. Here, $k$ is the wave-number, $l$ is the angular momentum quantum number and $\eta$ is the phase shift due to scattering. According to Friedel [13], to approximately count the number of states created by the impurity, consider a large sphere of radius $R$ with a defect at the center, and impose a condition $\psi_{k,l}(R) = 0$. Thus we obtain $kR - \frac{\eta}{r} + \eta l = n\pi$. The states $k$ thus obtained are real and not complex as it should be. Generally, scattering states have open boundary conditions that lead to their characterization in terms of complex energies. The imaginary part of their complex energy is called self energy and it arises because of the fact that the states can leak out to infinity and get absorbed by some detector irrespective of boundary conditions [12]. In this case also the interaction of the states within the large sphere of radius $R$ with the region outside the sphere will lead to a self energy. In absence of the scatterer, the scattering phase shift $\eta = 0$ and thus one gets Eq. (1) [13].

A more rigorous derivation, including the self energy is given by Buttiker et al. [7]. Earlier treatment of Dashen, Ma and Bernstein [14] and that of Avishai and Band [15] are also reviewed by these authors, in some of their works like Refs. [1, 6, 16]. These treatments are only valid for large systems. Souma and Suzuki [17] provides a straightforward extension of the work by Avishai and Band to quantum wires and also suffers from the same drawback. Ref. [6] gives

$$\frac{\partial}{\partial E} \theta_f(E) + Im \text{Tr} \hat{G}_a \frac{\partial \hat{\Sigma}^a}{\partial E} = Im \text{Tr} \hat{G}^a$$

$$= \pi [\rho(E) - \rho_0(E)] . \tag{2}$$

Here $\hat{G}^a = \left[ E - \hat{H}_{\text{system}} - \hat{\Sigma}^a(E) \right]^{-1}$, is the advanced Green’s function and $\hat{\Sigma}^a$ is the corresponding self energy. Note that $\hat{G}^a$ is the advanced Greens function for the system alone, where the modifications in the system due to the presence of the leads is included. Hence apart from this $Im \text{Tr} \hat{G}^a$ which is equal to the integrated disturbance in the LDOS created by the impurity, i.e., $\pi [\rho(E) - \rho_0(E)]$, there will be some disturbance in the LDOS in the leads which will depend on the Greens function of the lead and how it is affected by the system. This contribution is not important and also it gets screened away very easily as it is very small and the leads being ideal, carrier concentration is very high in the leads (this is often referred to as non-polarisable leads). The only assumption required to get Eq. (1) is to neglect $\frac{\partial \hat{\Sigma}^a}{\partial E}$ i.e. the energy dependence of the self energy. Now

$$\frac{\partial}{\partial E} \hat{\Sigma}^a = \frac{\partial}{\partial E} \left[ \tau_p g^a \tau_p \right] , \tag{3}$$

$\tau_p$ is the matrix element which couples the leads to the sample. In 1D, 2D and 3D $\tau_p$ is independent of energy in the WKB regime. $g^a_\sigma$ being the local Greens function of a semi-infinite ideal wire, its energy dependence is not very important and thus in 1D, 2D and 3D, in the WKB regime, FSR (11) is almost exact. There will be violations in the non-WKB regime, but since transport occurs in WKB regime, these violations are not important.

The scattering matrix $S$ for this single channel quasi-one-dimensional (Q1D) system is

$$S = \begin{pmatrix} \hat{t}_{11} & \hat{t}_{11} \\ \hat{t}_{11} & \hat{t}_{11} \end{pmatrix} . \tag{4}$$

Bagwell [3] has obtained

$$\hat{t}_{11} = 1 + \frac{\frac{1}{2k_\pi}}{1 + \sum_{n > 1} \frac{1}{2k_n} + i \frac{1}{2k_1}}, \tag{5}$$

and $\hat{r}_{11} = -1 + \hat{t}_{11}, \tag{6}$

where, $\Gamma_{nm} = \frac{2m_\pi}{\hbar w} \sin\left(\frac{\pi w}{2} \left(y_i + \frac{w}{2}\right)\right) \sin\left(\frac{\pi w}{2} \left(y_i + \frac{w}{2}\right)\right)$, $k_n = \sqrt{\frac{2m_\pi}{\hbar w} (E_n - E)}$, $E_n = \frac{\hbar^2 w^2}{2m_\pi^2} \gamma$, $\gamma$ is the strength of the delta potential placed at a distance $y_i$ from the center of the quantum wire of width $w$. We find that a similar expression exists for the transition amplitude from the propagating mode ($n=1$) to the nth evanescent mode, given by

$$t_{1n} = \frac{-\frac{1}{2k_1}}{1 + \sum_{n > 1} \frac{1}{2k_n} + i \frac{1}{2k_1}} . \tag{7}$$

When the impurity potential is positive it can only support scattering states. However when the impurity potential is negative, it can also support bound states, apart from the scattering states. For each $n$ we get a sub-band of scattering states ($E$ as a function of $k_n$). Similarly we get a bound state for each $n$, that are solutions to [3]

$$1 + \sum_{m=n} \frac{\Gamma_{nm}}{2k_m} = 0 \quad . \tag{8}$$

For $n=1$ we get a true bound state. The bound state for $n=2$ may or may not be a true bound state. If the impurity potential is such that the solution to Eq. (3) lie in the energy range where $n=1$ channel is propagating, then this bound state for $n = 2$, is degenerate with $n=1$ scattering state and it becomes a quasi-bound state.

We have also calculated to find

$$[\rho(E) - \rho_0(E)]_{total} = \sum_{p} \frac{2}{\hbar v_p} \int_{-\infty}^{\infty} dx \cos(2k_p x + \eta_p) \left| \frac{t_{11}}{k_e} \right| + \left| \frac{t_{11}}{k_e} \right|^2 . \tag{9}$$
Here \(v_p = \hbar k_p/m\). \(\sum p\) denotes sum over all propagating modes and \(\sum\) denotes sum over all evanescent modes. The 1st term on the R.H.S. is basically integrated change in the LDOS in the leads. Since the delta function potential is a point impurity, the integrated LDOS in the leads extends from \(-\infty\) to \(\infty\). One can do the integration to find \(\int_{-\infty}^{\infty} \pi \cos(2k_p x + \eta_p) = \pi \cos(\eta_p) \delta(k_p)\). So it is zero unless the quasi-bound state coincides with \(k_p = 0\). In the case of extended impurities one can see that this term gives an unimportant small contribution that does not change with energy. Also the carrier concentration in the leads is normally large enough to screen away a small oscillatory LDOS completely. So the relevant quantity that appears in FSR is

\[
\rho(E) - \rho_0(E) = \sum_p \frac{2}{\hbar v_p} \sum_e |t_{pe}|^2 \frac{1}{\kappa_e},
\]

(10)

This is actually the integrated local DOS around the impurity site and decaying away from the impurity site all the way up to \(\pm \infty\). In the regime of single propagating channel \(p\) can take only one value, i.e. \(p = 1\) and \(e = 2, 3, \ldots, \infty\). Thus we can independently calculate both sides of Eq. 1 starting from 1st principles, where we do not have to throw away dispersive behavior or energy dependence of self energy.

We first present below a discussion and definition of the WKB regime for a Q1D system, because it is an interesting subject on its own. When the incident electron propagates in a potential where the wavefunction changes very slowly in space then very little reflected wave is generated and that is taken to be the WKB regime. So a delta function potential in one-dimension (1D) has a WKB regime at higher energies, when the reflection probability is very small. In the inset of Fig.1, where we plot \(|\tilde{r}_{11}|^2\) versus incident energy we find that there are three regimes. One is to the left of point \(P_1\) where \(|\tilde{r}_{11}|^2\) is large and also strongly energy dependent. The other is between the points \(P_1\) and \(Q_1\), where \(\kappa_e^2 \gg \gamma\). These two regimes can be seen in 1D scattering (e.g., a delta function potential in 1D) and are the non-WKB and WKB regimes, respectively. The third regime is to the right of the point \(Q_1\), where again \(|\tilde{r}_{11}|^2\) is very small and is hence a WKB regime, but the energy dependence of \(|\tilde{r}_{11}|^2\) is very large. Such a regime cannot be seen in 1D and is a specialty of Q1D. So the energies that lie to the left of \(P_1\) is the non-WKB regime, where the electron feels the potential very strongly and is almost entirely reflected back. Energies to the right of the point \(P_1\) correspond to the WKB limit. Although, the system considered here is a Q1D system, corresponding to a scatterer in Q1D, there is an energy dependent scatterer in 1D. The bound states and scattering states of these two potentials are identical and this is an exact correspondence, valid in all regimes, quantum or semiclassical. And so when the reflection probability is small in Q1D, it is also small in the corresponding 1D potential. Then all the notions and results of WKB regime that we are familiar with in 1D are also true in Q1D.

In Fig.1 we find a large deviation of \(\pi [\rho(E) - \rho_0(E)]\) (dotted curve) from \(\frac{d\tau}{dE}\) (solid curve) at energies in the non-WKB regime (left of \(P_1\)). This is similar to what is seen in 1D, 2D or 3D. In the WKB regime, that is to the right of the point \(P_1\), although \(|\tilde{r}_{11}|^2\) is very small, its energy dependence is not as negligible as that of a potential in 1D (e.g., a delta function potential in 1D or a square well in 1D). Energy dependence of \(|\tilde{r}_{11}|^2\) automatically implies energy dependence of \(\tau_\rho\) (or \(\Sigma^n\)), i.e., dispersive behavior. So there is an appreciable difference between \(\pi [\rho(E) - \rho_0(E)]\) and \(\frac{d\tau}{dE}\).

Let us now analytically analyse the curves (solid and dashed) to the right of \(Q_1\). In this region \(\kappa_2 \to 0\). From Eq. (10) we find that only the 1st term in the series is relevant. That is

\[
\pi [\rho(E) - \rho_0(E)]_{\kappa_2 \to 0} \text{ diverges as } \left[ \frac{2\pi \Gamma_{11} \frac{1}{\hbar v_1 \Gamma_{22} \kappa_2}}{\pi} \right]_{\kappa_2 \to 0}\n\]

(11)

Thus the strong energy dependence in the energy beyond \(Q_1\) is due to the rapid population of the second subband through evanescent modes, as it approaches its propagating threshold. Hence, unlike the Fano resonance, this is not a quantum interference effect. This is like the Van Hove singularity at the band edge. Similarly one can find

\[
\frac{d\tau_\rho}{dE}_{\kappa_2 \to 0} = \left[ \frac{d}{dE} \text{arg}(\tilde{t}_{11}) \right]_{\kappa_2 \to 0}\n\]

(12)

diverges identically. Note that although \(\text{arg}(\tilde{t}_{11})\) can have a discontinuity, the derivative exists at all energies. Essentially the right derivative and left derivative is the same at the discontinuity. Hence we prove FSR is exact as \(\kappa_2 \to 0\). This is understood when we note that when \(\kappa_2 \to 0\), \(|\tilde{r}_{11}|^2\) goes to zero at the band edge. Also it is known that when \(\tilde{r}_{11} = 0\) then \(\tau_\rho\) maximizes, and energy dependence of \(\rho_0\) being negligible, \(\frac{d\tau}{dE} = 0\). Thus all the deviating terms being zero, the FSR is valid around the diverging DOS at the band edge.

For strong negative potentials, such that the bound state for \(n = 2\) is below the propagating threshold of \(n = 1\), the curves look similar to that in Fig. 1. For the negative \(\delta\) function potential with the bound state for \(n = 2\), in the propagating regime of \(n = 1\), we have plotted the two sides of Eq. (11) in Fig.2. \(|\tilde{r}_{11}|^2\) is shown in the inset. Note that \(|\tilde{r}_{11}|^2\) shows that at the point \(P\) the system is in extreme non-WKB regime where \(|\tilde{t}_{11}|^2\) goes to zero. At this energy there is a quasi-bound state and there is strong energy dependence of scattering matrix elements as well as self energy. According to earlier stated results, there should be violation of FSR here. The peak in \(\pi [\rho(E) - \rho_0(E)]\) at \(P\) occurs due to the quasi-bound state. We also see that at this very point \(P\) there is an exact agreement between L.H.S. & R.H.S. of Eq. (11). This can be even verified analytically. Substituting the bound state condition given in Eq. (8) into \(\frac{d\tau}{dE}\) as well as
in $\pi[\rho(E) - \rho_0(E)]$ separately, we get

$$\frac{d\theta}{dE} = \frac{m_e k_1}{\hbar^2} \frac{1}{\Gamma_{11}} \sum_{n>1} \frac{\Gamma_{nn}}{\kappa_n^2} = \pi[\rho(E) - \rho_0(E)] \quad (13)$$

This agreement between $\frac{d\theta}{dE}$ and $\pi[\rho(E) - \rho_0(E)]$ was argued to be equal for the case of a stub in ref. [1], at the transmission zero where the $\delta$ term in Eq. (2) was dropped from the very beginning [2]. Dropping the energy dependence of $\Sigma_n$ in non-WKB regime and verifying the validity of FSR is rather meaningless, as the violations do come from the energy dependence of $\Sigma_n$. Even after including these terms we get exact agreement at the transmission zero for the negative $\delta$ function potential in a quantum wire, although it is in extreme non-WKB regime. The reasons are as follows. At the transmission zero, since there is a quasi-bound state, $\Sigma_n$ becomes minimum and $\frac{d\Sigma_n}{dE} = 0$. All these arguments are also true.

The multichannel case was analysed in Ref. [11]. When two modes are propagating, the bound state coming from the 3rd sub-band, can be degenerate with the propagating channels. At that point there is no agreement between $\frac{d\theta}{dE}$ and $\pi[\rho(E) - \rho_0(E)]$. While $\pi[\rho(E) - \rho_0(E)]$ is not only positive definite, it also has a sharp peak meaning enhanced DOS at the energy corresponding to the bound state. The peak is completely missing from $\frac{d\theta}{dE}$ and $\frac{d\Sigma_n}{dE}$ turns out to be negative. Thus the disagreement is not just a quantitative one, but is a qualitative one.

Thus the purpose of this work was to verify FSR in single channel quantum wires in the presence or absence of Fano resonances. Fano resonance is a very general feature of quantum wires. At the Fano resonance all the quantities are strongly wave vector dependent as it is a purely quantum interference effect. Never the less, FSR is exact at the Fano resonance. This is contrary to the known fact that FSR is valid in semiclassical regimes where there is no strong dependence on wave vector. The exact agreement of the FSR in spite of the strong wave vector dependence is due to the fact that at the Fano resonance there is a quasi bound state that leads to a minimum in the self energy. Away from this quasi bound state there are strong violations. These are true for any negative potential in Q1D and the potential considered here and the associated calculations make this clear. For positive as well as negative delta function potentials, there is also strong wave vector dependence, close to the upper band edge of single channel propagation. This is due to the rapid population of the first evanescent mode at its propagation threshold and does not depend on the existence of Fano resonance. $d\Sigma/dE=0$ here because of the perfect transmission at the band edge, and hence the agreement in FSR. So the former case of agreement in the peak is an agreement in purely quantum regime, while that in the case of the latter peak is in the semiclassical regime. Away from the peaks there is always violation. It may be interesting to work out some extended potentials in Q1D [22].

One of the authors(S.B.) gratefully thanks Prof. Binayak Dutta Roy and Debasish Chaudhuri for useful discussions.

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[22] We have found that if we take two delta function potentials in a single channel quantum wire and place two of them close to each other, then for very large strengths of the two potentials, the system becomes almost reflectionless. This is very counter intuitive as large potentials are expected to give large reflections. It happens because strong potential couples the evanescent modes very strongly to the propagating mode at the positions of the delta potentials, and an incident electron is thrown into the evanescent channels rather than reflected. And since the two potentials are close to each other, the electron can easily tunnel from one potential site to the other and finally go to the transmission channel, again due to the large coupling between the evanescent and transmission channels. As far as FSR is concerned, qualitative results will be the same. At the quasi-bound states, the self energy has a minima, which means $d\Sigma/dE=0$, and
so the FSR will be exact at these points. There will be violations away from these points, the extent of which has to be seen through explicit calculations.

**Figure Captions**

Fig. 1. The dashed curve gives $\pi(\rho - \rho_0)$ and the solid curve gives $\frac{d}{dE}(-.5i ln Det[S])$. Both the functions are plotted versus $EW^2$ using $y_i = .21W$ and $\gamma = 1$. In the inset the corresponding $|f_{11}|^2$ is plotted. We have considered 500 evanescent modes.

Fig. 2. The solid curve gives $\pi(\rho - \rho_0)$ and the dashed curve gives $\frac{d}{dE}(-.5i ln Det[S])$. Both the functions are plotted versus $EW^2$ using $y_i = .21W$ and $\gamma = -1.5$. For this value of $\gamma$ there is a quasi-bound state at $EW^2 = 36.1022$. In the inset the corresponding $|f_{11}|^2$ is plotted. We have considered 500 evanescent modes.