Soliton like wave packets in quantum wires

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At a Fano resonance in a quantum wire there is strong quantum mechanical back-scattering. When identical wave packets are incident along all possible modes of incidence, each wave packet is strongly scattered. The scattered wave packets compensate each other in such a way that the outgoing wave packets are similar to the incoming wave packets. This is as if the wave packets are not scattered and not dispersed. This typically happens for the kink-antikink solution of the Sine-Gordon model. As a result of such non-dispersive behavior, the derivation of semi-classical formulas like the Friedel sum rule and the Wigner delay time are exact at Fano resonance. For a single channel quantum wire this is true for any potential that exhibit a Fano resonance. For a multichannel quantum wire we give an easy prescription to check for a given potential, if this is true. We also show that validity of the Friedel sum rule may or may not be related to the conservation of charge. If there are evanescent modes then even when charge is conserved, Friedel sum rule may break down away from the Fano resonances.

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I. INTRODUCTION

The Landauer-Buttiker approach to mesoscopic physics is rather novel. One of the great success of this approach is the Landauer-Buttiker conductance formula. To understand this approach further and the key to generalize this approach is the Friedel sum rule (FSR). It has been the subject of much study recently. While exact proofs can be given for bulk samples [1, 2, 3], in low dimensional systems some attempts to derive it ignore the effects of the leads [4, 5]. Buttiker and his co-workers, emphasize the effects of the leads and find a correction term to the FSR [6, 7]. They state that leads can result in non-conservation of charge in quantum regimes and in such regimes FSR will break down. When the system is in the WKB limit, then charge is conserved and FSR works very well. Recent explicit calculations [8] for an impurity in a quantum wire contradicted this result. A single attractive impurity in a quantum wire can produce many resonant states that can all be classified as Fano resonances [9, 10]. Such an impurity in a quantum wire has attracted many theoretical investigation [11]. Ref. [8] finds that the Friedel sum rule is exact at the Fano resonance which is a pure quantum interference phenomenon (and not a WKB regime), and very bad in the regimes away from the Fano resonance (that are in the WKB regime). Ref. [12] shows that other semi-classical formulas like the Wigner delay time (WDT) also become exact at the Fano resonance. An analysis of charge conservation and the origin of semiclassical behavior in a quantum regime is missing in Refs. [8, 12]. In this work we show that there is no connection between charge conservation and validity of FSR in the sense that FSR can be violated even when charge is conserved. We shall also show that although such an impurity in a quantum wire give strong back scattering that is quantum mechanical in nature, such scattering do not disperse a wave packet. We shall also show that this explains why semi-classical theories are exact in a purely quantum mechanical regime.

When one considers transport in mesoscopic systems then one typically considers a system as shown in Fig 1. The system between the points A and B is a grand canonical system coupled to reservoirs. The way we study grand canonical systems in text books is that the reservoir Hamiltonian and the system Hamiltonian can be decoupled. This allows one to construct a grand canonical partition function. But mesoscopic samples are so small that the actual modeling of the coupling to the reservoirs is necessary [13, 14, 15, 16]. The leads (here we show only two leads but there can be many) are ideal reservoirs is necessary [13, 14, 15, 16]. The leads (here we show only two leads but there can be many) are ideal wires that connect the system to the reservoirs. They inject and absorb electrons and also define the correct boundary conditions for the system. The region between A and B is an elastic scatterer. A particle injected by reservoir 1 will freely propagate along lead 1 and will be incident on the scatterer between A and B. The reflected part will be absorbed by reservoir 1 and the transmitted part will be absorbed by reservoir 2. The absorbed electrons are completely thermalized inside the reservoirs and their coherence is destroyed. Phase shifts are defined with respect to points A and B and not with respect to ±∞. Density of states (DOS) is also the local density of states (LDOS) integrated between the points A and B [8]. The scattering problem is completely defined with the points A and B [8]. Provided the total charge in the region between A and B (or the integrated LDOS in the region between A and B) is conserved. The region outside that can be parametrized with chemical potential (µ) and temperature (T). If µ and T are the same for the two reservoirs, then we get an equilibrium situation, and if they are different then we get non-equilibrium situation. All this will become explicit in our model calculation.
II. THE SCATTERING SOLUTION

As a simple realization of such a system (as shown in Fig. 1) in one dimension (1D) we can consider a double delta function potential in 1D between \( x = -l \) and \( x = l \) (see Fig. 2). The free regions \( x < -l \) and \( x > l \) are the leads. For a symmetric scatterer in 1D, the scattering matrix is

\[
S = \begin{pmatrix} R & T \\ T & R \end{pmatrix}
\]

where \( R \) is the reflection amplitude and \( T \) is the transmission amplitude of the scatterer.

If we consider a two channel quantum wire with a delta function potential. The scattering matrix will be 4X4 as shown below.

\[
S = \begin{bmatrix} R_{11} & R_{12} & T_{11} & T_{12} \\ R_{21} & R_{22} & T_{21} & T_{22} \\ T_{11} & T_{12} & R_{11} & R_{12} \\ T_{21} & T_{22} & R_{21} & R_{22} \end{bmatrix}
\]  

We are using a notation that \( S_{11} = R_{11} \) as it is a reflection amplitude for an electron incident along the first transverse mode from the left lead and scattered back to the first transverse mode in the left lead. Similarly, \( S_{12} = R_{12} \) as it is a reflection amplitude for an electron incident along the first transverse mode from the left lead and scattered back to the second transverse mode in the left lead. Similarly, \( S_{11} = T_{11} \) as it is a transmission amplitude for an electron incident along the first transverse mode from the left lead and scattered forward to the first transverse mode in the right lead. One can easily understand the rest. One can solve the scattering problem to find that for \( \alpha \) and \( \beta \) taking values 1 or 2,

\[
R_{\alpha\beta} = -\frac{i \Gamma_{\alpha\beta}}{2d \sqrt{\kappa_\alpha \kappa_\beta}}
\]  

If \( \alpha \neq \beta \) then

\[
T_{\alpha\beta} = -\frac{i \Gamma_{\alpha\beta}}{2d \sqrt{\kappa_\alpha \kappa_\beta}}
\]  

If \( \alpha = \beta \) then

\[
T_{\alpha\alpha} = 1 + R_{\alpha\alpha}
\]

Here

\[
\Gamma_{\alpha\beta} = \frac{2m \gamma}{\hbar^2} \sin\left(\frac{\alpha \pi}{w}(y_j + w/2)\right) \sin\left(\frac{\beta \pi}{w}(y_j + w/2)\right)
\]

\[
d = 1 + \sum_{\nu} \frac{\Gamma_{\nu\nu}}{2 \kappa_\nu} + i \sum_{\alpha} \frac{\Gamma_{\alpha\alpha}}{2 \kappa_\alpha}
\]

\[
\Gamma_{\nu\nu} = \frac{2m \gamma}{\hbar^2} \sin\left(\frac{\nu \pi}{w}(y_j + w/2)\right) \sin\left(\frac{\nu \pi}{w}(y_j + w/2)\right)
\]

\( \nu \) can take any integer value greater than 2 (i.e., \( \nu = 3, 4, 5, \ldots \)). \( \gamma \) is the strength of the delta function potential situated at \( x = 0 \) and \( y = y_j \). \( m \) is particle mass and \( w \) is the width of the quantum wire. \( k_1 = \sqrt{\frac{2m}{\hbar^2}(E - \frac{\pi^2}{w^2})} \) is the wave vector for the 1st propagating channel. \( k_2 = \sqrt{\frac{2m}{\hbar^2}(E - \frac{4\pi^2}{w^2})} \) is the wave vector for the 2nd propagating channel. \( \kappa_\nu = \sqrt{\frac{2m}{\hbar^2}(\frac{\nu^2\pi^2}{w^2} - E)} \) is the wave vector for the \( \nu \)th evanescent channel. \( E \) is the incident energy. The \( n \)th quasi bound state or the Fano resonance occur at energies that satisfy the following equation

\[
1 + \sum_{\nu=0}^{\infty} \frac{\Gamma_{\nu\nu}}{2 \kappa_\nu} = 0
\]  

At such an energy, there will be a large amount of charge localized around the impurity and decaying away from the impurity. One can define the points A and B as the cut off points beyond which the localized charge has decayed to negligible values. Also in real systems \( \nu \) will have some cut off points that can have several physical origins like decoherence or work function of the quantum wire. The \( \nu \)th injectivity at a point \( q = (x, y, z) \) is due to the incident electron of velocity \( v_\alpha \) (or \( -v_\alpha \)). It is defined as

\[
\sum_{\beta} \rho_{\alpha\beta}(q) = \frac{1}{\hbar |v_\alpha|} |\psi^{(\alpha)}(q)|^2
\]

where, \( h \) is Plank’s constant, \( v_\alpha = \frac{\hbar k_\alpha}{m} \), \( k_\alpha \) is incident wave vector, \( m \) is particle mass, \( q \) represents coordinate and \( \psi^{(\alpha)}(q) \) is quantum mechanical wave function due to unit current incident in the \( \alpha \)th injectivity at a point \( q \). It is defined as

\[
\rho(E) = \frac{1}{h |v_\alpha|} \int_{-\infty}^{\infty} |\psi^{(\alpha)}(q)|^2 dq
\]

And

\[
\rho^{GC}(E) = \sum_{\alpha=1}^{M} \frac{1}{h |v_\alpha|} \int_{A}^{B} |\psi^{(\alpha)}(q)|^2 dq
\]

Here suffix GC stands for “grand canonical”. Here \( M \) is the total number of incident channels possible.

III. FRIEDEL SUM RULE (FSR)

If the charge in the region between A and B is conserved then the scattering problem is completely defined with respect to the points A and B. FSR suggests that
the DOS in Eq. 12 can be calculated from $S$ matrix, without any knowledge of the $ψ^{(α)}(q)$ as the $S$ matrix elements can be determined experimentally [17, 18] as well as theoretically [14, 20].

The FSR can be stated as

$$\frac{dθ_f}{dE} \approx π[ρ^{GC}(E) − ρ_0^{GC}(E)] \quad (13)$$

where

$$θ_f = \frac{1}{2i} \log(Det[S]) \quad (14)$$

$S$ is the scattering matrix of a system and $E$ is incident electron energy. $ρ^{GC}(E)$ is integrated LDOS of a system in presence of scatterer as defined in Eq. 12 and $ρ_0^{GC}(E)$ is integrated LDOS of the same system in absence of scatterer, which naturally requires that impurity scattering conserves the total number of states in the system or the total charge in the system (or else $ρ$ need not be related to $ρ_0$ at all). In Eq. 13 we have used an approximate equality as there will be a correction term which we will discuss later. The beauty of Eq. 13 is its universality. At equality as there will be a correction term which we will discuss later. The beauty of Eq. 13 is its universality. At any resonance (or quasi bound state) [$ρ^{GC}(E) − ρ_0^{GC}(E)$] change by unity and hence $θ_f$ will change by $π$. Moreover, $\frac{dθ_f}{dE}$ can be determined from asymptotic wave function ($x → ∞$) and so one can completely avoid integrating the LDOS to find the DOS.

The purpose of this section is to explain the discrepancy observed in Ref. [8] about the FSR. Namely the FSR becomes exact in a purely quantum regime like the Fano regime and bad away from the Fano regime. According to our previous understanding, it should have been the opposite. Such an explanation requires a detailed analysis of charge conservation and quantum behavior as follows. A physical origin of such a behavior will become clear in the next section.

To understand where FSR may go wrong, we first inspect a derivation of the FSR [21]. We present it for 1D as the steps can be repeated for Q1D. Suppose there is an extended potential $V(x)$ (to be dimensionally correct in the subsequent analysis, $V(x) = eV(x)$, where $e$ is electronic charge). Assuming that $S_{α,β}(E, V(x))$ is analytic, we can make an expansion as

$$S_{α,β}(E, V(x) + δV(x)) = S_{α,β}(E, V(x)) + \int_{−∞}^{∞} dx'[\frac{∂S_{α,β}(E, V(x'))}{∂V(x')}] δV(x') + \ldots \quad (15)$$

Essentially this means breaking up the increment $δV(x)$ (although an infinitesimal perturbation, it is an extended potential) into many local increments $δV(x')$ and integrating the effect of all these local increments. $δV(x')$ is therefore a delta function potential at $x'$. Now without any loss of generality, we can say that $δV(x) = V_0$ for all $x$. In other words $δV(x)$ is a constant potential. Since $δV(x) = V_0$ for all $x$, the local perturbation $δV(x')$ is also equal to $V_0$, numerically. One has to remember that the two perturbations $δV(x) = V_0$ and $δV(x') = V_0$ are actually different. One of them is a global perturbation or an extended perturbation while the latter is a local perturbation. However, for $V_0 → 0$, one can neglect this difference between them to write

$$S_{α,β}(E, V(x) + V_0) − S_{α,β}(E, V(x)) \approx \frac{1}{V_0} \int_{−∞}^{∞} dx'[\frac{∂S_{α,β}(E, V(x'))}{∂V(x')}] \quad (16)$$

Note that now we have an approximate equality and this can be further justified by explicit calculations as shown below.

Now one may propose that instead of increasing the potential everywhere by an infinitesimal amount $V_0$, one may keep the potential constant and instead decrease the incident energy by $ΔE = V_0$. Thus

$$S_{α,β}(E − ΔE, V(x)) − S_{α,β}(E, V(x)) = −ΔE \quad (17)$$

One can prove that

$$−\frac{1}{4πi} (S^t_{α,β} \frac{∂S_{α,β}}{∂V(x')} − HC) = ρ_{α,β}(E) \quad (18)$$

where $ρ_{α,β}$ is the PLDOS. PDOS is therefore $ρ_{α,β}(E) = \int_{−∞}^{∞} ρ_{α,β}(x) dx$. One can take any potential in 1D and check that this equation is exact as done in Ref. [8]. Therefore, from Eqs. 17 and 18,

$$\frac{1}{4πi} (S^t_{α,β} \frac{∂S_{α,β}}{∂E} − HC) \approx ρ_{α,β}(E) \quad (19)$$

This on summing over $α$ and $β$ and further simplification gives

$$\frac{1}{2i} \frac{d}{dE} \log(Det[S]) ≈ π[ρ(E) − ρ_0(E)] \quad (20)$$

Thus we have derived FSR.

Replacing $∫ dx' \frac{∂S_{α,β}}{∂E}$ by $\frac{∂S_{α,β}}{∂E}$ is an approximation. Thus $\frac{∂θ_f}{dE}$ is not exactly equal to $π[ρ(E) − ρ_0(E)]$ and so naturally one can expect that $\frac{∂θ_f}{dE}$ is also not exactly equal to $[ρ^{GC}(E) − ρ_0^{GC}(E)]$. In fact [7],

$$\frac{dθ_f}{dE} = π[ρ^{GC}(E) − ρ_0^{GC}(E)] − Im(R_{LL} + R_{RR})/4E \quad (21)$$
We have used suffixes ‘LL’ and ‘RR’, instead of $\alpha$ and $\beta$. The reasons are obvious as $R_{LL}$ is for the electrons incident from the left and reflected back to the left lead, while $R_{RR}$ is for the electrons incident from the right and reflected back to the right lead. One may consider Eq. 21 as a new FSR but the correction term $[Im(R_{LL} + R_{RR})/4E]$ is not very universal. It can be different for different kinds of resonances. Secondly, in quasi 1D we will see that this correction term will also depend on internal details of the potential and can vary from sample to sample.

So the correction term is $Im(R_{LL} + R_{RR})/4E$. Ref. [7] and others assume that this term is due to the non-conservation of charge in the system. They assume (see Eqs. 11 and 12 in Ref. [7]) that this term can be related to self energy due to the escape probability of an electron in to the leads. So according to [7], in quantum regimes, this term can be large. An essential component of this work is to establish that this correction term is not due to non-conservation of charge. Although in 1D, 2D and 3D the correction term is large when the escape probability to the leads is large (that is charge is not conserved in the grand canonical system) and vice versa, this is not true in Q1D. We show below that the correction term can be large in Q1D even when charge is conserved and also the correction term can be zero in the Fano regime which is a quantum regime.

It is shown in the appendix that

\[
[(\rho(E) - \rho_0(E)) - [\rho^{GC}(E) - \rho_0^{GC}(E)] =
\]

\[
\frac{sin[2k]\ell}{k}(R_{LL} + R_{RR}) + \frac{cos[2k]\ell}{k}(iR_{LL} - iR_{RR})
\]

This has two implications. First is that since $\pi[\rho^{GC}(E) - \rho_0^{GC}(E)] - Im(R_{LL} + R_{RR})/4E \neq \pi[(\rho(E) - \rho_0(E)],$ it follows from Eq. 21 that

\[
\frac{d\theta_f}{dE} \neq \pi[\rho(E) - \rho_0(E)]
\]

It can only be an approximate equality as shown before. The second implication is that the correction term $-Im(R_{LL} + R_{RR})/4E$ is not due to the lack of charge conservation. This is explained below. When we integrate over all energy then we get that the RHS of Eq. 22 goes as $\delta(k)$. The global charge has to be conserved, implying $\int_{-\infty}^{\infty} dE[(\rho(E) - \rho_0(E)] = 0$. Hence from Eq. 22, $\int_{-\infty}^{\infty} dE[\rho^{GC}(E) - \rho_0^{GC}(E)]$ goes as $\delta(k).$ Since only positive energy states are propagating states that we are interested in, one can always take the integration over $E$ in the positive energy regime instead of taking it from $-\infty$ to $\infty$. As $k = 0$ is a non-propagating state, in the propagating regime $\int_{-\infty}^{\infty} dE[\rho^{GC}(E) - \rho_0^{GC}(E)] = 0.$ So charge is conserved in the grand canonical system. So the correction term in Eq. 21 is arising due to the error involved in the substitution in Eq. 17 and has nothing
to do with charge conservation. It is just an error due to an approximation in the algebra.

Although in the appendix we have considered a 1D system, all the steps can be repeated for a single channel Q1D system. Only the expressions for $R_{LL}$ and $R_{RR}$ will be different and $k = \sqrt{2m\gamma/(E - E_1)}$. So for a single channel quantum wire,

\[
d\theta_f/dE = \pi[\rho^{GC}(E) - \rho_0^{GC}(E)] - Im(R_{LL} + R_{RR})/4(E - E_1)
\]

First of all note the presence of sample specific parameter $E_1$ in the correction term that was ignored in Ref. [7]. This equation is the same whether evanescent modes are present or not present. However, only the expressions for $R_{LL}$ and $R_{RR}$ changes completely in presence and absence of evanescent modes. From Eq. 3

\[
-Im(R_{LL} + R_{RR}) = \frac{\Gamma_{11}E/(1 + \sum_{k_1 > 1} \Gamma_{k_1})}{1 + (\Gamma_{11}/2k_1)^2}
\]

For a delta function potential in 1D,

\[
-Im(R_{LL} + R_{RR}) = \frac{\Gamma_{1D}/k_1}{1 + (\Gamma_{1D}/2k_1)^2}
\]

where $\Gamma_{1D} = 2m\gamma/w$. In comparison with the 1D case, the only difference in quasi one dimension (Q1D) (compare Eqs. 25 and 26) is the term

\[
\sum_{\nu > 1} \Gamma_{\nu\nu}/2k_\nu
\]

If we remove this term then the correction term is negligible for $k_1 > \Gamma_{11}$ which is the semi-classical regime. Complications in Q1D arise because of the series term $\sum_{n > 1} \Gamma_{n}$. Even for $k_1 < \Gamma_{11}$, $(1 + \sum_{n > 1} \Gamma_{n})$ can become zero and then the correction term can become 0 in a purely quantum regime. At the Fano resonance this is exactly what happens, i.e., RHS of Eq. 25 becomes 0 precisely due to the fact that $(1 + \sum_{n > 1} \Gamma_{n})=0$ at the Fano resonance (see Eq. 9). Also note that although each term in the series decreases with energy, the sum does not decrease easily as the series is a divergent series. It goes as $log[N]$ where $N$ is the total number of terms in the series or the total number of evanescent modes [11]. One can make the transverse width $w \rightarrow \infty$ to create an infinite number of evanescent modes and then one can see from Eq. 25 that the correction term goes to zero implying that FSR is exact in 2D. In real quantum wires, we have to truncate the series at some value $N$. For any arbitrary number of evanescent modes, the correction term can be as large as $\Gamma_{11}/2k_1$ or $\pi[\rho^{GC}(E) - \rho_0^{GC}(E)]$, making the two qualitatively and quantitatively different, except in a narrow energy regime close to the upper band edge. At the upper band edge $\sum_{n > 1} \Gamma_{n}$ diverge as the first term in it (i.e., $\Gamma_{11}/2k_1$) diverges and hence RHS of Eq. 25 becomes 0.
IV. WIGNER DELAY TIME (WDT)

The fact that FSR becomes exact at the Fano resonance is very counterintuitive. FSR is similar to WDT and so it was also checked that WDT at the Fano resonance becomes exact [12]. The similarity between WDT and FSR can be seen from Eqs. 19 and 20.

\[
\sum_{\alpha \beta} \frac{1}{4\pi i} \left| S_{\alpha \beta}^l \right|^2 \frac{d}{dE} \text{arg}(S_{\alpha \beta}) - HC = 0
\]

\[
\sum_{\alpha \beta} \frac{1}{2\pi} \left| S_{\alpha \beta}^l \right|^2 \frac{d}{dE} \text{arg}(S_{\alpha \beta}) = \sum_{\alpha \beta} \int_{-\infty}^{\infty} \rho_{\alpha \beta}(x) dx \quad (28)
\]

\[
n\frac{d}{dE} \text{arg}(S_{\alpha \beta}) \text{ is the WDT for particles transmitted from the } \alpha \text{th channel to the } \beta \text{th channel and there are } \left| S_{\alpha \beta}^l \right|^2 \text{ of such particles. One can choose } n = 1. \text{ Here } \text{arg}(S_{\alpha \beta}) = \text{Arctan} \left[ \frac{1}{\text{Re}[S_{\alpha \beta}]} \right]. \text{ We have also seen that the LHS in Eq. 28 is the semi-classical limit of the LHS of Eq. 18 integrated over } x'. \text{ So in the semi-classical limit, WDT times the number of particles involved gives the PDOS. It was shown in Ref. [5], that in the Fano regime also the WDT } \left( \frac{1}{2\pi} \left| S_{\alpha \beta}^l \right|^2 \frac{d}{dE} \text{arg}(S_{\alpha \beta}) \right) \text{ gives the PDOS } \left( \int_{-\infty}^{\infty} \rho_{\alpha \beta}(x) dx \right) \text{ exactly, in spite the fact that Fano resonance is a quantum phenomenon. This happens for single channel quantum wires as well as for multi channel quantum wires. Another way to see that the WDT is semi-classical is that its derivation is based on non-dispersive wave-packets. Below we show how non-dispersive wave-packets are realized in the quantum regime of Fano resonance and as a result WDT becomes exact (that is WDT gives the PDOS correctly).}

We start by presenting a derivation of the WDT based on non-dispersive wave-packets. Let us consider an incident Gaussian wave packet in 1D representing an ensemble of non-interacting particles. \( a(k) \) is the weight of the \( k \)th component in the incident Gaussian wave packet.

\[
\psi_{in}(x,t) = \int_{-\infty}^{\infty} a(k) \exp[ikx - iwt] dk \quad (29)
\]

After the wave packet traverses a distance \( L \), its form will be

\[
\psi_{tr}(x,t) = \int_{-\infty}^{\infty} a(k) T(k) \exp[i(kx + L) - iw(t + t_0 + \Delta t)] dk
\]

(30)

Here, \( T(k) \) is the transmission amplitude of the potential in the region of length \( L \). \( t_0 \) is the time that the wave packet would have taken if the potential was absent. \( t_0 + \Delta t \) is the time that the wave packet takes in presence of the potential. If we go to the semi-classical limit then we should get close to classical behavior that implies \( \psi_{tr}(x,t) \) is also a Gaussian wave-packet like \( \psi_{in}(x,t) \). From this one can derive WDT. Normally, \( T(k) \) is complex and energy dependent. This is the essential cause of dispersion. The weight of the \( k \)th component in the transmitted wave packet are \( a(k) T(k) \) and hence \( \psi_{tr} \), is no longer a Gaussian wave packet. If \( T(k) \) is a real number, then the dispersion will be like a free particle as \( k \) and \( w \) in \( \psi_{tr} \) are identical to that of a free particle (\( w = \frac{\hbar k^2}{2m} \)). One simple example where this happens is when the incident energy is much smaller than the potential height, wherein one gets \( T(k) \to 0 \) and \( R(k) \to 1 \). In this case \( R(k) \) is real. One finds the WDT

\[
\Delta t = \hbar \frac{d}{dE} \text{arg}(R) = \frac{d}{dw} \text{arg}(R) \quad (31)
\]

and it correctly gives the PDOS (that is \( \frac{1}{2\pi} |R|^2 \frac{d}{dw} \text{arg}(R) = \int \rho_{\alpha \beta}(x) dx \)).

This explains why FSR is exact in case of single channel Fano resonance where the particle is completely reflected back due to an effective potential that is infinite. At the single channel Fano resonance \( R(k) = -1 \) and WDT give the correct PDOS. This also shows that the correctness of WDT and hence FSR at Fano resonance is always true in single channel quantum wires. It requires the presence of a transmission zero and that is always there for all potentials that support a Fano resonance. But the correctness of FSR or WDT does not only occur in single channel quantum wires where \( R(k) = -1 \) as in semi-classical limit, but it also happens in multi channel quantum wires where \( |R_{11}(k)| \neq 0 \) and \( |T_{11}(k)| \neq 0 \). So how for such a system WDT or FSR remain exact?

In order to show how one can get non-dispersive wave packets in the presence of quantum scattering, we take clue from the kink-antikink solution of the Sine-Gordon equation. Suppose we have a delta function potential in a 2 channel quantum wire. Let us have four identical Gaussian wave packets incident on it along all possible channels. That means two will be incident from the left and two will be incident from the right. Among the two that are incident from the left, one will be in the first channel or in the fundamental transverse mode and one will be in the 2nd channel that is the first excited transverse mode. Similarly for the two that are incident from the right. All these wave packets are scattered at the same time and we call this time \( t \). After scattering, the resultant wave packet on the right in the fundamental mode (say) and moving away from the potential and at a distance \( L \) from the delta function potential will be

\[
\psi_{tr}^{QW} = \int a_1(k_1) T_{11}(k_1) \exp[ik_1(x + L) - iw(t + t_0 + \Delta t_{T_{11}})] dk_1
\]

\[
+ \int a_2(k_2) T_{21}(k_2) \exp[ik_1(x + L) - iw(t + t_0 + \Delta t_{T_{21}})] dk_2
\]

\[
+ \int a_1(k_1) R_{11}(k_1) \exp[ik_1(x - L) - iw(t + t_0 + \Delta t_{R_{11}})] dk_1
\]

\[
+ \int a_2(k_2) R_{21}(k_2) \exp[ik_1(x + L) - iw(t + t_0 + \Delta t_{R_{11}})] dk_2
\]
Here $t_0 + \Delta t_{T_{12}}$ is for example the time taken by a particle in going from first channel in the left lead to the first channel on the right lead, and so on. One has to start with an infinitesimal potential so that with a small probability a particle goes from channel 2 on left to channel 1 on the right with an infinitesimal $\Delta t_{T_{12}}$. And then by increasing the potential to its actual value, one can get actual $\Delta t_{T_{12}}$ etc. It is easy to show that $a_1(k_1) = a_2(-k_1)$ and $a_2(k_2) = a_2(-k_2)$. So FSR as well as WDT will be correct if $\psi_{fr}$ is also a Gaussian wave packet. One way to get that is if $T_{11}(k), T_{21}(k), R_{21}(k)$ and $R_{11}(k)$ are simultaneously real. Because then the weight of the $k$th component is a real number times $a_1(k)$ and further those real numbers are complimentary to each other and also summed. That is if $T_{11}(k)$ increases then $T_{22}(k)$ decreases and the first two terms in Eq. 32 compensate each other and so on. One can also show that $T_{21} = R_{21}$, and $\arg(T_{21}) = \arg(R_{21}) = \arg(R_{11})$. In the following figure we show that $T_{11}, T_{21}, R_{21}$ and $R_{11}$ are simultaneously real at the Fano resonance. Since they are real, their squares add up to make 1. So they are also complimentary to each other and compensate each other. If $T_{11}$ is small the $R_{11}$ is large and so on. Actually, all the phase shifts vary strongly with energy as is expected in a quantum regime, but the variations are around 0 and becoming exactly 0 at the Fano resonance.

One can check the outgoing wave packets in the other channels also. They all show similar behavior at the Fano resonance. Although, the individual wave packets get strongly scattered, the four scatterings compensate each other in such a way that the outgoing waves are similar to the incoming waves. So the derivation of WDT holds good and so naturally the WDT also holds good. And then summing over all the particles making the wave packet, one naturally gets that FSR holds good. This provides a physical picture that helps us to understand why semi-classical formulas based on un-dispersed wave packets hold good in an extreme quantum regime. Semi-classical formulas are always much simpler and easy to understand as it has classical analogies.

V. CONCLUSION

For larger systems, that is when the sample size is larger than the inelastic mean free path, it has been argued that the scattering matrix approach do not take into account the conservation of charge [22]. FSR can break down due to non-conservation of charge [23]. In this work we show that even for mesoscopic systems, that is when sample size is smaller than inelastic mean free path, although charge is conserved, the scattering matrix approach does not give the DOS exactly. In a quantum wire, the correction term due to the evanescent modes is quite complicated and it is not possible to make any general statement about it like correction term is negligible in semi-classical regime and large in quantum regimes. Quite counter intuitively, the correction term in Eq. 25, becomes 0 at the Fano resonance as a result of which the FSR becomes exact. We do not know of any system where this correction term can become exactly 0. We have shown that in single channel quantum wire, this is true for all potential that exhibit a Fano resonance as it only requires the presence of a transmission zero. We have also taken a scatterer in a multi channel quantum wire that has Fano resonance, wherein all the $S_{0n}$s are non zero and also strongly energy dependent. But the correction term is once again exactly 0 making the FSR exact at the Fano resonance. We provide a physical understanding of this based on non-dispersive wave packets that are crucial for the derivation of semi-classical formulas like FSR and WDT. This gives us a general prescription to check for a given Fano resonance in a multi-channel quantum wire, if semi-classical formulas will be exact or not. Although, the quantum mechanical scattering can strongly disperse the different partial waves, the resultant of all possible partial waves in the Hilbert space and their scattering compensate each other in such a way that the resultant wave-packet is un-dispersed.

The advantage of using FSR to know the DOS of a system has certain advantages. It makes it un-necessary to find the local wave-functions inside a scatterer and also removes the problem of integrating the LDOS to find the DOS. Also FSR is expected to work in presence of electron-electron interactions [24]. An easy way to see this is to consider the Kohn-Sham theorem [25], which essentially means that an electron passing through an interacting system, actually passes through a one body effective potential that accounts for exchange and correlation effects exactly.

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VII. APPENDIX

Let us calculate the DOS $\rho(E)$ for the system in Fig. 2. We first consider the electron incident from the left (as shown in Fig. 2), with incident wave vector $k$. The PDOS in this case is

$$\rho^{(1)}(E) = \frac{1}{\hbar v} \int_{-L}^{L} |ae^{ikx} + be^{-ikx}|^2 dx$$

$$+ \int_{-\infty}^{-l} |e^{ikx} + Re^{-ikx}|^2 dx + \int_{l}^{\infty} |Te^{ikx}|^2 dx$$

(33)

$T$ is the same whether incident from left or incident from right. We next consider the electron incident from the right, with incident wave vector $-k$. The PDOS in this
The indefinite integrals on \( \sin[x] \) and \( \cos[x] \) can be done by breaking them up in exponential functions to give

\[
\rho(E) = \frac{1}{h^2} \int_{-\infty}^{\infty} dx \rho(kx) \int_{-\infty}^{\infty} dx \rho(-kx)
\]

Thus we have proved that

\[
\rho(E) - \rho_0(E) = \rho^{GC}(E) - \rho_0^{GC}(E)
\]

where

\[
\rho'(E) = \int_{-\infty}^{\infty} |ae^{ikx} + be^{-ikx}|^2 dx - 2 \int_{-\infty}^{\infty} dx = \frac{\hbar v}{2\pi} (\rho^{GC}(E) - \rho_0^{GC}(E))
\]

The indefinite integrals on \( \sin[x] \) and \( \cos[x] \) can be done by breaking them up in exponential functions to give

\[
\rho(E) = \frac{1}{h^2} \int_{-\infty}^{\infty} dx \rho(kx) \int_{-\infty}^{\infty} dx \rho(-kx)
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\]
$T_{11}, R_{11}, T_{21}$ and $R_{21}$ are simultaneously real at the Fano resonance.
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