

Nondispersive backscattering in quantum wires

P. Singha Deo

Unit for Nano Science and Technology, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake City, Kolkata 98, India

(Received 9 October 2006; revised manuscript received 6 February 2007; published 28 June 2007)

At a Fano resonance in a quantum wire, there is strong quantum-mechanical backscattering. 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 collision of the sine-Gordon model. As a result of such nondispersive behavior, the derivation of semiclassical formulas, such as 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 exhibits 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 the 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, the Friedel sum rule may break down away from the Fano resonances.

DOI: 10.1103/PhysRevB.75.235330

PACS number(s): 61.66.-f, 61.72.Ff

I. INTRODUCTION

The Landauer-Buttiker approach to mesoscopic physics is rather novel. One of the great successes of this approach is the Landauer-Buttiker conductance formula. To understand this approach further, 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,¹⁻³ in low-dimensional systems, some attempts to derive it ignore the effects of the leads.^{4,5} Buttiker and co-workers emphasize the effects of the leads and find a correction term to the FSR.⁶⁻⁸ They state that in quantum regimes, FSR will break down.⁸ When the system is in the WKB limit, then FSR works very well.⁸ Recent explicit calculations⁹ 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.^{10,11} Such an impurity in a quantum wire has attracted many theoretical investigations.¹²⁻¹⁵ Reference 9 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 worse in the regimes away from the Fano resonance (that are in the WKB regime). Reference 16 shows that other semiclassical formulas such as 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. 9 and 16. 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 gives strong backscattering that is quantum mechanical in nature, such scattering does not disperse a wave packet. We shall also show that this explains why semiclassical 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 textbooks 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.¹⁷⁻²⁰ 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 de-

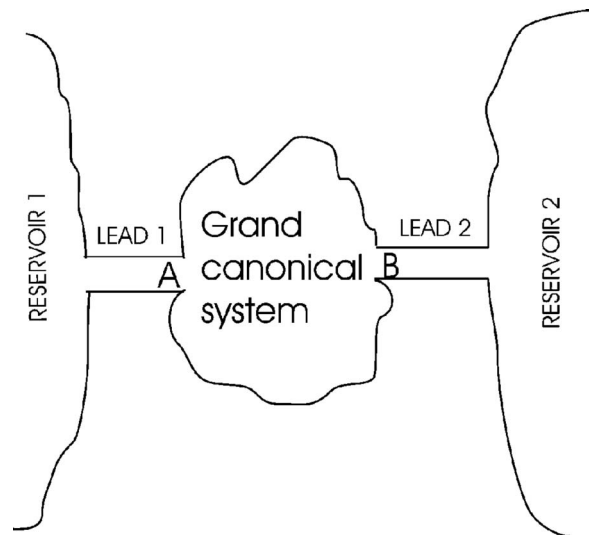


FIG. 1. A grand canonical system, extending from *A* to *B*, connected to two reservoirs on two sides with ideal leads.

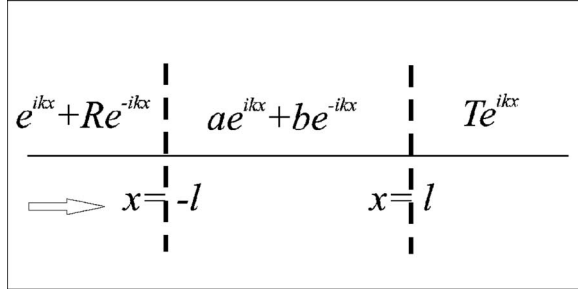


FIG. 2. A realization of the system shown in Fig. 1 in one dimension. $x=-l$ corresponds to the point A in Fig. 1 and $x=l$ corresponds to the point B.

stroyed. Phase shifts are defined with respect to points A and B and not with respect to $\pm\infty$.⁶ Density of states (DOS) is also the local density of states (LDOS) integrated between the points A and B.⁶ The scattering problem is completely defined with the points A and B,⁶ 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 a nonequilibrium situation. All this will become explicit in our model calculation.

II. SCATTERING SOLUTION

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

$$S = \begin{pmatrix} R & T \\ T & R \end{pmatrix}, \quad (1)$$

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

Recent developments in fabrication techniques allow us to fabricate a two-dimensional (2D) quantum wire. This is essentially done by making the confinement potential in the third direction so narrow that only one mode is populated and there are no degrees of freedom in the third direction. In the following, when we refer to quantum wire, it means a 2D quantum wire where transverse modes are quantized like that of a square well potential and modes along the length of the wire are propagating plane waves.

If we consider a two-channel quantum wire with a delta function potential, the scattering matrix will be 4×4 as shown below,

$$S = \begin{bmatrix} R_{11} & R_{12} & T_{11} & T_{12} \\ R_{21} & R_{22} & T_{21} & T_{22} \\ T_{11} & T_{12} & R_{11} & R_{12} \\ T_{21} & T_{22} & R_{21} & R_{22} \end{bmatrix}. \quad (2)$$

We are using a notation where $S_{11}=R_{11}$ as it is a reflection amplitude for an electron incident along the first transverse

mode from the left lead (lead 1) 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, $S_{13}=T_{11}$ 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 (lead 2). One can easily understand the rest. One can solve the scattering problem¹¹ to find that for α and β taking values of 1 or 2,

$$R_{\alpha\beta} = -\frac{i\Gamma_{\alpha\beta}}{2d\sqrt{k_\alpha k_\beta}}. \quad (3)$$

If $\alpha \neq \beta$, then

$$T_{\alpha\beta} = -\frac{i\Gamma_{\alpha\beta}}{2d\sqrt{k_\alpha k_\beta}}. \quad (4)$$

If $\alpha = \beta$, then

$$T_{\alpha\alpha} = 1 + R_{\alpha\alpha}. \quad (5)$$

Here,

$$\Gamma_{\alpha\beta} = \frac{2m\gamma}{\hbar^2} \sin\left[\frac{\alpha\pi}{W}\left(y_j + \frac{W}{2}\right)\right] \sin\left[\frac{\beta\pi}{W}\left(y_j + \frac{W}{2}\right)\right], \quad (6)$$

$$d = 1 + \sum_\nu \frac{\Gamma_{\nu\nu}}{2\kappa_\nu} + i \sum_\alpha \frac{\Gamma_{\alpha\alpha}}{2k_\alpha}, \quad (7)$$

$$\Gamma_{\nu\nu} = \frac{2m\gamma}{\hbar^2} \sin\left[\frac{\nu\pi}{W}\left(y_j + \frac{W}{2}\right)\right] \sin\left[\frac{\nu\pi}{W}\left(y_j + \frac{W}{2}\right)\right]. \quad (8)$$

ν can take any integer value greater than 2 (i.e., $\nu = 3, 4, 5, \dots$). γ 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 first propagating channel. $k_2 = \sqrt{\frac{2m}{\hbar^2}E - \frac{4\pi^2}{W^2}}$ is the wave vector for the second propagating channel. $\kappa_\nu = \sqrt{\frac{\nu^2\pi^2}{W^2} - \frac{2mE}{\hbar^2}}$ is the wave vector for the ν th evanescent channel. E is the incident energy.

In principle, the sum over the evanescent modes includes an infinite number of evanescent modes. If all the infinite evanescent modes are included, then the delta potential cannot scatter. However, the higher evanescent modes involve such a high amount of transverse energy given by $\frac{\hbar^2\nu^2\pi^2}{2mW^2}$ that such high-energy electrons cannot be realized in a quantum wire. They will either dissipate or overcome the work function of the wire to be ejected from the wire. So, there is a natural cutoff for the infinite series. Given any cutoff, there are potential strengths for which our results discussed below are valid. This is essentially because the finite number of evanescent modes just renormalize the strength of the delta function potential. Given such an energy cutoff, we can still take the 2D limit by making $W \rightarrow \infty$ and then the above expressions (3)–(8) do give the 2D result wherein a delta function potential cannot scatter.²¹

The n th quasibound state or the Fano resonance occurs at energies that satisfy the following equation:

$$1 + \sum_{\nu=n}^{\nu=\infty} \frac{\Gamma_{\nu\nu}}{2\kappa_{\nu}} = 0. \quad (9)$$

At such an energy, there will be a large amount of charge localized around the impurity and decaying away from the impurity. One has to define the points A and B as described in Ref. 9. Also, in real systems, ν will have some cutoff as discussed above. The α th injectivity at a point $q \equiv (x, y, z)$ is due to the incident electron of velocity v_{α} (or $-v_{\alpha}$). It is defined as [one can easily see that if we sum both sides of Eq. (10) over α , then we get LDOS and hence Eq. (10) defines injectivity, and an alternate definition can be found from Eq. (18)]

$$\sum_{\beta} \rho_{\alpha\beta}(q) = \frac{1}{h|v_{\alpha}|} |\psi^{(\alpha)}(q)|^2, \quad (10)$$

where h is Plank's constant, $v_{\alpha} = \frac{\hbar k_{\alpha}}{m}$, k_{α} 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 α th channel. $\rho_{\alpha\beta}(q)$ is known as the partial local density of states (PLDOS). For different possible values of incident wave vector, we get different injectivities. Summing up for all the injectivities, we get the local density of states (LDOS). Integrating LDOS over entire spatial coordinates, we get DOS. So DOS will be

$$\rho(E) = \sum_{\alpha=1}^M \int_{-\infty}^{\infty} \frac{1}{h|v_{\alpha}|} |\psi^{(\alpha)}(q)|^2 dq \quad (11)$$

and

$$\rho^{GC}(E) = \sum_{\alpha=1}^M \int_A^B \frac{1}{h|v_{\alpha}|} |\psi^{(\alpha)}(q)|^2 dq. \quad (12)$$

Here, suffix GC stands for ‘‘grand canonical.’’ Here, M is the total number of incident channels possible.

III. FRIEDEL SUM RULE

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 the S matrix, without any knowledge of the $\psi^{(\alpha)}(q)$ as the S matrix elements can be determined experimentally^{22,23} as well as theoretically.^{24,25}

The FSR can be stated as^{9,26,27}

$$\frac{d\theta_f}{dE} \approx \pi[\rho^{GC}(E) - \rho_0^{GC}(E)], \quad (13)$$

where

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

S is the scattering matrix of a system, and E is the incident electron energy. $\rho^{GC}(E)$ is the integrated LDOS of a system

in the presence of a scatterer, as defined in Eq. (12), and $\rho_0^{GC}(E)$ is the integrated LDOS of the same system in the absence of a scatterer, which naturally requires that impurity scattering conserves the total charge in the grand canonical system (or else ρ^{GC} need not be related to ρ_0^{GC} 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 any resonance (or quasibound state), $[\rho^{GC}(E) - \rho_0^{GC}(E)]$ change by unity and hence θ_f will change by π . Moreover, $\frac{d\theta_f}{dE}$ can be determined from asymptotic wave function ($x \rightarrow \infty$), 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. 9 about the FSR. Namely, the FSR becomes exact in a purely quantum regime such as the Fano regime and worse away from the Fano regime. According to our previous understanding (see, for example, Ref. 8), 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.²⁶ We present it for 1D as the steps can be repeated for quasi-one-dimension (Q1D). Suppose there is an extended potential $V(x)$. Assuming that $S_{\alpha,\beta}(E, V(x))$ is analytic, we can make an expansion as

$$\begin{aligned} S_{\alpha,\beta}(E, V(x) + \Delta V(x)) \\ = S_{\alpha,\beta}(E, V(x)) + \int_{-\infty}^{\infty} dx' \left[\frac{\partial S_{\alpha,\beta}(E, V(x'))}{\partial V(x')} \delta V(x') \right] + \dots \end{aligned} \quad (15)$$

We have chosen the electronic charge e to be the unit of charge. Equation (15) means breaking up the increment $\Delta V(x)$ (although an infinitesimal perturbation, it is an extended potential) into many local increments $\delta V(x')$ and integrating the effect of all these local increments. $\delta V(x')$ is therefore a delta function potential at x' . Now, without any loss of generality, we can say that $\Delta V(x) = V_0$ for all x . In other words, $\Delta V(x)$ is a constant potential. Since $\Delta V(x) = V_0$ for all x , the local perturbation $\delta V(x')$ is also equal to V_0 numerically. One has to remember that the two perturbations $\Delta V(x) = V_0$ and $\delta V(x') = V_0 \delta(x')$ are actually different. One of them is a global perturbation or an extended perturbation, while the latter is a local perturbation. However, for $V_0 \rightarrow 0$, one can neglect this difference between them to write

$$\begin{aligned} \frac{S_{\alpha,\beta}(E, V(x) + V_0) - S_{\alpha,\beta}(E, V(x))}{V_0} \\ \approx \int_{-\infty}^{\infty} dx' \left[\frac{\partial S_{\alpha,\beta}(E, V(x'))}{\partial V(x')} \right]. \end{aligned} \quad (16)$$

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 $\Delta E = V_0$. Thus,

$$\begin{aligned} & \frac{S_{\alpha,\beta}(E - \Delta E, V(x)) - S_{\alpha,\beta}(E, V(x))}{-\Delta E} \\ &= \frac{S_{\alpha,\beta}(E, V(x) + \Delta V(x)) - S_{\alpha,\beta}(E, V(x))}{V_0} \\ &\approx \int_{-\infty}^{\infty} dx' \left[\frac{\partial S_{\alpha,\beta}(E, V(x'))}{\partial V(x')} \right]. \end{aligned} \quad (17)$$

One can prove that²⁶

$$-\frac{1}{4\pi i} \left(S_{\alpha\beta}^\dagger \frac{\partial S_{\alpha\beta}}{\partial V(x')} - HC \right) = \rho_{\alpha\beta}(x), \quad (18)$$

where $\rho_{\alpha\beta}$ is the PLDOS. The partial density of states (PDOS) is therefore $\rho'_{\alpha\beta}(E) = \int_{-\infty}^{\infty} \rho_{\alpha\beta}(x) dx$. One can take any potential in 1D and check that this equation is exact as done in Ref. 6. Therefore, from Eqs. (17) and (18),

$$\frac{1}{4\pi i} \left(S_{\alpha\beta}^\dagger \frac{dS_{\alpha\beta}}{dE} - HC \right) \approx \rho'_{\alpha\beta}(E). \quad (19)$$

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

$$\frac{1}{2i} \frac{d}{dE} \log(\text{Det}[S]) \approx \pi[\rho(E) - \rho_0(E)]. \quad (20)$$

Thus, we have derived FSR.

Replacing $\int dx' \frac{\partial S_{\alpha\beta}}{\partial V(x')}$ by $-\frac{\partial S_{\alpha\beta}}{\partial E}$ is an approximation. Thus, $\frac{d\theta_f}{dE}$ is not exactly equal to $\pi[\rho(E) - \rho_0(E)]$, and so naturally one can expect that $\frac{d\theta_f}{dE}$ is also not exactly equal to $[\rho^{GC}(E) - \rho_0^{GC}(E)]$. In fact,⁷

$$\frac{d\theta_f}{dE} = \pi[\rho^{GC}(E) - \rho_0^{GC}(E)] - \text{Im} \frac{(R_{LL} + R_{RR})}{4E}. \quad (21)$$

We have used suffixes LL and RR , instead of α and β . 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 another FSR, but the correction term $\text{Im}[(R_{LL} + R_{RR})/4E]$ is not very universal. It can be different for different kinds of resonances. Secondly, in Q1D, 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 $\text{Im}[(R_{LL} + R_{RR})/4E]$. Reference 7 and others state that this term is due to the nonconservation of charge in the grand canonical system. They state [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 into the leads. So, according to Refs. 7 and 8, 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 nonconservation of charge in the grand canonical system. Although in one, two, and three dimensions 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 in the grand canonical system, and also the correction term can be zero in the Fano regime which is a quantum regime.

It is shown in the Appendix that

$$\begin{aligned} & [\rho(E) - \rho_0(E)] - [\rho^{GC}(E) - \rho_0^{GC}(E)] \\ &= -\frac{\sin[2kl]}{k} (R_{LL} + R_{LL}^*) + \frac{\cos[2kl]}{k} (iR_{RR} - iR_{RR}^*). \end{aligned} \quad (22)$$

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

$$\frac{d\theta_f}{dE} \neq \pi[\rho(E) - \rho_0(E)]. \quad (23)$$

It can only be an approximate equality as shown in Eq. (20). The second implication is that the correction term $-\text{Im}[(R_{LL} + R_{RR})/4E]$ is not due to the lack of charge conservation in the grand canonical system. This is explained below. When we integrate over all energies, then we get that the right-hand side (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 ∞ . As $k=0$ is a nonpropagating state, in the propagating regime, $\int_{\epsilon}^{\infty} dE [\rho^{(GC)}(E) - \rho_0^{(GC)}(E)] = 0$. 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 in the grand canonical system. It is just an error due to an approximation in the algebra.

Although in the Appendix we have considered a one-dimensional 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 $k_1 = \sqrt{\frac{2m_e}{\hbar^2} E - \frac{\pi^2}{W^2}}$. So, for a single-channel quantum wire,

$$\frac{d\theta_f}{dE} = \pi[\rho^{GC}(E) - \rho_0^{GC}(E)] - \text{Im} \frac{R_{LL} + R_{RR}}{4 \left(E - \frac{\hbar^2 \pi^2}{2mW^2} \right)}. \quad (24)$$

First of all, note the presence of sample specific parameter $\frac{\hbar^2 \pi^2}{2mW^2}$ in the correction term. This equation is the same whether evanescent modes are included or not included. However, only the expressions for R_{LL} and R_{RR} changes completely if we include or exclude the evanescent modes. From Eq. (3),

$$-\text{Im}[R_{LL} + R_{RR}] = \frac{\frac{\Gamma_{11}}{k_1} \left(1 + \sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}\right)}{\left(1 + \sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}\right)^2 + \left(\frac{\Gamma_{11}}{2k_1}\right)^2}. \quad (25)$$

For a delta function potential in 1D,

$$-\text{Im}[R_{LL} + R_{RR}] = \frac{\frac{\Gamma_{1D}}{k_1}}{1 + \left(\frac{\Gamma_{1D}}{2k_1}\right)^2}, \quad (26)$$

where $\Gamma_{1D} = \frac{2m\gamma}{\hbar^2}$. In comparison with the 1D case, the only difference in Q1D [compare Eqs. (25) and (26)] is the term

$$\sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}, \quad (27)$$

which is due to the evanescent modes. If we remove this term, then the correction term is negligible for $k_1 > \Gamma_{11}$, which is the semiclassical regime. Complications in Q1D arise because of the series term $\sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}$. Even for $k_1 < \Gamma_{11}$, $\left(1 + \sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}\right)$ 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 $\left(1 + \sum_{\nu>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}\right) = 0$ at the Fano resonance [see Eq. (9)]. Alternately, one can also see this from the Fisher-Lee relationship, but Eqs. (24)–(26) help us to demonstrate the difference between 1D and Q1D and hence argue in terms of quantum behavior or semiclassical behavior. Also, note that although each term in the series in Eq. (27) decreases with energy, the sum does not decrease 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.¹³ 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 two-dimensions. 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 $\frac{d\theta_f}{dE}$ 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, $\sum_{n>1} \frac{\Gamma_{\nu\nu}}{2\kappa_\nu}$ diverges as the first term in it (i.e., $\frac{\Gamma_{22}}{2k_2}$) diverges and hence the RHS of Eq. (25) becomes 0.

IV. WIGNER DELAY TIME

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.¹⁶ The similarity between WDT and FSR can be seen from Eqs. (19) and (20),

$$\sum_{\alpha\beta} \frac{1}{4\pi i} \left[S_{\alpha\beta}^\dagger \frac{dS_{\alpha\beta}}{dE} - HC \right] = \sum_{\alpha\beta} \frac{1}{2\pi} \left[|S_{\alpha\beta}|^2 \frac{d}{dE} \arg(S_{\alpha\beta}) \right] \approx \sum_{\alpha\beta} \int_{-\infty}^{\infty} \rho_{\alpha\beta}(x) dx. \quad (28)$$

$\hbar \frac{d}{dE} \arg(S_{\alpha\beta})$ is the WDT for particles transmitted from the α th channel to the β th channel, and there are $|S_{\alpha\beta}|^2$ of such particles. One can choose $\hbar = 1$. Here, $\arg(S_{\alpha\beta}) = \arctan \left[\frac{\text{Im}[S_{\alpha\beta}]}{\text{Re}[S_{\alpha\beta}]} \right]$. We have also seen that the left-hand side (LHS) in Eq. (28) is the semiclassical limit of the LHS of Eq. (18) integrated over x' , α , and β . So, in the semiclassical limit, WDT times the number of particles involved gives the PDOS. It was shown in Ref. 9 that in the Fano regime, also, the WDT $\left[\frac{1}{2\pi} |S_{\alpha\beta}|^2 \frac{d}{dE} \arg(S_{\alpha\beta}) \right]$ gives the PDOS $\left[\int_{-\infty}^{\infty} \rho_{\alpha\beta}(x) dx \right]$ exactly, in spite of the fact that Fano resonance is a quantum phenomenon. This happens for single-channel quantum wires as well as for multichannel quantum wires. Another way to see that the WDT is semiclassical is that its derivation is based on nondispersive wave packets. Below we show how nondispersive 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 nondispersive wave packets. Let us consider an incident Gaussian wave packet in 1D representing an ensemble of noninteracting particles. $a(k)$ is the weight of the k th Fourier component in the incident Gaussian wave packet,

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

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

$$\psi_{tr}(x, t) = \int_{-\infty}^{\infty} a(k) T(k) \exp[ik(x+L) - i\omega(t+t_0 + \Delta t)] dk. \quad (30)$$

Here, $T(k)$ is the transmission amplitude of the potential in the region of length L . t_0 is the time that the free wave packet would have taken if the potential was zero in the region of length L . $t_0 + \Delta t$ is the time that the wave packet takes in the presence of the potential. If we go to the semiclassical limit, then we should get close to classical behavior that implies $|T(k)| = 1$ and $\psi_{tr}(x, t)$ 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 is $a(k)T(k)$ and, hence, ψ_{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 ψ_{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 $T(k) \rightarrow 0$ and $R(k) \rightarrow -1$. In this case, $R(k)$ is real. One finds the WDT

$$\Delta t = \hbar \frac{d}{dE} \arg(R) = \frac{d}{dw} \arg(R), \quad (31)$$

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

This explains why FSR is exact in the 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 zero transmission that is always there for all potentials that support a Fano resonance. However, the correctness of FSR or WDT does not only occur in the case of single-channel quantum wires where $R(k)=-1$ as in the semiclassical limit, but it also happens in multichannel quantum wires where $|R_{11}(k)| \neq 1$ and $|T_{11}(k)| \neq 0$. So how for such a system WDT or FSR remains exact?

In order to show how one can get nondispersive wave packets in the presence of quantum scattering, we take a clue from the kink-antikink solution of the sine-Gordon equation. Suppose we have a delta function potential in a two-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 second channel, that is, the first excited transverse mode, and 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

$$\begin{aligned} \psi_{tr}^{OW} = & \int a_1(k_1) T_{11}(k_1) \exp[ik_1(x+L) - iw_1(t+t_0 + \Delta t_{T_{11}})] dk_1 \\ & + \int a_2(k_2) T_{21}(k_2) \exp[ik_1(x+L) \\ & - iw_1(t+t_0 + \Delta t_{T_{21}})] dk_1 \\ & + \int a_1(k_1) R_{11}(k_1) \exp[ik_1(x+L) - iw_1(t+t_0 \\ & + \Delta t_{R_{11}})] dk_1 + \int a_2(k_2) R_{21}(k_2) \exp[ik_1(x+L) - iw_1(t \\ & + t_0 + \Delta t_{R_{11}})] dk_1. \end{aligned} \quad (32)$$

Here, $t_0 + \Delta t_{T_{11}}$ is, for example, the time taken by a particle in going from the 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 the left to channel 1 on the right and traverses the region of length L in time t_0 . It is easy to show that $a_1(k_1) = a_1(-k_1)$ and $a_2(k_2) = a_2(-k_2)$. Also, note that $T_{21}(k_2) = T_{12}(k_1)$, $R_{21}(k_2) = R_{12}(k_1)$, and $\Delta t_{T_{21}} = \Delta t_{R_{11}}$ fol-

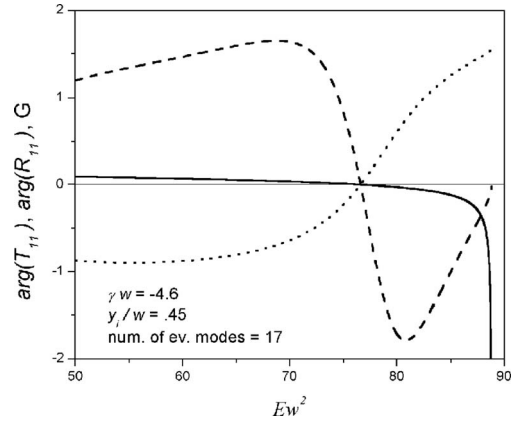


FIG. 3. This figure is for a delta function potential in Q1D ($\gamma = -4.6$, $y_i = 0.45$, the number of propagating modes is 2, and the number of evanescent modes is 17). Here, $G = 1 + \sum_{\nu=n}^{\infty} \frac{\Gamma_{\nu\nu}}{2k_\nu}$, that is, the LHS of Eq. (9). It is shown by the solid line. When it crosses the energy axis then we get a bound state. $\arg(T_{11})$ (dashed curve) and $\arg(R_{11})$ (dotted curve) become simultaneously 0 at the bound state or at the Fano resonance. This implies that T_{11} , R_{11} , T_{21} , and R_{21} are simultaneously real at the Fano resonance.

low from unitarity and time reversibility. So, FSR as well as WDT will be correct if ψ_{tr}^{OW} is also a Gaussian wave packet. Now, nondispersive behavior does not only mean that a Gaussian wave packet is transmitted as a Gaussian wave packet, but a wave packet of any shape (Lorentzian, square, etc.) will be transmitted without changing its shape. Hence, without any loss of generality, we can take the initial weights $a_2(k_2)$ or $a_1(k_1)$ to be constants, which implies

$$\begin{aligned} \psi_{tr}^{OW} = & \int T_{11}(k_1) \exp[ik_1(x+L) - iw_1(t+t_0 + \Delta t_{T_{11}})] dk_1 \\ & + \int [T_{12}(k_1) + R_{11}(k_1) + R_{12}(k_1)] \exp[ik_1(x+L) \\ & - iw_1(t+t_0 + \Delta t_{R_{11}})] dk_1. \end{aligned} \quad (33)$$

One way to get that ψ_{tr}^{OW} is the same as the initial incident wave packets is that if $T_{11}(k_1)$, $T_{21}(k_2)$, $R_{21}(k_2)$, and $R_{11}(k_1)$ are simultaneously real, because then the weight of the k th component is a real number. The main source of dispersion is always the phases of scattering amplitudes, with the energy dependence of their absolute values being always weak. Besides, there could be some fluctuation in $|T_{11}(k_1)|$, $|T_{21}(k_2)|$, $|R_{21}(k_2)|$, and $|R_{11}(k_1)|$ individually in the quantum regimes, but their sum is weakly energy dependent in all regimes (classical or quantum) and becoming constant at the Fano resonance. Similarly, the four wave packets in Eq. (32) compensate each other to make ψ_{tr}^{OW} a Gaussian wave packet. One can also show that $T_{21} = R_{21}$, and $\arg(T_{21}) = \arg(R_{21}) = \arg(R_{11})$. In Fig. 3, 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 complementary to each other and compensate each other. 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. Then, summing over all the particles making the wave packets, one naturally gets that FSR holds good. This provides a physical picture that helps us to understand why semiclassical formulas based on undispersed wave packets hold good in an extreme quantum regime. Semiclassical formulas are always much simpler and easy to understand as they have 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 does not take into account the conservation of charge.²⁸ FSR can break down due to non-conservation of charge.²⁹ 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, such as correction term is negligible in the semiclassical regimes and large in quantum regimes. Quite counterintuitively, 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 a single-channel quantum wire, this is true for all potentials that exhibit a Fano resonance as it only requires the presence of a zero transmission. We have also taken a scatterer in a multichannel quantum wire that has Fano resonance, wherein all the $S_{\alpha\beta}$'s are nonzero and also strongly energy dependent. However, 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 nondispersive wave packets that are crucial for the derivation of semiclassical formulas such as FSR and WDT. This gives us a general prescription to check for a given Fano resonance in a multichannel quantum wire if semiclassical 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 undispersed.

The advantage of using FSR to know the DOS of a system has certain advantages. It makes it unnecessary 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 the presence of electron-electron interactions.³⁰ An easy way to see this is to consider the Kohn-Sham theorem,³¹ 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.

ACKNOWLEDGMENT

The author is grateful to ICTP, Italy for support where a part of this work was done.

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

$$\rho^{(1)}(E) = \frac{1}{h|v|} \left[\int_{-l}^l |ae^{ikx} + be^{-ikx}|^2 dx + \int_{-\infty}^{-l} |e^{ikx} + R_{LL}e^{-ikx}|^2 dx + \int_l^{\infty} |Te^{ikx}|^2 dx \right]. \quad (\text{A1})$$

Here, $v = \hbar k/m$. T is the same whether incident from the left or incident from the right. We next consider the electron incident from the right, with incident wave vector $-k$. The PDOS in this case is

$$\rho^{(2)}(E) = \frac{1}{h|v|} \left[\int_{-l}^l |ae^{-ikx} + be^{ikx}|^2 dx + \int_l^{\infty} |e^{-ikx} + R_{RR}e^{ikx}|^2 dx + \int_{-\infty}^{-l} |Te^{-ikx}|^2 dx \right]. \quad (\text{A2})$$

Therefore, DOS is given by

$$\begin{aligned} \rho(E) = \rho^{(1)}(E) + \rho^{(2)}(E) = & \frac{1}{hv} \left[2 \int_{-\infty}^{\infty} dx + 2\rho' \right. \\ & + R_{LL}^* \int_{-\infty}^{-l} \cos[2kx] dx + iR_{LL}^* \int_{-\infty}^{-l} \sin[2kx] dx \\ & + R_{RR} \int_l^{\infty} \cos[2kx] dx + iR_{LL}^* \int_l^{\infty} \sin[2kx] dx \\ & + R_{LL} \int_{-\infty}^{-l} \cos[2kx] dx - iR_{LL} \int_{-\infty}^{-l} \sin[2kx] dx \\ & \left. + R_{RR}^* \int_l^{\infty} \cos[2kx] dx - iR_{RR}^* \int_l^{\infty} \sin[2kx] dx \right], \end{aligned} \quad (\text{A3})$$

where

$$\begin{aligned} \rho' = & \int_{-l}^l |ae^{ikx} + be^{-ikx}|^2 dx - 2 \int_{-l}^l dx \\ = & \frac{hv}{2\pi} [(\rho^{GC}(E) - \rho_0^{GC}(E))]. \end{aligned} \quad (\text{A4})$$

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

$$\rho(E) = \frac{1}{hv} \left[2 \int_{-\infty}^{\infty} dx + 2\rho' - \frac{\sin[2kl]}{k} (R_{LL} + R_{LL}^*) + \frac{\cos[2kl]}{k} (iR_{RR} - iR_{RR}^*) \right]. \quad (\text{A5})$$

Thus, we have proven that

$$\rho(E) - \rho_0(E) = \rho^{GC}(E) - \rho_0^{GC}(E) - \frac{\sin[2kl]}{k} (R_{LL} + R_{LL}^*) + \frac{\cos[2kl]}{k} (iR_{RR} - iR_{RR}^*). \quad (\text{A6})$$

-
- ¹M. Kohmoto and T. Koma, arXiv:math-ph/0508030.
²V. I. Okulov, arXiv:cond-mat/0401174 (unpublished).
³R. Dashen, S.-K. Ma, and H. J. Bernstein, Phys. Rev. **187**, 345 (1969).
⁴S. Souma and A. Suzuki, Phys. Rev. B **65**, 115307 (2002).
⁵Y. Avishai and Y. B. Band, Phys. Rev. B **32**, 2674 (1985).
⁶V. Gasparian, T. Christen, and M. Buttiker, Phys. Rev. A **54**, 4022 (1996).
⁷A. L. Yeyati and M. Buttiker, Phys. Rev. B **62**, 7307 (2000).
⁸T. Taniguchi and M. Buttiker, Phys. Rev. B **60**, 13814 (1999).
⁹S. Bandopadhyay and P. S. Deo, Phys. Rev. B **68**, 113301 (2003).
¹⁰P. Singha Deo, Solid State Commun. **107**, 69 (1998).
¹¹P. F. Bagwell, Phys. Rev. B **41**, 10354 (1990).
¹²P. F. Bagwell and R. K. Lake, Phys. Rev. B **46**, 15329 (1992).
¹³D. Boese, M. Lischka, and L. E. Reichl, Phys. Rev. B **61**, 5632 (2000), and references therein.
¹⁴C. S. Chu and R. S. Sorbello, Phys. Rev. B **40**, 5941 (1989).
¹⁵E. Granot, Phys. Rev. B **71**, 035407 (2005); Physica E (Amsterdam) **31**, 13 (2006).
¹⁶P. Singha Deo, Int. J. Mod. Phys. B **19**, 899 (2005).
¹⁷Colin Benjamin and A. M. Jayannavar, Phys. Rev. B **68**, 085325 (2003); **65**, 153309 (2002).
¹⁸M. Buttiker, Phys. Rev. B **32**, 1846 (1985).
¹⁹E. Akkermans, A. Auerbach, J. E. Avron, and B. Shapiro, Phys. Rev. Lett. **66**, 76 (1991).
²⁰A. A. Clerk, X. Waintal, and P. W. Brouwer, Phys. Rev. Lett. **86**, 4636 (2001).
²¹M. Y. Azbel, Phys. Rev. B **43**, 2435 (1991); **43**, 6717 (1991); Phys. Rev. Lett. **67**, 1787 (1991).
²²K. Kobayashi, H. Aikawa, S. Katsumoto, and Y. Iye, Phys. Rev. B **68**, 235304 (2003).
²³K. Kobayashi, H. Aikawa, A. Sano, S. Katsumoto, and Y. Iye, Phys. Rev. B **70**, 035319 (2004).
²⁴B. F. Bayman and C. J. Mehoke, Am. J. Phys. **51**, 875 (1983).
²⁵R. Englman and A. Yahalom, Phys. Rev. B **61**, 2716 (2000).
²⁶M. Buttiker, H. Thomas, and A. Pretre, Z. Phys. B: Condens. Matter **94**, 133 (1994); M. Buttiker, Pramana, J. Phys. **58**, 241 (2002).
²⁷Here, we are using the textbook definition of FSR. See, for example, J. M. Ziman, *Principles of the Theory of Solids*, 2nd ed. (Cambridge University Press, Cambridge, 1979). The Buttiker-Thomas-Pretre (BTP) formula [Eq. (18)], on the other hand, is a unique formula for the LDOS. One can, of course, integrate the LDOS to get the DOS, but this is not a substitute for the FSR. This is rather an alternate approach to integrating the squared absolute value of the local wave function to get the DOS. The beauty of the FSR is that one can avoid calculating the LDOS or the local wave function and directly arrive at the DOS and hence thermodynamic properties from the asymptotic wave functions or S matrix. The essence of the BTP formula is that it helps us to understand ac response, fluctuations, nonlinear effects, etc., in terms of the scattering matrix.
²⁸M. P. Das and F. Green, J. Phys.: Condens. Matter **15**, L687 (2003).
²⁹R. Egger and H. Grabert, Phys. Rev. Lett. **79**, 3463 (1997).
³⁰J. S. Langer and V. Ambegaokar, Phys. Rev. **121**, 1090 (1961).
³¹P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L. J. Sham, *ibid.* **140**, A1133 (1965).