Larmor precession time, Wigner delay time and the local density of states in a quantum wire

P. Singha Deo

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

(Dated: December 30, 2021)

Buttiker-Thomas-Pretre (BTP) \cite{94} proposed that the concepts behind the Larmor precession time tell us that it is possible to define exactly the local density of states (LDOS) in terms of the scattering matrix. However, we take into account evanescent modes and show that for an impurity in a quantum wire, this is in principle not exactly true. We also prove that the Wigner delay time gives correct superluminal times at the Fano resonances, in spite of the fact that the stationary phase approximation is not valid there.

PACS numbers:

I. INTRODUCTION

Scattering phase shift in a scattering problem carry a lot of physical informations and are as important as scattering cross section or scattered intensity. However, phase shifts were always difficult to measure directly, until very recently \cite{11,12}. Elastic scattering plays a prominent role in mesoscopic systems, wherein the inelastic processes are quenched by reducing the temperature and the sample size \cite{3}. Transport processes and thermodynamic properties of such samples can be formulated in terms of elastic scattering \cite{6,7}. Resonances in these systems, due to elastic processes, will be mainly Fano resonances and Breit-Wigner resonance is a special case of Fano resonance \cite{6,7}. Impurities in such systems act like point scatterers and delta function like potentials are studied in this regard \cite{8,9}. Such a negative delta function potential can create Fano resonance.

II. SCATTERING PHASE SHIFT AT FANO RESONANCE

In this section we shall review some early works that lead us to study the present problem. Readers who are already familiar in this area can skip this section.

Phase shifts for Fano resonance was first studied with respect to parity effect. Electronic states in a one-dimensional (1D) ring with an Aharonov-Bohm flux piercing the ring exhibit the parity effect according to which if the magnetization of the ring with N electrons is diamagnetic (or paramagnetic) then the magnetization with N + 1 electrons is paramagnetic (or diamagnetic). Leggett conjectured that this is true even in presence of interaction between electrons as well as defects or disorder in the ring \cite{10}. Now suppose another quantum system S is coupled to the 1D ring R such that the states of S can leak into R and become flux dependent. Ref. \cite{12} shows that the states of the combined system (S+R) does not always have the property of reversing the magnetization with the addition of a single electron. It was found that the electrons in the ring undergo usual phase changes associated with their quantum mechanical motion. These phase changes are i) Aharonov-Bohm phase, ii) statistical phase, which means electrons being fermion, acquire a phase change of $\pi$ when they cross each other and iii) relative phase change due to the wave like property of the electrons, that depend on their wave vector or their kinetic energy. It was also shown \cite{10} that apart from these phase changes, there are discontinuous phase changes by $\pi$, at the zeroes of the Fano resonances (say at energy $E_0$) that will be there when the ring (with the system S attached to it) is severed at a point and two leads are attached to the two broken ends \cite{11}. If Fermi energy of $N$ body state is below $E_0$, and that of the $N + 1$ body state is above $E_0$, then the magnetization of the $N$ body state and the $N + 1$ body state is the same, and otherwise opposite. Thus Leggett’s arguments can be generalized to systems that are of the form $S+R$, with the conclusion that this new discontinuous phase change is a new phase different from the ones mentioned in i), ii) or iii) \cite{11}. When S and R are not 1D systems but becomes quasi-1D (Q1D), even then this provides a general theory to understand coupled systems \cite{11}.

In an experiment \cite{11}, a quantum dot was coupled to a ring (S+R is now a dot+ring) and the conductance oscillations of the system with an Aharonov-Bohm flux was measured. Yeyati and Buttiker \cite{12} try to interpret the conductance oscillations in terms of the flux dependence (or magnetization) of the electronic levels of the combined system (dot + ring) using the Friedel sum rule (FSR). The phase change at the resonances of the dot could be roughly understood but the phase change between the resonances of the dot could not be understood. Other works tried to assign this in between resonance phase change to processes like charge decapture (the system throws away unit charge) \cite{11}. Ref. \cite{11} and \cite{11} predicted that the resonances are actually Fano resonances and the phase change between the resonances can be explained by the new phase at the transmission zeroes and it will be an abrupt drop. It was confirmed in a later experiment that this phase drop occur over an energy scale, that is much smaller than any energy scale present in the system \cite{11}. Finite width of the leads and evanescent modes has to be considered to explain the abrupt phase changes occurring between each consecutive reso-
nances. Ref. [7] considers there is a pole between the zeroes and that is where a charge is captured and the resonance phase changes smoothly by $\pi$ in agreement with FSR. But the discontinuous phase drops being a new kind of phase, does not have anything to do with charge capture or decapture. Later on this was proved to be true whenever we have time reversal symmetry [16, 17]. Also the fact that simple 1D calculations will not explain the phase drop between each two consecutive resonances was shown [13]. Rigorous experimental verification has also emerged in favor of Fano resonances in quantum dots [19].

In fact unitarity is also required to produce such discontinuous phase changes [20]. It was subsequently seen that when an unitary channel continuously evolves into a non-unitarity channel, then along with it, the transmission zeroes evolve into minima (difference with Breit-Wigner resonance is that the minima has a complex zero, that is for a complex value of incident energy, transmission zeroes evolve into minima (difference with Breit-Wigner resonance is that the minima has a complex zero, that is for a complex value of incident energy, transmission amplitude is zero), and discontinuous phase drops evolve into continuous phase drops [21]. As an example, one can consider a two channel quantum wire with a delta potential (see Fig. 1) at the middle of the quantum wire. Since the two channels of the quantum wire are opposite parity states like the ground state and the first excited state of a quantum well, the two channels are decoupled. If an electron is incident from the left in the first channel then amplitude of transition to the second channel i.e., $t_{12}$ (state 1 to state 4) or $r_{12}$ (state 1 to state 2) is zero, making the first channel preserve unitarity. Whenever $|t_{11}|^2$ has a zero, the phase of $t_{11}$ drops (or decreases) discontinuously by $\pi$. Now if the delta potential is shifted slightly from the center of the quantum wire, then parity is no longer a good quantum state and $t_{12}$ etc are no longer zero. So by continuously displacing the delta potential from the center, one can destroy the individual unitarity of each channel and thus make the discontinuous phase drops continuously evolve into fast continuous phase drops. These phase drops can be seen in Fig. 2 at an energy $E_a \approx 85$. Even dephasing can result in the loss of unitarity [21] and can explain the small width of the phase drops observed in the experiment. For the two propagating channel case,

$$\frac{\partial \theta_f}{\partial E} = \frac{1}{2\pi} \left[ |r_{11}|^2 \frac{\partial \arg(r_{11})}{\partial E} + |r_{22}|^2 \frac{\partial \arg(r_{22})}{\partial E} 
+ 4|r_{12}|^2 \frac{\partial \arg(r_{12})}{\partial E} + |t_{12}|^2 \frac{\partial \arg(t_{11})}{\partial E} 
+ |t_{22}|^2 \frac{\partial \arg(t_{22})}{\partial E} \right]$$

Here $\theta_f$ stands for Friedel phase. For the delta potential at the center of the wire, the discontinuous drops in $\arg(t_{11})$ or $\arg(t_{22})$ occur when $|t_{11}|^2=0$ and $|t_{22}|^2=0$ and so it is obvious from Eq. 1 that there are no drops in $\theta_f$. In that case, obviously the drops in $\arg(t_{11})$ or $\arg(t_{22})$ do not have anything to do with $\theta_f$ and hence charge decapture. But for the $\delta$ potential off center, since $|t_{11}|^2$ or $|t_{22}|^2$ are not zero when there are drops in their arguments, it is not obvious that these drops do not have anything to do with charge decapture. However only after all the simplification, one finds that

$$\frac{\partial \theta_f}{\partial E} = \frac{\partial \arg(r_{a\beta})}{\partial E}$$

That means $\theta_f$ only depends on the phase of reflection amplitudes and hence is completely independent of the phase drops in the transmission amplitudes. So once again the phase drops do not imply a drop in $\theta_f$ or charge decapture [21].

One also knows from earlier known results that FSR in mesoscopic systems is valid only in semi-classical regimes. And so Fano resonance being a purely quantum interference phenomenon, one would expect larger violations of FSR at the Fano resonances. Instead what Refs. [22] shows is that FSR is exact at the energy corresponding to the Fano resonance, but there are large violations away from this energy. Refs. [22] also explained that the correctness of FSR at the Fano resonance is due to the fact that there is a quasi bound state here, and hence the self energy due to the leads become minimum and hence its energy derivative becomes 0. This is obviously true for any potential that supports Fano resonances. The exactness of FSR at the Fano resonance ($E_a \approx 85$) and the deviation away from it is also shown in Fig. 2 (compare the dotted and dashed curves) for the two propagating channel case. The results are the same for any number of propagating channels. The regime around $E_a \approx 85$ is a purely quantum regime like the regime $E_a < 40$. However, in the regime around $E_a \approx 85$, which is the Fano resonance regime, FSR holds good unlike the regime $E_a < 40$, which is unexpected. $40 < E_a < 80$ is the semiclassical regime and violation of FSR here is also unexpected.

### III. THE PROBLEM

Apart from the DOS we know that time scales associated with a particle crossing a quantum mechanical potential can also be determined from the scattering phase shifts. For example, in the stationary phase approximation (i.e., phase shifts do not strongly depend on energy) $\frac{\partial}{\partial E} \arg(t_{a\beta})$ gives the Wigner delay time (WDT) for the particle to be transmitted from state $\alpha$ to state $\beta$. A negative slope in $\arg(t_{a\alpha})$, like that in the solid and dash-dotted curve at $E_a \approx 85$ in Fig. 2, means superluminality, i.e., the particle can travel faster than light across the potential, according to the WDT. However, once again, since Fano resonance is a quantum interference effect, dispersion will be very strong and stationary phase approximation will not hold good at the Fano resonances, and one cannot be sure if these negative slopes actually correspond to super-luminality. To be sure of superluminality, established theories say that one should
see if we get negative delay times from the Buttiker-Thomas-Pretre (BTP) formalism. They proposed that the Larmor precession time can be determined exactly from the scattering matrix and give the correct local delay times in all regimes \cite{4} and delay time can be determined by integrating the local delay times. It gives

\[ \nu(\alpha, E, r, \beta) = -\frac{1}{4\pi i} Tr[S_{\alpha\beta}^* \delta S_{\alpha\beta} / \delta V(r) - HC] \]  

(3)

where \( \nu(\alpha, E, r, \beta) \) is proportional to the time spent by the particle (i.e., delay time) going from state \( \alpha \) to state \( \beta \), while encountering the potential at \( r \). If we sum it up for all \( \alpha \) and \( \beta \) then it should give the LDOS at \( r \), exactly \cite{4, 21}. Originally, it was derived by considering the effect of a small magnetic field on the outgoing spin wave function. But more generally, for any potential, to obtain the LDOS at \( r \), we have to create a \( \delta \) function potential like local perturbation at \( r \) and see the change in the scattering matrix \( S \) of the entire system. Thus the delta function potential, apart from representing point defects, is also very ideal to study BTP formula and delay time.

Given the fact that the scattering phase shift at the Fano resonance often violate established theories, is the BTP formula correct in Q1D? And secondly, is there superluminality at Fano resonance? WDT suggests that there could be limitless superluminality but can we trust WDT at the Fano resonance?

\section{IV. THE SCATTERING SOLUTION}

The scattering problem is defined in Fig. 1. For this system in Fig. 1 \cite{3},

\[ t_{\alpha\beta} = r_{\alpha\beta} = -\frac{i\Gamma_{\alpha\beta}}{2d\sqrt{k_\alpha k_\beta}} \]  

(4)

where for the transmissions, \( \alpha \neq \beta \) and

\[ t_{\alpha\alpha} = r_{\alpha\alpha} + 1 \]  

(5)

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

(6)

For a quantum wire with hard wall confinement, \( \Gamma_{mn} = (2m_e/c)(h/\hbar^2)\sin[\pi m_e(y_i + w/2)]\sin[\pi n_e(y_i + w/2)] \), \( m_e \) is electron mass, \( k_n = (2m_e/c)(E - E_m) \), \( \kappa_n = (h^2/2m_e)(n^2\pi^2/w^2) \), \( E \) is incident energy. \( \Gamma_{\alpha\alpha} \) is sum over all the evanescent modes.

\textbf{Explicit calculations of LDOS:} We derive LDOS explicitly from the internal wavefunctions for unit incident flux by using \cite{17}

\[ \rho(E, x = 0, y = y_i) = \sum_\alpha \frac{2}{\hbar\nu_\alpha} |\psi_\alpha(x = 0, y = y_i)|^2 \]  

(7)

Where \( \psi_\alpha(x, y) \) is the wavefunction when incident electron is in the \( \alpha \)th channel. It can be taken from Ref. \cite{6} and can be further simplified to give

\[ \rho(E, 0, y_i) = \sum_\alpha \frac{2}{\hbar\nu_\alpha} \sum_m t_{\alpha m} \sin\left(\frac{m\pi}{w}(y_i + w/2)\right)^2 \]  

(8)

where \( \nu_\alpha = h\kappa_\alpha/m_e \) and \( \frac{2\pi}{w} \),

\[ t_{\alpha e} = \frac{-\Gamma_{ee}}{1 + \sum_e \frac{\Gamma_{ee}}{2\kappa_e} + i \sum_\alpha \frac{\Gamma_{\alpha\alpha}}{2\kappa_\alpha}} \]  

(9)

In Eq. 8, sum over \( \alpha \) runs over the propagating modes only while that for \( m \) is for all modes.

\textbf{LDOS from BTP formula:} We consider two propagating channels to present our results but we have checked that the results are the same for any number of channels including just one channel. For this case, Eq. 3 after summing over \( \alpha \) and \( \beta \) gives

\[ \nu(E, 0, y_i) = -\frac{1}{\pi i} \left[ r_{11}^* r_{22}^* + r_{22}^* r_{11}^* + 4r_{12}^* r_{12}' + r_{11}^* r_{11}' + r_{22}^* r_{22}' - HC \right] \]  

(10)

where primes mean derivatives wrt \( \gamma \) and \( \delta \gamma \) gives

\[ \nu(E, x, y) = -\frac{1}{\pi i} \left( r_{11}^* r_{22}^* + r_{22}^* r_{11}^* + 4r_{12}^* r_{12}' + r_{11}^* r_{11}' + r_{22}^* r_{22}' - HC \right) \]  

(11)

If we make a substitution of the type

\[ - \int dx' dy' \frac{\delta}{\delta V(x', y')} \rightarrow \frac{d}{dE} \]  

then we derive FSR. But this substitution being an approximation, the FSR is also approximate.

First of all, note that the role of evanescent modes on the derivative of the scattering matrix elements is that it renormalizes \( \delta \gamma \) according to the following relation.

\[ \delta \gamma \sum_e \frac{g_{ee}}{2\kappa_e} = \delta \gamma / (\text{say}) \]  

(12)

where \( g_{ee} = 2m_e/c\sin[\pi m_e(y_i + w/2)] \). Note that the sum \( \sum_e \frac{g_{ee}}{2\kappa_e} \) is not a converging series. It diverges as \( \log[N] \) as \( N \rightarrow \infty \). Here \( N \) is the total number of evanescent modes. And so derivative w.r.t \( \gamma \) will not exist for any arbitrary number of modes. Thus the expansion required to derive BTP formula is not defined at all energies and thus the concept of Larmor precession time fails. That means LDOS cannot be defined in terms of \( S \) matrix.

\section{V. VERIFICATION OF BTP FORMULA}

The derivation of Eq. 3 assumes that a small perturbation to the actual system, allows us to expand a scattering matrix element as

\[ S_{\alpha\beta}^\pm(E, V(x_i, y_i) \mp \delta V(x_i, y_i)) = S_{\alpha\beta}(E, V(x_i, y_i)) \]  

\[ \mp \int dx'_i dy'_i \delta S_{\alpha\beta}(E, V(x'_i, y'_i)) / \delta V(x'_i, y'_i) \delta V(x'_i, y'_i) + . \]  

(11)

If we make a substitution of the type

\[ - \int dx' dy' \frac{\delta}{\delta V(x', y')} \rightarrow \frac{d}{dE} \]  

then we derive FSR. But this substitution being an approximation, the FSR is also approximate.

First of all, note that the role of evanescent modes on the derivative of the scattering matrix elements is that it renormalizes \( \delta \gamma \) according to the following relation.

\[ g_{ee} \sum_e \frac{g_{ee}}{2\kappa_e} = \delta \gamma / (\text{say}) \]  

(13)
We shall also show that the expansion in Eq. 11 is valid at the Fano resonance and also explicit calculations of LDOS prove the correctness of BTP formula only at the Fano resonance. For this note that at the bound state \( \sum \frac{d}{dE} = -\delta \gamma \), irrespective of the number of evanescent modes. Thus at the Fano resonance, convergence exists and the expansion in 11 holds good. Which means that at the Fano resonance, the BTP formula will give the correct delay time and hence also the LDOS. We verify this explicitly by numerically calculating the RHS of 8 and 10. For example, let us truncate the series at the 3rd term, that is we consider 2 evanescent modes only. In that case we show in Fig. 3 that the BTP formula is accurate. To calculate the derivative we have taken 3rd term, that is we consider 2 evanescent modes only.

It is possible to provide further analytical arguments in support of our result. The RHS of Eq. 10 can be calculated by expanding the RHS of 16 and considering this explicitly by numerically calculating the RHS of 8 and 10. For example, let us truncate the series at the 3rd term, that is we consider 2 evanescent modes only. In that case we show in Fig. 3 that the BTP formula is accurate. To calculate the derivative we have taken 3rd term, that is we consider 2 evanescent modes only.

\[ \delta \gamma = 0.001 \] (see Fig. 4). This can be cross checked by using Eq. 13. Note that now although the two curves do not coincide with each other exactly, they do coincide exactly at the energy corresponding to the bound state (i.e., where both curves peak). Of course one can take a smaller value of \( \delta \gamma \) and get a better agreement between the two curves, but then again the same disagreement will be there if more evanescent modes are considered. Since the sum is not a converging sum, this will be a never ending story. One can see that \( \frac{\delta S_{\alpha \beta}}{\delta \gamma} \) do not exist for an infinite number of evanescent modes as \( \frac{\delta \gamma}{\delta \gamma} \) diverge as \( \log[N] \).

It was also shown in ref. [22] that the two curves, but then again the same disagreement will be there if more evanescent modes are considered. Since the sum is not a converging sum, this will be a never ending story. One can see that \( \frac{\delta S_{\alpha \beta}}{\delta \gamma} \) do not exist for an infinite number of evanescent modes as \( \frac{\delta \gamma}{\delta \gamma} \) diverge as \( \log[N] \).

\[ \nu(E, 0, y_i) = -\frac{1}{2\pi i} \sum_{\alpha \beta} Tr[S_\alpha^\dagger S_\beta \delta S_{\alpha \beta}] \] (14)

or

\[ \nu(E, 0, y_i) = \frac{\delta}{\delta V(0, y_i)}[-\frac{1}{2\pi i} \log Det[S]] \] (15)

It was also shown in ref. [22]

\[ \frac{-1}{2i} \log Det[S] = -\arctan \frac{\text{Im}[r_{\alpha \beta}]}{\text{Re}[r_{\alpha \beta}]} + \text{constant} \] (16)

This means that the functional derivative in 15 can be calculated by expanding the RHS of 16 and considering only the linear term in \( \delta \gamma \), provided all higher order terms are finite. In the regime \( (1 + \sum_{\alpha} \frac{1}{2\kappa_\alpha} > \sum_{\alpha} \frac{1}{2\kappa_\alpha} \), this expansion can be done using (4) and (6), to give

\[ \arctan \frac{\text{Im}[r_{\alpha \beta}]}{\text{Re}[r_{\alpha \beta}]} = \frac{\pi}{2} - \sum_{\alpha} \frac{\Gamma_{\alpha}}{2\kappa_\alpha} \sum_{\alpha} \frac{\Gamma_e}{2\kappa_e} + 1 + \frac{1}{3} \left( \sum_{\alpha} \frac{\Gamma_{\alpha}}{2\kappa_\alpha} \right)^3 \left( \sum_{\alpha} \frac{\Gamma_e}{2\kappa_e} \right)^3 \ldots \] (17)

It can be seen that the coefficients of higher order terms as well as the coefficients of linear terms in \( \delta \gamma \), diverge as \( \log[N] \) as well as higher powers of \( \log[N] \), which implies that the functional derivative does not exist.

Wang et al [23] has pointed out some regimes where the BTP formula is violated due to the lack of gauge invariance. They also calculated the correction terms in those regimes. However, they overlooked the violations that can arise due to non-existence of functional derivatives, and we point it out in this paper. Only way out is to truncate the number of evanescent modes to keep the error within acceptable limits.

VI. GENERALIZATION

The scattering matrix \( S \) of an extended system can be written as \( S = S_1 \otimes S_2 \otimes S_3 \), where \( S_2 \) is the scattering matrix of an infinitesimal region at \( r \), \( S_1 \) and \( S_3 \) are the scattering matrices of the regions to the left and right of \( r \), respectively. Hence \( S_2 \) is the scattering matrix of a \( \delta \) function potential that we have to further perturb infinitesimally to see the changes in \( S_2 \). All the change in \( S \) will be due to this change in \( S_2 \). Thus complications of the BTP formula will depend on its complications for a \( \delta \) function potential. If we want to integrate LDOS over an extended region then one has to take \( \delta \) function potential like perturbations at many many places of the region and sum the changes they produce on the S matrix. The error will be added.

VII. WDT AT FANO RESONANCE GIVES CORRECT SUPERLUMINARITY

We have shown in section 5 that the BTP formula is exact at the Fano resonance. So the LHS in 12, operating on \( S_{\alpha \beta} \) will give the correct delay time as well as will be observed in an experiment. The substitution in 12, is exact at the Fano resonance follows from earlier results [22] that the FSR is exact at Fano resonance. Hence the RHS of 12, operating on \( S_{\alpha \beta} \) will also give the correct delay time as well as will be observed in an experiment. Hence, in spite of all non-stationary phase behavior, the WDT will exactly correspond to physical delay times at the Fano resonance and the negative slopes in Fig. 2 do mean that there is strong superluminality that can be observed.

VIII. LARGE VIOLATIONS OF FSR DUE TO EVANESCENT MODES

We see in Fig. 2 that away from the Fano resonance, there are large violations in FSR. Once we have explored the BTP formula we can now analyze the cause of it. First of all we would like to state that we are dealing with a system that is coupled to reservoirs (a grand canonical system) where the reservoirs can inject charge or absorb charge. So charge is not conserved, \( \rho - \rho_0 \) can be arbitrary, and it may not be possible to relate it to \( \frac{d\theta}{dE} \).
very strictly. But of course, as in all grand canonical sys-
tems, at equilibrium charge and energy are as good as
conserved and we can talk of Friedel sum rule. Eqn 12
suggests that if there is a sample connected to semi-infinite
quasi 1D leads then
\[ \frac{d\theta_E}{dE} = \pi [\rho(E) - \rho_0(E)]_{\text{global}} = \]
\[ \pi \sum_\alpha \frac{2}{\hbar v_\alpha} \int_{-\infty}^{\infty} \left[ |\psi(r)|^2 - |\psi_0(r)|^2 \right] dr \] (18)
where \( r \) represents coordinate. Now the sample that ex-
tends from \(-r_s\) to \(+r_s\) is a grand canonical system and
one can show that when the leads are single channel then
(in the absence of evanescent modes)
\[ \frac{d\theta_E}{dE} = \pi [\rho(E) - \rho_0(E)] = \]
\[ \pi \sum_\alpha \frac{2}{\hbar v_\alpha} \int_{-r_s}^{r_s} \left[ |\psi(r)|^2 - |\psi_0(r)|^2 \right] dr - \frac{S - S^\dagger}{4(E - E_1)} \] (19)
\[ \frac{S - S^\dagger}{4(E - E_1)} \] is the error due to the substitution in Eq. 12.
It depends on parameters like \( E_1 \) that depends on the
internal details of the potential. For multichannel leads,
all the \( E_\alpha \)s appear in the correction term. This amount
is a negligible amount for practical purposes and the substi-
tution in 12 can still be used without involving large
errors. We show below that in the presence of evanescent
modes, there will be larger errors when we make the substi-
tution in 12.

Ref. 22 did some explicit calculations to show
\[ [\rho(E) - \rho_0(E)]_{\text{global}} = \sum_\alpha \frac{2}{\hbar v_\alpha} \int_{-\infty}^{\infty} \text{propagating modes} \]
\[ + \sum_\alpha \frac{2}{\hbar v_\alpha} \int_{-\infty}^{\infty} \text{evanescent modes} \] (20)
that gives
\[ [\rho(E) - \rho_0(E)]_{\text{global}} = \sum_\alpha \frac{2|\rho_{\alpha\alpha}|}{\hbar v_\alpha} \int_{-\infty}^{\infty} dx \cos(2k_\alpha x + \eta_\alpha) \]
\[ + \sum_\alpha \frac{2}{\hbar v_\alpha} \sum_e \frac{|t_{\alpha e}|^2}{\kappa_e} \]. (21)
Here \( v_\alpha = \hbar k_\alpha/m_e \). \( \sum_\alpha \) denotes sum over all propa-
gating modes and \( \sum_e \) denotes sum over all evanes-
cent modes. \( r_{\alpha\alpha} = |\rho_{\alpha\alpha}| e^{-\eta_\alpha} \) is the \( \alpha \)th diagonal element in
the \( S \)-matrix. \( t_{\alpha e} \) is the transition amplitude from the
\( \alpha \)th propagating mode to the \( e \)th evanescent mode.

So now if we follow the scheme of 19 then \( \rho(E) - \rho_0(E) = 0 \) as \( r_s \to 0 \). But if we consider
\[ [\rho(E) - \rho_0(E)] = \sum_\alpha \frac{2}{\hbar v_\alpha} \sum_e \frac{|t_{\alpha e}|^2}{\kappa_e} \]. (22)
then we get the dotted curve in Fig 2. The first term on
the RHS of 21, gives the charge lost to the reservoir. One
can do the integration to find \( \int_{-\infty}^{\infty} dx \cos(2k_\alpha x + \eta_\alpha) = \pi \cos(\eta_\alpha) \delta(k_\alpha) \). So for \( k_\alpha > 0 \), charge is fully conserved.
The difference in the dotted and dashed curves in Fig.2,
is the error due to the substitution 12. The error is still
\( \frac{S - S^\dagger}{4(E - E_1)} \) in case of single channel leads and this error is
due to the substitution in 12.

Substitution 12 means that change in scattering matrix
element due to infinitesimal increase (decrease) in inci-
dent energy, is the same as change in scattering matrix
element due to constant infinitesimal decrease (increase)
in potential over entire space. And also the constant de-
crease in potential over entire space can be integrated as
small changes locally and adding up the effect due to all
such local changes.

If we could have chosen a \( \delta V(r) \) at \( r < -r_s \) that dis-
turbs the propagating modes at \( r \) and does not disturb
the evanescent modes at \( r \) then the error in substitution
12 would have been as negligible as it is in 1D. This is
because although the evanescent modes exist in the leads
they are to be considered as not existing in the leads but
existing in the sample (this is clear from 19, 20, 21, 22).
Indeed we see that in Eq 6, if we ignore any change in
the second term on the RHS (which is due to evanescent
modes) then the scattering matrix elements look exactly
like that of a delta function potential in 1D. But once we
include the evanescent modes on the RHS of 6, we get
diverging terms in the scattering matrix if we change \( E
\) or \( V \), and the substitution described in the above para
involves much greater error as compared to 1D.

IX. SUMMARY AND CONCLUSIONS

The BTP formalism is very crucial to understand
mesoscopic transport beyond the Landauer conductance
formula, that is beyond the linear and DC response. So
far it has been verified for simple 1D systems or sys-
tems where there are localized states completely decou-
pled from the leads. Violations of BTP formula can also
occur in situations where there is absence of gauge
invariance. We have shown that BTP formalism is not
exact in Quasi-one-dimension (Q1D) due to the presence
of evanescent modes. These evanescent modes make
the scattering matrix singular in nature and the series
expansions in Eq. 11. required to show the equality
between \( \rho \) and \( \nu \) breaks down. If there are only a few
evanescent modes in the system, then the formula may
be acceptable for practical purposes. For extended poten-
tials and large number of evanescent modes, it may not
be practical. It definitely cannot be used as a definition
for DOS. DOS has to be defined in terms of the internal
wave function and Hamiltonian. Scattering matrix will
not contain all the information. We have also proved
that in spite of all non-stationary phase effects, WDT
\((\frac{d}{dt} \text{arg}(t_{\alpha\alpha}))\) correctly give the superluminal
times and there is superluminality at the energy where the phase
drops of transmission amplitudes occur (for example at $E_a=85$ in Fig. 2). Experimentalists have always tried to find situations wherein they can create larger superluminality. A delta function potential in a Q1D wire can create limitless superluminality. So far, experiments to observe superluminality, only considered systems with Breit-Wigner type resonances.

Finally in this paragraph, we also make some comments on possible future research, that are not related to the theme of this work. Features of superluminality in case of Fano type resonances should be explored experimentally. Also as it seems that semi-classical formulas like WDT and FSR are valid at Fano resonances, in spite of strongly energy dependent scattering phase shifts, it is possible that an incident wave packet is not dispersed by scattering at Fano resonance. Parts of it will be transmitted to different channels without shape distortions. Rather, if wavepackets are simultaneously incident on the scatterer from different channels, then after scattering the outgoing wavepackets in different channels will be similar to the incoming wavepackets. Their centroids may remain unchanged before and after scattering. This normally happens for solitons and very rare in quantum mechanics.

References

[1] A. Yacoby et al., Phys. Rev. Lett. 74, 4047 (1995)
[2] G. Cernicchiaro, T. Martin, K. Hasselbach, D. Mailly, and A. Benoit, Phys. Rev. Lett. 79, 273-276 (1997)
[3] S. Datta, Electronic transport in mesoscopic systems, Cambridge university press, 1995.
[4] M. Büttiker, H. Thomas, and A Pretre, Z. Phys B 94, 133 (1994); M. Büttiker, Pramana Journal of Physics, 58, 241 (2002).
[5] M.P. Das and F. Green, J. Phys.: Condens. Matter 15, L687 (2003).
[6] P.F. Bagwell, Phys. Rev. B 41, 10354 (1990).
[7] P. Singha Deo, Physica E 1, 301 (1997); P. Singha Deo, Solid State Commun. 107, 69 (1998).
[8] D. Boese, M. Lischka, and L.E. Reichl, Phys. Rev. B 61, 5632 (2000).
[9] A.J. Leggett, in Granular Nano-Electronics, Vol. 251 of NATO Advanced Studies Institute, Series B: Physics, edited by D.K. Ferry, J.R. Barker and C. Jacoboni (Plenum, New York, 1991), p. 297.
[10] P.S. Deo, Phys. Rev. B 53, 15447 (1996).
[11] P.A. Sreeram and P. Singha Deo, Physica B 228, 345 (1996).
[12] L. Yeyati and M. Büttiker, Phys. Rev. B 52, R14360 (1995).
[13] G. Hackenbroich, W.D. Heiss and H.A. Weidenmuller, Phys. Rev. Lett. 79 127 (1997) and references therein; P.G. Silvestrov and Y. Imry, Phys. Rev. Lett. 85, 2565 (2000).
[14] P. Singha Deo and A.M. Jayannavar Mod. Phys. Lett. B 10, 787 (1996).
[15] R. Schuster et al., Nature(London) 385, 417 (1997).
[16] H.W. Lee, Phys. Rev. Lett. 82, 2358 (1999).
[17] T. Taniguchi and M. Buttiker, Phys. Rev. B 60, 13814 (1999).
[18] A.L. Yeyati and M. Büttiker, PRB, 62, 7307 (2000).
[19] K. Kobyashi, H. Aikawa, S. Katsumoto, and Y. Iye, Phys. Rev. B 68, 235304 (2003).
[20] P. Singha Deo, cond-mat/0005123.
[21] P.S. Deo, S. Bandopadhyay and S. Das, IJMP B, 16, 2247 (2002).
[22] S. Bandopadhyay and P.S. Deo, Phys. Rev. B 68, 235304 (2003); PhD thesis of S. Bandopadhyay (under preparation).
[23] J. Wang, Q. Zheng and H. Guo, Phys. Rev. B 55, 9763 (1997).
[24] T. Gramespacher and M. Büttiker, Phys. Rev. B 56, 13026 (1997); V. Gasparian, T. Christen and M. Büttiker, Phys. Rev. A 54 4022 (1996).
[25] Texier and Buttiker in Phys. Rev. B 67, 245410 (2003).
[26] L. J. Wang, et al., Nature 406, 277 (2000); A. M. Steinberg, P. G. Kwiat and R. Y. Chiao, Phys. Rev. Lett. 71, 708 (1993); S. Chu and S. Wong, Phys. Rev. Lett. 48, 738 (1982).

Figure captions

Fig. 1. Here we show a quantum wire of width $w$ with a delta function potential $V(x, y) = \gamma \delta(x) \delta(y - y_1)$ situated at $x$. We consider scattering effects when the incident electron is from the left. The sub-bands on the left of the impurity is denoted as 1 for the first mode and 2 for the second mode. Similarly the sub-bands on the right of the impurity is denoted as 3 for the first mode and 4 for the second mode.

Fig. 2. The dotted curve gives $G = G_0$ for the second mode. Similarly the sub-bands on the right of the impurity is denoted as 3 for the first mode and 4 for the second mode.

Fig. 3. The system under consideration is shown in Fig. 1. with two propagating modes. Solid line gives $H = \rho(E, 0, y_1)$, that LDOS calculated from internal wavefunction, in units of $h = (2 m w^2 / h^2)$. Dashed line gives $J = \nu(E, 0, y_1)$, i.e., LDOS calculated using BTP formula, in units of $j = h$. All parameters are the same as that considered in Fig. 2. The x-axis is energy in units of $a = w^2$.

Fig. 4. Here we consider 5000 evanescent modes and $\gamma = -1.5$. Everything else is the same as in Fig. 3.
