

Generic Transmission Zeros and In-Phase Resonances in Time-Reversal Symmetric Single Channel Transport

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We study phase coherent transport in a single channel system using the scattering matrix approach. It is shown that identical vanishing of the transmission amplitude occurs generically in quasi-1D systems if the time reversal is a good symmetry. The transmission zeros naturally lead to abrupt phase changes (without any intrinsic energy scale) and in-phase resonances, providing insights to recent experiments on phase coherent transport through a quantum dot. [S0031-9007(99)08737-2]

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In 1995, it was first demonstrated in an experiment using the Aharonov-Bohm (AB) interference effect that the electron transport through a quantum dot contains a phase coherent component [1]. This experiment, however, was found to have some problem due to the so-called phase locking effect [2]. Two years later, the experiment was refined using the four probe measurement scheme so that the phase of the transmission amplitude through the dot can be measured in a reliable way [3]. It was found that the phase increases by π whenever the gate voltage to the dot sweeps through a resonance and that the profile of the phase increase is well described by the Breit-Wigner resonance formula [4].

Unexpected properties were also discovered. The behavior of the phase evolution is identical (up to 2π) for a large number of resonances, and between each pair of adjacent in-phase resonances there is an abrupt phase change by π , whose characteristic energy scale is much smaller than all other energy scales available in the experiment. On the other hand, the 1D Friedel sum rule [5],

$$\Delta Q/e = \Delta \arg(t)/\pi, \quad (1)$$

predicts that all neighboring resonances are off phase by π , which differs from the experimental findings. Thus two central questions arise: First, how can in-phase resonances occur? Does it imply that the Friedel sum rule is not valid for the quantum dot? Second, why do abrupt phase changes occur and why are they so sharp?

Many theoretical investigations addressed these questions. It was suggested that the Friedel sum rule is still valid and the abrupt phase changes are due to "hidden" electron charging events that do not cause conductance peaks [2]. It was also speculated that the in-phase resonances are due to the strong Coulomb interaction [6], the finite temperature [7], or the Fano resonance [8,9]. There was also a claim that they are due to peculiar properties of the AB ring instead of their being a true manifestation of the phase of the transmission amplitude [10]. Regarding the characteristic energy scale, it was claimed that the width of the abrupt phase change is the true measure of the intrinsic resonance width Γ while the measured resonance peaks are thermally broadened [11].

In this paper, we present a new theory based on the Friedel sum rule and the time-reversal symmetry. (In Ref. [3], the magnetic flux threading the dot is only a small fraction of a flux quantum.) One of the key observations is that the 1D Friedel sum rule (1) is not strictly valid for quasi-1D systems due to the appearance of the transmission zeros.

To demonstrate this, we first discuss mirror reflection symmetric systems without magnetic fields. Since the parity is a good quantum number, the scattering states can be decomposed into even and odd scattering states: for $|x| > R$, $\psi_e(x) = e^{-ik|x|} + e^{2i\theta_e} e^{ik|x|}$ and $\psi_o(x) = \text{sgn}(x)[e^{-ik|x|} + e^{2i\theta_o} e^{ik|x|}]$. (For $|x| < R$, there are scattering potentials which may have a higher dimensional nature as in Ref. [3].) The outgoing waves are phase shifted, and the Friedel sum rule ($\Delta Q_e/e = \Delta\theta_e/\pi$, $\Delta Q_o/e = \Delta\theta_o/\pi$) shows that whenever an even (odd) parity quasi-bound state is occupied, θ_e (θ_o) shifts by π (Fig. 1).

Alternatively, left and right scattering states can be used, which are superpositions of the even and odd scattering states: $\psi_l(x) = [\psi_e(x) - \psi_o(x)]/2$, $\psi_r(x) = [\psi_e(x) + \psi_o(x)]/2$. From these relations, one finds that the transmission amplitude t and t' for the left and right scattering states are

$$t = t' = ie^{i\theta} \sin \phi, \quad (2)$$

where $\theta \equiv \theta_e + \theta_o$ and $\phi \equiv \theta_e - \theta_o$. In terms of the new angles, the Friedel sum rule becomes

$$\Delta Q/e = \Delta\theta/\pi. \quad (3)$$

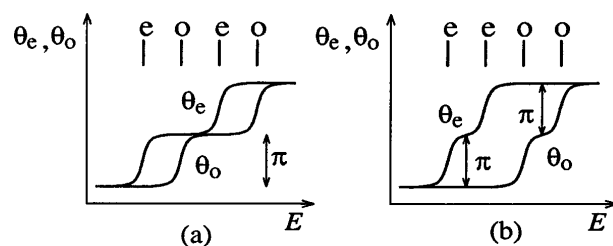


FIG. 1. (a) In true 1D systems, even and odd resonance levels alternate in energy. (b) In quasi-1D systems, they do not necessarily alternate, leading to the transmission zeros since $t \propto \sin(\theta_e - \theta_o)$.

In true 1D systems, even and odd resonant states alternate in energy and the angle ϕ can be limited to the range $0 < \phi < \pi$ [Fig. 1(a)]. Then $\Delta\theta = \Delta \arg(t)$ and the 1D Friedel sum rule (1) is recovered.

In quasi-1D systems, on the other hand, even and odd levels do not necessarily alternate in energy. One concrete example is a dot with the anisotropic harmonic confining potential. The energy levels of the dot are given by $E(n_x, n_y) = \hbar\omega_x(n_x + 1/2) + \hbar\omega_y(n_y + 1/2)$ where $\omega_x \neq \omega_y$. Here n_x determines the parity of a level while n_y is a free parameter as far as the parity is concerned. Because of the presence of this free parameter, situations like Fig. 1(b) occur generically, where some of the adjacent levels share the same parity. Notice that the difference between θ_e and θ_o increases from almost zero to almost 2π and then decreases to almost zero. Since the change is continuous, points should exist where the difference ϕ is π exactly. At these points, $\sin \phi$ vanishes identically and as these points are scanned, $\sin \phi$ reverses its sign, causing the abrupt phase change of t . It is straightforward to verify that the transmission zeros occur whenever neighboring states share the same parity.

As a result of the transmission zeros, one finds

$$\Delta Q/e = \Delta\theta/\pi \neq \Delta \arg(t)/\pi. \quad (4)$$

Thus the 1D Friedel sum rule (1) is not strictly valid for quasi-1D systems. One immediate consequence is that there are *two* possibilities for adjacent resonances. They can be either off phase by π or in phase, and in the latter case, a transmission zero occurs in between. Another important implication is that there is *no* intrinsic energy scale for the abrupt phase change, since the transmission zero corresponds to a singular point as far as the phase is concerned. It also explains naturally the experimental observation that the abrupt phase changes occur when the amplitude of the AB oscillation almost vanishes [3].

We next generalize the discussion to systems without the mirror reflection symmetry. The electron transport in single channel systems can be described by the 2×2 scattering matrix \mathbf{S} ,

$$\mathbf{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = e^{i\theta} \begin{pmatrix} e^{i\varphi_1} \cos \phi & ie^{-i\varphi_2} \sin \phi \\ ie^{i\varphi_2} \sin \phi & e^{-i\varphi_1} \cos \phi \end{pmatrix}, \quad (5)$$

where the matrix elements are parametrized in a most general way compatible with $\mathbf{S}^\dagger \mathbf{S} = \mathbf{S} \mathbf{S}^\dagger = \mathbf{I}$. When the time reversal is a good symmetry, $t = t'$ [12] and the angle φ_2 can be set to zero. Then Eq. (2) is recovered. Also the general Friedel sum rule [13],

$$\Delta Q/e = [\Delta \ln \text{Det}(\mathbf{S})]/2\pi i, \quad (6)$$

reduces to Eq. (3). Thus one again finds that both possibilities of the off-phase resonances and the in-phase resonances are compatible with the Friedel sum rule and the time-reversal symmetry.

To examine whether the in-phase resonances can appear generically, one has to investigate whether the transmis-

sion zeros are generic. The following gedanken experiment is useful for discussion. Imagine that one changes the confining potential $V(x, y; \lambda) = V_s(x, y) + \lambda V_n(x, y)$ of a dot adiabatically by turning on the parameter λ where $V_s(x, y) = V_s(-x, y)$ and $V_n(x, y) \neq V_n(-x, y)$. For $\lambda = 0$, the potential is mirror symmetric and for $\lambda \neq 0$, the mirror symmetry is broken. Let us assume that transmission zeros in the mirror symmetric potential disappear after λ is turned on. Then, Figs. 2(a) and 2(b) represent the typical behaviors of the transmission amplitude in the complex t plane for $\lambda = 0$ and $\lambda = \delta\lambda \ll 1$, respectively. Notice that there is no transmission zero in 2(b) since the trajectory of t is shifted off the origin. As the energy is scanned from A to B , $\Delta\theta = 0$ in Fig. 2(a). In Fig. 2(b), on the other hand, $\Delta\theta = \pi$ and thus $\Delta Q = e$. The corresponding energy levels of the dot are depicted in the insets. While there is no energy level between A and B for $\lambda = 0$, a new level is present between A and B in the level diagram for $\lambda = \delta\lambda$ since $\Delta Q = e$. Upon the infinitesimal change of the confining potential, however, new energy levels cannot appear suddenly although they can drift up and down. Thus this sudden appearance of a new energy level is unphysical and to avoid this, the trajectory for $\lambda = \delta\lambda$ should pass through the origin. This argument applies all along the turning on process and it shows that the transmission zeros should still appear generically even if the system is not mirror symmetric.

One can also argue for the in-phase resonances directly, which then establishes the appearance of the transmission zeros since these two features are linked to each other. With the time-reversal symmetry, the wave functions can be taken as real. In true 1D systems, the number of wave function nodes increases by 1 when a new level appears (oscillation theorem [14]), and each node increases the phase of the transmission amplitude by π . In quasi-1D systems, on the other hand, there are two classes of nodes: "spanning" nodes [Fig. 3(a)] that connect two opposite boundaries of the dot, and "nonspanning" nodes [Fig. 3(b)] that touch either only one particular boundary or no boundary at all. Such nonspanning nodes can

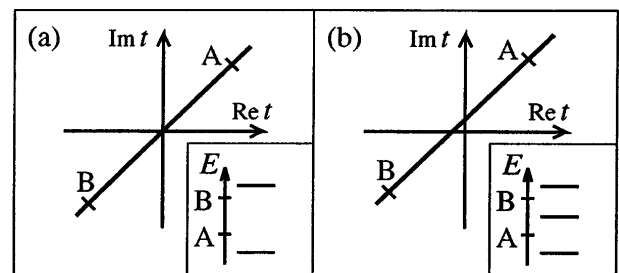


FIG. 2. Behaviors of the transmission amplitude in the complex t plane for $\lambda = 0$ (mirror symmetric systems) (a) and $\lambda = \delta\lambda \ll 1$ (nonsymmetric systems) (b). The behavior in (b) however leads to an unphysical consequence (see text). Insets show the corresponding energy level diagrams.

be created, for example, by excitations in the transverse direction or by negative impurity potentials in the interior of the dot. The two classes of nodes affect the phase of the transmission amplitude in different ways. While each spanning node shifts the phase by π , nonspanning nodes do *not* affect the phase at all. In the experiment [3], the transverse size of the quantum dot is estimated to be much larger than the Fermi length. In such a case, nonspanning nodes are equally plausible as spanning nodes, and accordingly in-phase resonances can occur as generically as off-phase resonances.

Until now, we have demonstrated the generic appearance of the transmission zeros and in-phase resonances based on the Friedel sum rule and the time-reversal symmetry. Next we demonstrate that multiple resonances also lead to the transmission zeros naturally if the time reversal is a good symmetry. (This demonstration, in fact, constitutes an alternative derivation of the same conclusion without using the Friedel sum rule.) Near a resonance, the scattering matrix becomes $\mathbf{S}(E) = \mathbf{S}_{\text{bg}} - i\mathbf{B}_0/(E - E_0 + i\Gamma_0/2)$ where the 2×2 matrix \mathbf{S}_{bg} ($\mathbf{S}_{\text{bg}}^\dagger \mathbf{S}_{\text{bg}} = \mathbf{I}$) is the energy independent background contribution [15]. If the off-diagonal matrix elements of \mathbf{S}_{bg} are sufficiently small, $\mathbf{S}(E)$ describes the Breit-Wigner resonance. For multiple resonances, the scattering matrix becomes

$$\mathbf{S}(E) = \mathbf{S}_{\text{bg}} - \sum_{k=1}^N \frac{i\mathbf{B}_k}{E - E_k + i\Gamma_k/2}. \quad (7)$$

Here we emphasize that the matrix residues $-i\mathbf{B}_k$ are not independent. Instead they should be highly correlated so that $\mathbf{S}^\dagger(E)\mathbf{S}(E) = \mathbf{I}$ for arbitrary real E . (This is the origin of the limited phase relations between resonances.) From the unitarity relation and the time-reversal symmetry, one finds five constraints: $|t(E)|^2 = |t'(E)|^2$; $|r(E)|^2 = |r'(E)|^2$; $|t(E)|^2 + |r(E)|^2 = 1$; $t(E)/t'(E)^* + r(E)/r'(E)^* = 0$; $t(E) = t'(E)$.

It turns out that to examine the implications of the constraints, it is more convenient to express the matrix elements of $\mathbf{S}(E)$ in the product representation by summing up all $N + 1$ terms in Eq. (7),

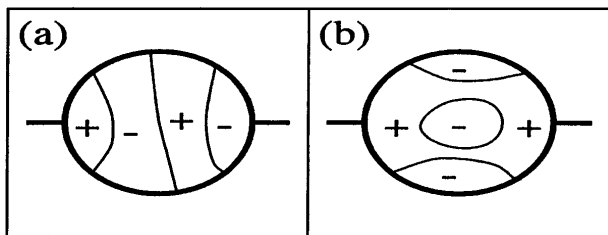


FIG. 3. Two classes of wave function nodes (thin solid line) in two dimensions. The marks (+) and (-) represent the fact that the wave functions in the marked areas have positive and negative values, respectively. Notice that while each spanning node in (a) shifts the resonance phase by π , the introduction of nonspanning nodes (b) does not affect the resonance phase. Straight lines on the left and right represent 1D electrodes.

$$t(E) = t'(E) = t_{\text{bg}} \prod_{k=1}^N \frac{E - \epsilon_k + i\mu_k/2}{E - E_k + i\Gamma_k/2},$$

$$r(E) = r_{\text{bg}} \prod_{k=1}^N \frac{E - \epsilon_k + i\nu_k/2}{E - E_k + i\Gamma_k/2}, \quad (8)$$

$$r'(E) = r'_{\text{bg}} \prod_{k=1}^N \frac{E - \epsilon_k + i\nu'_k/2}{E - E_k + i\Gamma_k/2},$$

where $(\nu_k)^2 = (\nu'_k)^2$ [16]. Then by imposing the constraints and the condition of no degenerate resonance levels [17], one finds

$$\mu_k = 0 \quad \text{for all } k, \quad (9)$$

which implies that all zeros of $t(E)$ are located on the real energy axis. (We mention that impurities and irregular boundaries of the dot generate the level repulsion that lifts the degeneracy. The degeneracy is lifted further by the Coulomb blockade effect.)

Evolution of the transmission amplitude is determined from the locations of poles and zeros. Thus this analysis produces the following prediction (Fig. 4): If there is a transmission zero (B and D) in between, two neighboring resonances ($A-C$ and $C-E$) are in phase, and otherwise, they are off phase ($E-F$). Notice that these predictions are identical to those of the Friedel sum rule.

It is instructive to compare the transmission zeros from the Breit-Wigner resonances and the Fano resonances [8,9]. Within an energy window that contains two Breit-Wigner resonances, $t(E) = -i(\mathbf{B}_k)_{21}/(E - E_k + i\Gamma_k/2) - i(\mathbf{B}_{k+1})_{21}/(E - E_{k+1} + i\Gamma_{k+1}/2)$. By summing up the two contributions, one finds $t(E) = \alpha(E - \beta)/[(E - E_k + i\Gamma_k/2)(E - E_{k+1} + i\Gamma_{k+1}/2)]$ where $\beta = \beta^*$ due to the time-reversal symmetry. Thus the transmission zero at $E = \beta$ is due to the completely “destructive interference” of the *two* resonance levels.

The transmission zeros also arise from the Fano resonance [8,9], to which the same expression (7) applies. Unlike the Breit-Wigner resonances, however, the off-diagonal matrix elements of \mathbf{S}_{bg} are not small. Thus near

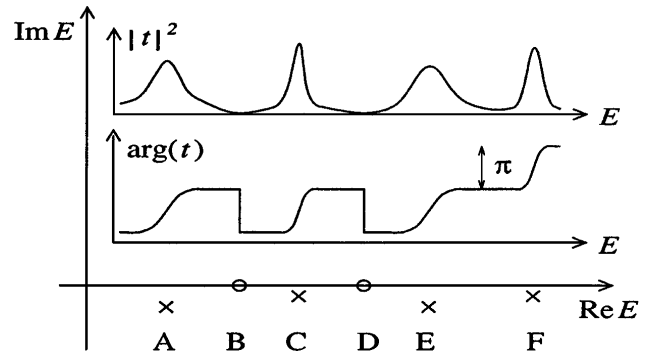


FIG. 4. Zeros (o) and poles (x) of the transmission amplitude $t(E)$ in the complex energy plane. Insets show the corresponding behaviors of the magnitude $|t|^2$ and the phase $\arg(t)$ as a function of real energy E .

a Fano resonance, one finds $t(E) = (\mathbf{S}_{\text{bg}})_{21} - i(\mathbf{B}_k)_{21} / (E - E_k + i\Gamma_k/2) = \alpha(E - \beta) / (E - E_k + i\Gamma_k/2)$ where $\beta = \beta^* \approx E_k$. One finds again the transmission zero. It should be noted however that the transmission zero is now due to the destructive interference of the background contribution (continuous state of the energy channel) and the pole contribution (localized state for Ref. [8] and t stub for Ref. [9]). Notice also that the Fano resonance peak is highly asymmetric since $\beta \approx E_k$, which disagrees with the experiment [3].

Below we discuss briefly effects of the electron-electron interaction and magnetic fields on the transmission zeros. Langer and Ambegaokar [13] have shown that even in the presence of the interaction, the general Friedel sum rule (6) is valid at $E = E_F$ provided that quasiparticle excitations at the Fermi energy remain well defined. Then all analyses for noninteracting systems apply equally to interacting systems if one fixes the probing energy E at E_F and instead varies the depth of the potential well, which amounts to replacing E by $E_F - \eta eV_g$. (Figure 2 can be used to argue against the disappearance of the transmission zeros upon the adiabatic interaction turning on. In this case, $\Delta Q = e$ in Fig. 2(b) can be interpreted as the sudden charge density jump.)

Magnetic fields, on the other hand, affect the transmission zeros in a fundamental way since it breaks the time-reversal symmetry. In this case, $t \neq t'$ and the angle φ_2 in Eq. (5) can have nonzero values. Then the transmission zeros are generically replaced by the rapid but continuous change of φ_2 by π , and thus a finite energy scale appears for the abrupt phase changes. The precise energy scale depends on the detailed electron dynamics inside the dot, which goes beyond the scope of this paper.

Lastly, we discuss the large dominance of the in-phase resonances over the off-phase resonances in Ref. [3]. Hackenbroich *et al.* [18] proposed that avoided crossings of single particle levels may result in a long sequence of resonances carrying the *same* internal wave function. In view of the present analysis, this mechanism is overrestrictive since it restricts not only the number of spanning nodes but also the number of nonspanning nodes as well. We speculate that a less restrictive and possibly more widely applicable mechanism may exist which exploits the “degree of freedom” given by the nonspanning nodes. Further investigation in this direction is necessary.

In summary, we demonstrated that the transmission zeros and the in-phase resonances are generic features in the time-reversal symmetric single channel transport if the transverse size of a scatterer (dot) is sufficiently larger than the Fermi wavelength.

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 - [16] Equation (8) does not mean however that there is always the same number of zeros and poles. From Eq. (7), it can be explicitly verified that when $t_{\text{bg}} \rightarrow 0$, one of ε_k diverges as $1/t_{\text{bg}}$, making the numerator in the expression for $t(E)$ [Eq. (8)] essentially $(N - 1)$ th polynomial and reducing the number of zeros by 1. When matrix elements of \mathbf{B}_k satisfy certain conditions, the number of zeros can be reduced further.
 - [17] The constraints alone allow nonzero μ_k provided that $\mathbf{S}(E)$ itself includes the factor $(E - \varepsilon_k + i\mu_k/2) / (E - \varepsilon_k - i\mu_k/2)$ that is of the magnitude of 1 for arbitrary real E . This factor is equal to $\mathbf{I} - i\mathbf{A}_k / (E - \varepsilon_k - i\mu_k/2)$ where $\mathbf{A}_k = -\mu_k \mathbf{I}$. One then finds that the pole $\varepsilon_k + i\mu_k/2$ represents doubly degenerate resonance levels since the rank of the residue matrix is equal to the degeneracy [15] and the rank of \mathbf{A}_k is two.
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