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Reflection phase of scattering electrons in a single-channel atomic wire

H. Q. Xu,[1,2,*] I. C. Fasth,[1] D. Csontos,[1] L. B. Zhang,[2] and Y. Zhao[2]
[1]*Division of Solid State Physics, Lund University, Box 118, S-221 00 Lund, Sweden*
[2]*Department of Physics, Dalian University of Technology, Dalian 116023, China*
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A theoretical study of the phase property of the reflection coefficient of a single-channel quantum system is presented. This reflection phase information is required for a complete characterization of the scattering problem in the system. It is found that the phase of the reflection coefficient of the system shifts abruptly by π when the reflection probability passes through a zero. It is also found that in certain systems this phase discontinuity can appear even when no zero and no phase discontinuity are present in the transmission coefficient. Possible experiments for the observation of the reflection phase discontinuity are discussed.

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As the characteristic feature size of electronic devices continues to shrink, interest has focused on the nature of electron transport through essentially one-dimensional nanometer-scale channels such as atomic wires[1–8] and carbon nanotubes.[9–12] It is now well known that quantum effects have significant influence on the electric properties of nanometer-scale devices. A notable example is that the conductance of atomic point contacts, in which a "neck" of atoms between two electrodes is just a few atomic diameter wide, is quantized in units of $2e^2/h$.[1–7] Both the atomic point contacts consisting of only a single-atom neck and that consisting of a 20-Å-long single-atom chains have been observed.[1–7] A link between the chemical valence of the atoms and the number of conductance channels in single-atom wires has also been demonstrated.[4] These findings are reminiscent of the properties of phase-coherent ballistic electron transport in semiconductor mesoscopic point contacts and have shown that it becomes possible to study the influence of quantum effects on electron transport using nanometer-scale atomic systems.

One of the current interests in the study is the phase properties of scattering electrons in single-channel atomic wires containing a quantum confinement structure. Such an atomic system can be fabricated by, e.g., local probe methods, which, as demonstrated in Ref. 13, allow us to build systems of the same complexity as used by nature. It was discovered[14,15] that the phase of the transmission of electrons in a single-channel quantum wire with an attached quantum dot exhibits two interesting features: first, the phase acquired by electrons traversing the quantum dot increases smoothly by π along a resonance peak; second, the phase changes abruptly by π in the tail of the resonant peak, where the transmission amplitude of the system vanishes. The first feature was explained by Schuster *et al.* in Ref. 14 using the Breit-Wigner resonance formula, while the second one was totally unexpected. Several theoretical models[16–26] have been proposed to explain the observed phase drops. It was shown,[16,17] based on analytical and numerical calculations for quantum dots embedded in a single-channel wire, that the sharp phase drops occur exactly when the transmission amplitude vanishes. Later, it was shown that identical vanishing of the transmission amplitude can occur generically in single-channel systems if the time reversal is a good symmetry, and that the Friedel sum rule is not strictly valid for the systems as a result of the appearance of the transmission zeros.[20,21] In addition, models that take into account specific properties of the dot states in a semichaotic structure were also proposed and a mechanism for the phase drops based on large differences in the coupling of the dot states to the continuous states of the leads was discussed.[22,24] Very recently, studies of the transmission phase have also been made for quantum dot systems with Kondo correlations.[27,28] However, all these studies have not addressed the phase properties of the reflected electrons.

In this work, we report on a study of the phase properties of the reflection coefficient of single-channel quantum devices. This phase information is needed for a complete characterization of a scattering problem in a quantum system. In a two-terminal device, the reflection amplitude can be obtained from the transmission amplitude using the current conservation law. However, the reflection phase cannot be found from the transmission phase, unless the relation between the two phases is known. We will present our results for the reflection phase found by direct calculations. We will show that the phase discontinuity can also occur in the reflection coefficient of quantum devices, and that in certain systems this discontinuity can occur even when no discontinuity is present in the transmission coefficient. We will finally discuss possible devices for experimental observations of the reflection phase discontinuity.

It is worthwhile to recall some generic properties of the transmission phase of a quantum system. The electron transport in single-channel atomic systems can be described by a unitary 2×2 matrix, which can be expressed in a most general way as

$$\mathbf{S}=\begin{pmatrix} r & t' \\ t & r' \end{pmatrix}=e^{i\theta}\begin{pmatrix} ie^{i\varphi_1}\sin\phi & e^{i\varphi_2}\cos\phi \\ e^{-i\varphi_2}\cos\phi & ie^{-i\varphi_1}\sin\phi \end{pmatrix}, \tag{1}$$

with real parameters θ, φ_1, φ_2, and ϕ.[20–22] When the systems are symmetric under time reversal, $t=t'$ and φ_2 can be set to zero. The scattering matrix $\mathbf{S}$ is linked to the charge Q of the system via the Friedel sum rule,

$$\delta Q/e=[\delta \ln \mathrm{Det}(\mathbf{S})]/2\pi i. \tag{2}$$

Thus, the phase of the transmission coefficient θ_t, as in $t = |t|e^{i\theta_t}$, and the Friedel phase θ_F are not independent,

$$\theta_t = \theta_F - \frac{\pi}{2} - \pi\Theta(-\cos\phi), \tag{3}$$

where $\Theta(x)$ is the step function of x.[20–22] It is seen that in difference from the Friedel phase, which is a continuous function, the phase of the transmission coefficient may exhibit discontinuity. A prerequisite for the occurrence of the discontinuity is the existence of transmission zeros, at which $\cos\phi = 0$.

Calculations and analysis have shown that transmission zeros can appear in a system with a multilevel quantum dot coupled to two one-dimensional leads, provided that all the coupling elements between the dot and the leads are taken into account.[18,26] However, it has been rigorously proved that the transmission coefficient of a double barrier confined, in-line, one-dimensional wire with multiple quasibound states does not have zeros at energies for which the leads are open for conduction.[21,23] A deep understanding of the physical origin of transmission zeros is then needed in order to resolve these seemingly contradictory results. If a detailed analysis is made, one can find that in each of the models used in Refs. 16–23 there exist at least two coherent paths for electrons passing through the confined dot region from one lead to the other one. Thus the transmitted wave is a result of interference between different coherent electron paths. However, in the system consisting of an in-line double-barrier confined one-dimensional wire, there exists only one coherent path for the electrons passing through the confinement region, which can be the one associated with resonant tunneling or the one at off-resonance. Thus no effect of multiple-path interference can be seen in the transmitted wave of the system. The above analysis leads us to conclude that zeros in the transmission through a confined region arise from interference between different coherent paths that contribute to the transmission. This conclusion can be generalized and stated as follows: if a wave emitted from a confined region consists of contributions from different coherent paths, destructive interference can lead to zero wave emitting.

A chain of single monovalence atoms can be considered as a single-channel quantum wire. By creating two weak-coupling junctions inside the chain or at the connections between the chain's ends and two conducting leads, one realizes an in-line one-dimensional double-barrier structure. Thus, the transmission of the system can show resonant oscillations, but certainly should not have zeros between resonant peaks. As a consequence, no phase discontinuity can appear in the transmission of the system. The situation will be different if the single-atom chain contains a cavity, such as an atomic cluster or an attached conducting molecule. In this case, the transmission can have zero and phase discontinuity, as a result of the presence of multiple coherent electron paths in the cavity region.

For a single-channel quantum wire, it can be derived that the phases of the reflection coefficients, θ_r and $\theta_{r'}$, as in $r = |r|e^{i\theta_r}$ and $r' = |r'|e^{i\theta_{r'}}$ are given by

$$\theta_r = \theta_F + \varphi_1 - \pi\Theta(-\sin\phi) \tag{4}$$

and

$$\theta_{r'} = \theta_F - \varphi_1 - \pi\Theta(-\sin\phi). \tag{5}$$

It is seen that $\theta_r - \theta_{r'} = 2\varphi_1$. Similar to the transmission coefficient, a prerequisite (but not a sufficient condition) for the occurrence of the discontinuities in the two reflection phases is the existence of reflection zeros, at which $\sin\phi = 0$.

It is interesting to see whether or not reflection zeros can appear in an in-line one-dimensional double-barrier structure made from a single-atom chain. We have discussed, in the above, that such a resonant atom-chain structure does not possess the transmission zeros, as a result of that there exists only one coherent path for electrons passing through the confined region. The situation becomes different when the reflection of the electron wave is considered. Here, the reflection wave is a result of interference between two coherent paths: direct reflection from first barrier and resonant reflection from the confined region. Thus the reflection coefficient can be zero if the interference is fully destructive. In fact, a fully destructive interference does exist in the reflection of in-line one-dimensional double-barrier systems symmetric under mirror reflection. Thus, a symmetric, resonant atom-chain system can have reflection zeros.

The question is then that will the phase of the reflection coefficient of an in-line one-dimensional double-barrier structure made from a single-atom chain be discontinuous at the reflection zeros? We will answer this question with numerical calculations. In the calculations, we employ a tight-binding model. The model consists of three regions: a finite chain of single monovalence atoms, i.e., a confinement region (C), and two single-channel semi-infinite leads on the left (L) and the right (R). The Hamiltonian of the system is given by

$$\begin{aligned} H = & \sum_{n(n,\, n+1 \in C)} [\varepsilon_C a_n^\dagger a_n - \lambda(a_{n+1}^\dagger a_n + \text{H.c.})] \\ & + \sum_{n(n,\, n+1 \in L,R)} [\varepsilon_0 a_n^\dagger a_n - \lambda(a_{n+1}^\dagger a_n + \text{H.c.})] \\ & - v_L(a_{n_L}^\dagger a_{n_C} + \text{H.c.}) - v_R(a_{n_R}^\dagger a_{n_C} + \text{H.c.}), \end{aligned} \tag{6}$$

where $a_n^\dagger$ (a_n) is the creation (annihilation) operator for an electron at site n, ε_C and ε_0 are the on-site energies in the confined region and the two leads, and λ is the hopping integral. The first term is the Hamiltonian of the finite atomic chain; the second term is the Hamiltonian of the two leads; the couplings between the finite atomic chain and the two leads are given by the remaining two terms with coupling parameters v_L and v_R and site indices $n_C \in C$, $n_L \in L$, and $n_R \in R$.

The transmission coefficients of the system, t and t', can be calculated as in Ref. 23 using, e.g., the Fisher-Lee relation.[29] The reflection coefficients, r and r', can be calculated using a procedure as described in Ref. 30. For an in-line double-barrier structure, it can be shown that the reflection coefficient r can be written as

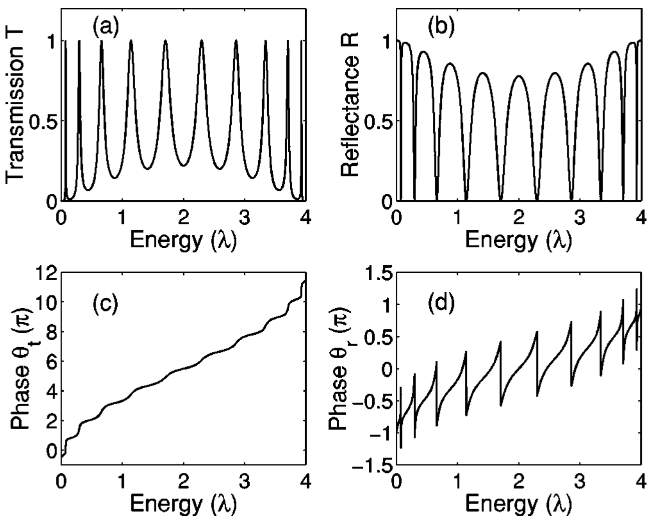

FIG. 1. Scattering parameters of the single-channel symmetric double-barrier structure. The confined region is modeled by a wire of ten single on-site energy sites and is coupled to two semi-infinite leads in an in-line configuration.

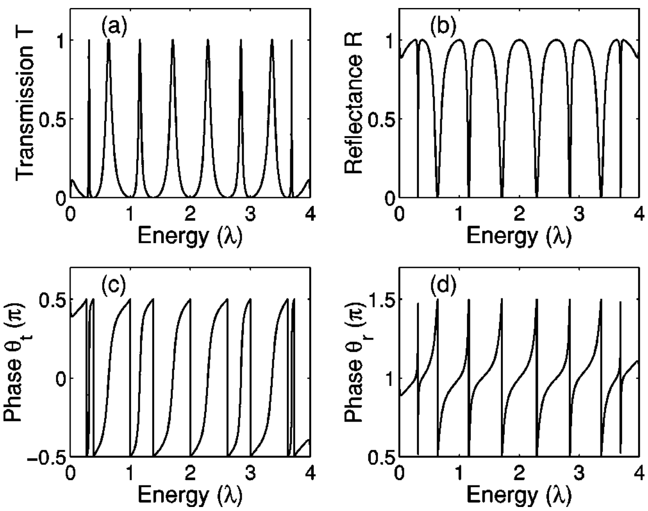

FIG. 2. Scattering parameters of the quantum-confined single-channel wire structure. The confined region is modeled by a wire of ten single on-site energy sites and is coupled via tunneling junctions to two semi-infinite leads in a crossbar configuration.

$$r=-\frac{E-\tilde{\varepsilon}+\lambda e^{-ik^L a}}{E-\tilde{\varepsilon}+\lambda e^{ik^L a}}, \tag{7}$$

where $\tilde{\varepsilon}=\varepsilon_C+\varepsilon_\Sigma$ with ε_Σ given by

$$\varepsilon_\Sigma=\cfrac{v_L^2}{E-\varepsilon_C-\cfrac{\lambda^2}{E-\varepsilon_C-\cfrac{\lambda^2}{\ddots\,\cfrac{\lambda^2}{E-\varepsilon_C-\Sigma^R(E)}}}}. \tag{8}$$

In the above equation, the self-energy $\Sigma^R(E)$ can be found from

$$\Sigma^R(E)=v_R^2 G^R(E), \tag{9}$$

where

$$G^R(E)=[E-\varepsilon_R-\lambda^2 G^R(E)]^{-1} \tag{10}$$

is the Green's function at the first site of the right-hand-side lead. A similar expression can also be derived for the reflection coefficient r'.

Figure 1 shows the results of the calculations for an in-line single-channel double-barrier model with a chain of ten atomic sites, sandwiched in between two single-channel leads with an in-line configuration. In the calculations, the on-site energies, ε_C and ε_0, are assumed to have a value of 2λ. The coupling parameters are assumed to be $v_L=v_R=-0.5\lambda$. Thus the system is symmetric with respect to the direction of the current. The transmission and reflection probabilities of the system are shown in Figs. 1(a) and 1(b), respectively. It is seen, as expected, that the transmission probability exhibits ten resonant peaks of unit height, and that the reflection probability exhibits ten zero reflection dips, occurring at the same energies as of the corresponding transmission peaks. The phase shifts of the transmission and reflection coefficients of the system are shown in Figs. 1(c) and 1(d), respectively. It is seen that the phase shift of the transmission coefficient is continuous. This result is consistent with the fact that there exist no zeros in the transmission probability, and is in agreement with previous studies.[21,23] However, in strong contrast, the phase shift of the reflection coefficient exhibits discontinuities; it drops abruptly by π precisely when the reflection probability passes through a zero.

It is of interest to ask the question that can both the discontinuity of the transmission phase and the discontinuity of the reflection phase be observed in a single monovalence-atom wire device? For an answer to this question, we consider a single-channel device model with a different structure. The same finite wire of ten atoms as in Fig. 1 is assumed in the model. However, instead of the in-line structure, the wire couples to the two semiinfinite leads in a crossbar configuration. Figure 2 shows the results of the calculations for the system. It is seen that the transmission probability exhibits eight peaks with unit height, but oscillating widths. This result can be understood in terms of the local density of states on the finite wire.[30] In principle, the system has ten states localized within the finite wire. However, not all the ten states appear as resonances in the transmission. This is due to the fact that two of these states have their energies outside of the conduction band of the leads. An interesting feature seen in these calculations is that zeros appear in both the transmission and reflection probabilities. As we have already discussed, these zeros can be understood as arising from destructive interferences between coherent electron paths. An important result found in these calculations is that both the transmission phase and the reflection phase show abrupt phase drops by π at the corresponding transmission and reflection zeros. The co-occurrence of the transmission zeros and the sharp transmission phase drops is in agreement with the experimental observation by Schuster *et al.* and previous calculations. However, the presence of both the transmission phase drops and the reflection phase drops in a single-quantum system, as predicted in this work, has not yet been observed. We have also done the calculations for a number of other crossbar single-channel atom-wire devices and the same phase properties of the transmission and reflection coefficients as in Fig. 2 have been found.

It is challenging to measure the phase of the reflection coefficient of a single-channel quantum-wire system, although the measurement of the transmission phase has been successfully carried out for a single-channel system with an attached quantum dot. The phase drops of the reflection coefficient are very sensitive to the symmetry of quantum-wire systems. For example, in a single-channel double-barrier confined atom-wire system, a tiny difference between the two barriers will destroy the reflection zeros and therefore the reflection phase discontinuities. A simple, but promising system for the observation of the discontinuities in the reflection phase is the one obtained by attaching a finite piece of atomic (or molecular) wire to a long perfect atomic (or molecular) wire in a crossbar or a *T*-junction configuration. This system is similar to the device studied in Fig. 2 without double-barrier confinement. However, our calculations have shown that the transmission and reflection phases of such a system exhibit the same discontinuous behavior as seen in Fig. 2.

In summary, we have presented a theoretical study for the phase properties of the transmission and reflection coefficients of single-channel quantum-confined systems. Our study has shown that the reflection phase is discontinuous at reflection zeros. This phase discontinuity can even appear in a system where the transmission phase is completely continuous. Single-channel devices, such as atomic-wire crossbar and *T*-shaped junctions, are proposed for experimental observation of the phase discontinuity in the reflection coefficient.

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*Corresponding author. Email address: Hongqi.Xu@ftf.lth.se

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