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Effects of intrasubband coupling on the scattering phases and density of states in a quantum wire

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ABSTRACT

The properties of scattering phases and density of states in a quantum wire with an attractive scatterer are analyzed. We consider two bound states which couple to a scattering channel and give rise to two Fano resonances. It is shown that varying the parameters of the scatterer (such as its strength and position) produces significantly different effects on the phase behavior and density of states, depending on the subband they occur. These effects stem mainly from the difference between the coupling matrix elements of the two resonant levels with the propagating channel mode.

1. Introduction

It is established by now that the wave nature of electrons plays a significant role in the interpretation of transport properties of very small electronic devices. In order to fully characterize these properties both the phase and magnitude of the electron wave function are required to be known. The behavior of the wave-function phase in an actual quantum transport device was originally investigated for an electron transmitted through a quantum dot [1–4]. These important experiments demonstrated the presence of a coherent component in the current through a quantum dot while, at the same time, a strange behavior of the transmission phase was revealed; namely, the transmission phase drops suddenly by π in the conductance valleys.

In relation to these experiments, several theoretical efforts have been devoted to investigating the behavior of the various phases that appear in the scattering matrix [5–10]. The existence of two important phases with very distinctive behavior was emphasized [5,6]; namely, the phase of the transmission amplitude and the phase that appears in the Friedel sum rule [11]. The major difference between the phases is that even though the Friedel phase is a continuous function of the system parameters the phase of the transmission amplitude can depart from the Friedel phase [5,6] and exhibit a nonanalytic behavior at energies where the modulus of the transmission vanishes.

The simultaneous occurrence of a transmission zero and a sudden phase drop was interpreted in terms of the properties of a Fano resonance [12]. A Fano resonance is caused by the quantum interference of two transmission channels, a resonant one, associated with a discrete level, and a nonresonant one, associated with a continuum band. It is the destructive interference between the two transmission channels that leads to the Fano type of transmission zero and the associated phase discontinuities.

The above-mentioned behavior of the transmission phase may also appear in a quantum wire with a scatterer [13,14]. In the presence of a scatterer, a bound state in one subband (imaginary wave number in the wire leads) can coexist with an unbound state in another subband. A Fano resonance in this case arises when the closed and the open channels are coupled, the channels being the propagating and cut-off subbands. However, it has been shown that the effect of the scattering potential on a Fano resonance strongly depends on the subband [15] through the bound state-continuum coupling. Thus, it is natural to expect that the scattering phases also depend sensitively on the subband they occur. One important issue, therefore, is in what manner does the phase evolution in one subband differs from the phase evolution in another subband in the context of ballistic transport through quantum wires.

The purpose of this Letter is to extend our previous work [14] and investigate the behavior of the scattering phases in a quantum wire thus providing further insight into the present problem.

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The coupling between channels is provided by an attractive scatterer. We consider the case of one open and two closed channels, the latter two being dominated by their bound states. In this two-subband regime, by varying the parameters of the scattering potential (such as its strength and position), we investigate and compare the behavior of the scattering phases that occur in the first and second subbands.

Specifically, it is shown that the phase behavior in a particular subband is determined by: i) the strength of the coupling to the respective quasibound level, and ii) the strength of the interaction of a channel mode with the scatterer. As a result, the phase evolution in one subband exhibits substantially different behavior than that of the phase evolution in another subband.

2. Model and calculation

2.1. Coupled-channel model

We consider a ballistic uniform quantum wire in which electrons are confined along the y direction (transverse direction) but are free to propagate along the x direction. In the presence of a scattering potential, the Schrödinger equation describing the electron motion is

$$H(x,y)\Psi(x,y)=E\Psi(x,y), \tag{1}$$

where $H(x,y)$ is the Hamiltonian given as

$$H(x,y)=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V_c(y)+V(x,y). \tag{2}$$

In Eq. (2), $V_c(y)$ is the confining potential and $V(x,y)$ is the scattering potential. The transverse potential $V_c(y)$, providing confinement of the electron motion along the y direction, gives rise to channel modes $\phi_n(y)$,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+V_c(y)\right]\phi_n(y)=E_n\phi_n(y), \tag{3}$$

where E_n is the threshold energy for mode n. Expanding the wave function $\Psi(x,y)$ of Eq. (1) in terms of the channel modes and substituting the expansion into Eq. (1) we obtain the following coupled-channel equations for $\psi_n(x)$,

$$(E-E_n-\widehat{K})\psi_n(x)=\sum_{l=0}^{\infty}V_{nl}(x)\psi_l(x), \tag{4}$$

where $\widehat{K}=-(\hbar^2/2m)d^2/dx^2$ and $V_{nl}(x)$ are the coupling matrix elements given by $V_{nl}(x)=\int dy\,\phi_n^*(y)V(x,y)\phi_l(y)$. These matrix elements form effective coupling potentials for the longitudinal electron motion and also provide the interaction between channels.

We assume that only the first channel mode (i.e., the mode with $n=0$) can be found in a scattering state. These states can be found from Eq. (4) by considering the decoupling limit. In addition to the open channel $n=0$, we consider two closed ones $n=1$ and 2, which are dominated by their bound states $\Phi_{01}(x)$ and $\Phi_{02}(x)$, respectively, with $\widetilde{E}_j$ the bound-state energies ($j=1,2$). The bound states can also be found from Eq. (4). Truncating the sum in Eq. (4) at $n=2$ and solving the resulting system of three equations (see [15] for details and Appendix A of that reference) we obtain the transmission amplitude as

$$t(E)=t^{bg}\frac{(E-\widetilde{E}_1)(E-\widetilde{E}_2)-\bar{\varepsilon}}{(E-E_R^{(1)}+i\Gamma_1)(E-E_R^{(2)}+i\Gamma_2)-W_{12}^2}, \tag{5}$$

where $\bar{\varepsilon}$ is real and proportional to the coupling potential V_{12}, and $E_R^{(j)}=\widetilde{E}_j+\delta_j$ are the shifted quasibound-state (resonant) energies. The shift and width, δ_j and Γ_j, of the jth bound-state energy are determined from the self-energy term. Also, in Eq. (5) W_{12} denotes the sum of two matrix elements,

$$W_{12}=\langle\Phi_{01}|V_{12}|\Phi_{02}\rangle+\langle\Phi_{01}|V_{10}\widehat{G}_0V_{02}|\Phi_{02}\rangle. \tag{6}$$

The first matrix element represents the direct coupling of the two bound states, while the second matrix element represents the indirect coupling of the bound states via the open channel.

2.2. Scattering phases and density of states

For a single transport channel the scattering matrix is represented as a 2×2 unitary matrix at an energy E,

$$S(E)=\begin{pmatrix} r(E) & t'(E)\\ t(E) & r'(E)\end{pmatrix}. \tag{7}$$

The unitarity condition, $S^\dagger=S^{-1}$, guarantees conservation of particle current and implies that the eigenvalues of the scattering matrix S are on the unit circle. We assume that both time-reversal and inversion symmetries hold and, in this case, one has additionally $t=t'$ and $r=r'$.

The Friedel phase is defined by

$$\theta_f(E)=\frac{1}{2i}\ln\det\{S(E)\}, \tag{8}$$

where, for a time-reversal symmetric system, $\det\{S(E)\}=-t(E)/t^*(E)$. The derivative of the Friedel phase with respect to the energy of the incident electron can be related to the energy derivatives of the scattering matrix. The density of states can also be expressed in terms of the scattering matrix. From this we can obtain a relation that connects the energy derivative of the Friedel phase and the scattering matrix with the density of states,

$$\frac{\partial\theta_f(E)}{\partial E}=\pi\rho(E). \tag{9}$$

With the help of the transmission amplitude given in Eq. (5), the Friedel phase of Eq. (8) can be expressed as

$$\theta_f(E)=\theta_f^{bg}(E)+\sum_{j=1}^{2}\arctan\left(\frac{E-E_R^{(j)}}{\Gamma_j}\right)-\frac{\pi}{2}, \tag{10}$$

where $\theta_f^{bg}(E)$ originates from the background contribution and varies slowly with energy across a resonance. We also assumed for simplicity that the interaction, W_{12}, between the bound states is small compared with the relevant energy scale $|\widetilde{E}_1-\widetilde{E}_2|$ and therefore W_{12} can safely be neglected. Using Eqs. (9) and (10) we obtain the density of states as

$$\rho(E)=\frac{1}{\pi}\sum_{j=1}^{2}\frac{\Gamma_j}{(E-E_R^{(j)})^2+\Gamma_j^2}, \tag{11}$$

which is a superposition of two Lorentzians with peak positions at the resonant energies i.e., at $E=E_R^{(j)}$.

On the other hand, the phase of the transmission amplitude can be obtained by expressing Eq. (5) as $t=|t|e^{i\theta_t(E)}$ where

$$\theta_t(E)=\theta_t^{bg}(E)+\theta_t^r(E). \tag{12}$$

One can easily verify that $\theta_t^{bg}=\theta_f^{bg}$, which will henceforth be denoted as θ^{bg}. Note that the form of θ^{bg} depends on the specific type of scattering potential.