Interpretation of the Fano lineshape reversal in quantum waveguides

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(Received 31 December 2006; published 9 March 2007)

Fano lineshape parameter (q) reversal is a proxy for interaction beyond the usual interference of indistinguishable quantum pathways. Reversal of the Fano parameter has been observed recently in quantum dots (QDs). We show that such a profile reversal may come about from the interaction of interloping over-the-top states (shape resonances) in the "nonresonant" channel with the QD bound states, interacting with the continuum channel (Feshbach resonances). Using this mechanism, we show that with minimal modifications of the QD parameters, we can affect the presence or absence of interloping resonances and hence lineshape profile reversal, as a way of coherence engineering.

DOI: 10.1103/PhysRevB.75.113305 PACS number(s): 73.63.Kv, 33.40.+f, 72.15.Qm, 73.23.−b

Quantum dots (QDs) are lithographically fabricated semiconducting structures in which electrons are confined in three dimensions.[1–3] The confinement of electrons in QDs leads to the quantization of charge-Coulomb blockade (CB) and energy-level structure reminiscent of energy-level diagram in atoms. In a similar analogy, coupled QD form artificial molecules, whose molecular bonding can be controlled.[4] Transitions between QD levels can be induced and controlled by applying a magnetic field or manipulated by electrostatic tuning of the electronic phase.[5] Because QDs are fabricated and maintained in continuous contact with the environment, decoherence is a major concern. Electron dephasing has implications for proposals, which aim to integrate cascades of such nanodevices into larger circuits for executing scalable quantum logic operations. The interaction between the localized and delocalized electrons in QDs and other mesoscopic systems, such as in a QD embedded in Aharonov-Bohm (AB) rings[6,7] and in nanotubes,[8] bears resemblence to the interaction of discrete and continuum electrons in atoms or molecules undergoing collision or photoabsorption.[9–11]

Fano resonances, ultimate proxies for the existence of quantum interference, ubiquitous already in atomic and molecular systems, have also been observed when magnetic impurities are introduced[12] in quantum dots[6,7,13–15] and carbon nanotubes.[8] The Kondo effect, which arises from the interaction of electrons in a metal and a magnetic impurity, leads to charge and spin localization around the impurity atom as resonances.[16,17] The famous "0.7 anomaly," the previously unexplained shoulder in conductance of electrons through constrictions—quantum point contacts (QPCs)—has been associated with the existence of quasibound states in the QPC.[18,19] Fano modulations, because they arise from coherent interference, could influence the operation of spin-filter devices,[20,21] which aim to perform spin polarization using electrical means only.

A unique feature of Fano interference resonance is the so-called profile, or q reversal, whereby the asymmetry of Fano lineshapes changes. The Fano q reversal, an observable signature not just of quantum interference but also of channel interaction, has been studied and observed in atomic and molecular physics[10,11] and has been linked to complicated interloping or interferometric interaction between quantum continuum channels and electronic states. Recently, conductance measurements in a quantum dot embedded in an AB ring[6,7] observed a reversal of Fano resonance profile in the CB regime, where Coulombic oscillations in QD in one AB arm are interfered with the direct conductance in the other AB arm. Other measurements of electron transport in a one-lead QD in a two-dimensional (2D) heterostructure[7,15] (2DEG) observed also a reversal of Fano resonances, in the CB open dot regime.

In this work, we demonstrate that the Fano q reversal occurs in QDs, in the open dot regime, through an interloping interaction between over-the-top shape resonances, which appear in the "nonresonant" open channels and Feshbach resonances, which exist in the "resonant" closed channels (Fig. 1). A nonresonant channel could be the source-drain leads and a resonant channel could be the discrete levels in a QD. We show that with minimal modifications of the QD geometry, we could induce Fano lineshape profile reversal and hence alter the electron transport in dramatic fashion.

The asymmetric profile of these resonances is a measure of the degree of configuration interaction, and Fano[22] was the first to provide an analytical expression for the spectral intensity,

$$I(\epsilon) = I_0 \frac{(q+\epsilon)^2}{1+\epsilon^2}, \tag{1}$$

where I_0 is some background intensity, ϵ is a reduced energy which vanishes at the position of the resonance, and q is the Fano profile parameter, a measure of the continuum and discrete configuration interactions. When $q \to 0$, a resonance dip or window appears, and when $q \to \infty$, the familiar Lorentzian profile is obtained. A positive (negative) value of q indicates that the intensity of the line falls (rises) as the energy is increased from $\epsilon = 0$.

Consider a model of a two-dimensional rectangular QD of width W_{QD} and length L connected to two leads of width W (Fig. 1). Our model is constructed on a single-electron scattering picture—the many-body effects are obviously at

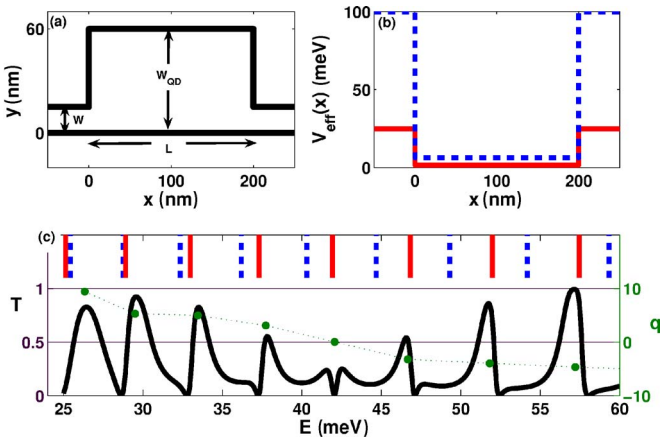

FIG. 1. (Color online) The electron transmission spectrum (C) through a QWG is modeled as a 2D structure with left and right leads and a rectangular QD (a). The first two interacting transverse modes are shown in (b), with open (closed) mode in solid (dashed) line. The profile reversal at an energy of 42 meV in the leads is from the interaction of an open-channel interlopper resonance with closed-channel Feshbach resonances (c). The positions of open-channel (solid) and closed-channel (dashed) resonances are indicated. The values of the Fano parameter q are shown in (c) (full circles).

play—but by focusing on the quantum interloping interaction, we will show that, nevertheless, complex Fano lineshape reversal occurs. The potential inside this quantum waveguide (QWG) is zero and infinite elsewhere. We study the scattering of electrons from the left lead (LL) through the QD and out of the right lead (RL) and calculate the transmission spectrum of such a monoenergetic beam of electrons in the S-matrix formalism.[23] The QWG is sectored into the LL and RL and QD regions, for which analytical solutions to the Schrödinger equation exist,

$$\Psi_L(x,y) = \sqrt{\frac{2}{W}}\sum_n \sin\left(\frac{n\pi y}{W}\right)\begin{Bmatrix} a_n^L b_n^L \\ b_n^R a_n^R \end{Bmatrix}\begin{Bmatrix} e^{ik_n x} \\ e^{-ik_n x} \end{Bmatrix},$$

$$\Psi_{\mathrm{QD}}(x,y) = \sum_m \sqrt{\frac{2}{W_{\mathrm{QD}}}}\sin\left(\frac{m\pi y}{W_{\mathrm{QD}}}\right)(c_n e^{iq_m x} + d_n e^{-iq_m x}), \tag{2}$$

where momentum components in the transverse modes n and m in the RL and LL, and in the QD, respectively, are

$$k_n^{L,R} = \sqrt{2m^* E/\hbar^2 - (n\pi/W)^2},$$

$$q_m = \sqrt{2m^* E/\hbar^2 - (m\pi/W_{\mathrm{QD}})^2}, \tag{3}$$

and m^* is the effective mass of the electron taken to be that of an electron gas in a GaAs substrate, i.e., $m^* = 0.067$ a.u. Once the wave functions and their derivatives have been matched at the sector boundaries, the S-matrix connecting the outgoing flux to the incoming flux is constructed as

$$\begin{pmatrix} \vec{b}^L \\ \vec{b}^R \end{pmatrix} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}\begin{pmatrix} \vec{a}^L \\ \vec{a}^R \end{pmatrix}. \tag{4}$$

The transmission from the LL mode n to all the RL modes can then be calculated[24] as follows:

$$T_n = \sum_m \frac{k_m^R + k_m^{R*}}{k_n^L + k_n^{L*}}[\mathbf{S}_{21}]_{m,n}\cdot[\mathbf{S}_{21}^*]_{m,n}. \tag{5}$$

An immediate observation, from the form of the numerator in the above fraction, is that only open channels (modes) in the RL contribute to the transmission. In order to elucidate the underlying physics, we restrict ourselves to a range in energy where there is only one open channel in the left and right leads.

Consider an electron moving from the left lead, traversing the QD to reach the right lead. The motion in the y direction is restricted by the infinite walls of the QWG, allowing us to construct an effective potential for the electron current passing through the QD from $x=-\infty$ to $x=+\infty$, $V_n^{eff}(x) = \hbar^2\pi^2 n^2/(2m^* W(x)^2)$, where the mode number n enumerates the different channels and $W(x)$ is the change in the QWG width as the electron advances from left to right. The couplings between the different channels are the usual derivative couplings in the Born-Oppenheimer approximation,[25] but are provided here through the nondiagonal elements of the S matrix, which are proportional to the transverse-mode overlap integrals. Each channel is described by a finite square well of depth $\Delta V_n^{eff} = \hbar^2\pi^2 n^2/2m^*(1/W^2 - 1/W_{\mathrm{QD}}^2)$ and of length L.

If the width of the leads, W, and the QD, W_{QD}, do not differ much, the square-well channels will be separated in energy from each other. In practice, $W \ll W_{\mathrm{QD}}$ and therefore the channels interlay. This interlaying of channels is the origin of the rich and complicated transmission spectrum cross sections in QWG [Fig. 1(c)]. Still, the asymmetric profiles that one observes in the transmission spectra generally have the same sign of the q parameter,[15] signaling the absence of an interloping effect and raising the question as to *what circumstances bring about a change in the sign of q*.

Infinite number of transverse modes (channels) in two dimensions can produce an arbitrarily complicated transmission spectrum. The essential physics of channel interaction and quantum interference that leads ultimately to the q-reversal phenomenon can be as well understood by simplifying the discussion to the scattering of electrons from only two channels. This means truncating the sums in Eqs. (2) to two terms in m and n. This truncated model contains many of the elements of interaction and interference in the problem.

Figure 1(c) shows the transmission spectra for the rectangular QD, as described above. A reversal of the sign of q occurs at $E \approx 42$ meV. The positions of the shape resonances in the first channel (solid lines) and of the bound states in the closed channel (dashed lines) are also marked. The bound-state positions serve as the zeroth-order approximation to the Feshbach resonance positions. The shape resonances are usually associated with the peaks in the transmission spectrum, as can be seen from a single-channel approximation comprising of Lorentzian peaks centered around the positions of

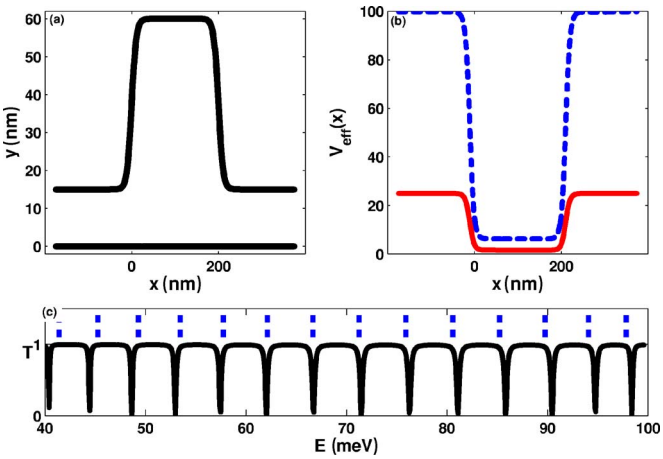

FIG. 2. (Color online) A model QWG containing left and right leads coupled smoothly to a QD (a). The first two interacting transverse modes are shown in (b), with the open mode (solid line) and the closed mode (dashed line). The transmission spectrum (c) shows a series of resonance dips which correspond well to the positions of the bound states in the closed channel, as indicated. No reversal of the Fano profiles appears.

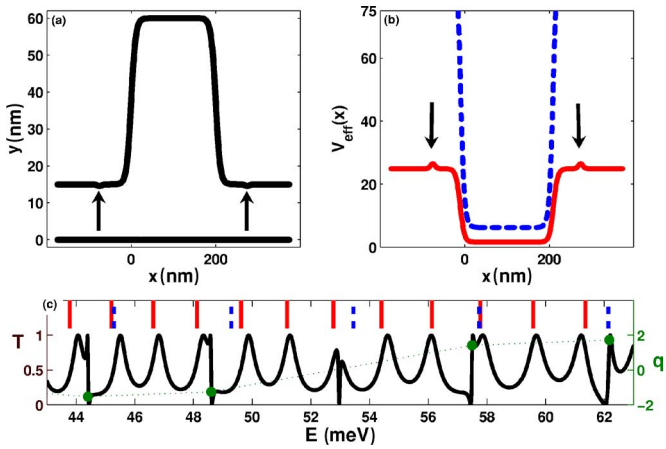

FIG. 3. (Color online) A smooth QD coupled lead with a small perturbation (marked by arrows) (a), which introduces small barriers (marked by arrows) in the effective potential shown in (b). The transmission is fully affected by the perturbation (see Fig. 2), and in particular, produces a reversal of the Fano profiles. The values of q are also shown on top of the transmission spectrum (c) (full circles). Large $|q|$ values are not shown. The sign of q, however, only changes after crossing $E \approx 53$ meV.

shape resonance (not shown here). When closed channels appear, channel interaction obscures this association of the peaks in the transmission with the shape resonances. Specifically, at the energy of the aforementioned q reversal, the transmission goes to zero nearly precisely, at the position of the shape resonance. An analysis of the poles of the S matrix for a coupled two square-well model with constant interaction[26] has shown the existence of two different types of poles which can be related to the open- and closed-channel poles, respectively,[26] and also shows the appearance of a mirror symmetry in the cross section, centered at specific energies, for different interaction strengths. In our case, channel interaction is more complicated, yielding the profile reversal.

To examine the effect of the shape resonances on the transmission, we compare the transmission spectrum of the rectangular QD described above and a smoothed "rectangular" QD in Fig. 2(a). For the smoothed QD, the width of the QWG is given by $W(x)=W+0.5(W_{\mathrm{QD}}-W)[\tanh \xi x-\tanh \xi(x-L)]$, where the smaller ξ is, the smoother the potential becomes. Figure 2(c) shows the transmission spectra of the smoothed QD for $\xi=0.005$. The profiles appearing in Fig. 2(c) are resonance dips, sometimes referred to as antiresonances[14,27] corresponding to $q \sim 0$. By comparing the positions of the bound states in the closed channel to the positions of the resonances in the spectrum, the absence of shape resonances can be confirmed. Thus in a two-channel approximation of conductance in a smoothed 2D QD, the q reversal results from the interaction between shape and Feshbach resonances.

The two models presented so far show that Fano q reversal could occur when the over-the-top and Feshbach resonances interact. More generally, the profile's reversal is the result of an interference between resonances in the "resonant" channel and resonances in the so-called nonresonant channel (NRC). The source of these NRC resonances differs from system to system; for example, in the model presented above, they result from the sharp curvature of the potential and, in the case of the 0.7 anomaly, they result from the Friedel oscillations in the QPC.[19]

Although rectangular QDs are of common use in modeling different phenomena in 2DEG, see, for example Refs. 28 and 29, the actual form of the potentials in the experiments are not necessarily sharp. We now wish to explore other possibilities in which interloping shape resonances can occur in the smooth model presented above.

Shape resonances can also appear due to barriers in the potential. These barriers (in the effective potential) can come about in an experiment as a result of coupling the QD to a reservoir by tiny leads, i.e., QPC or by some imperfection, causing a potential variation in the leads. A possible imperfection is when part of the lead is "thinner" than the rest of the lead, leading to barriers in the effective potential. We evaluate the transmission through a third structure, which simulates the possible effect of a small perturbation in the leads on the transmission in the smooth QD model discussed above [see Figs. 3(a) and 3(b)]. The difference between the transmission spectra of the slightly perturbed and unperturbed smooth QDs is remarkable considering the size of the perturbation. An inspection of the spectrum for this model shows a q reversal around $E \approx 53$ meV. As discussed above for the case of the rectangular QD, a one-to-one correspondence between the positions of spectral resonances [Fig. 3(c)] and the positions of noninteracting shape and Feshbach resonances is tenuous. This is the result, and consequentially a sign, of strong interaction and quantum interference between the different resonances, leading in Figs. 1 and 3 to q reversals occurring nearly at the position of a shape resonance, where the transmission goes to zero.

In summary, we have demonstrated in a series of open quantum dot simulations that intricate coherent quantum interference patterns, modulated due to strong interloping

channel interaction, result in the electronic transport through QD. It is shown that shape-induced and over-the-top states in the nonresonant channels interfere strongly with discrete QD levels in the closed resonant channels to produce modulation of transmission probability. We demonstrate that with slight modifications of the QD geometries, such as introducing small constrictions in the leads, we could arbitrarily introduce or remove the interloping shape resonances and hence create or destroy lineshape reversal in the transport conductance. This offers intriguing possibilities in coherence engineering in QWG systems.

This work was supported by the U.S. National Science Foundation through a grant for ITAMP at Harvard University and Smithsonian Astrophysical Observatory and by the fund of promotion of research at the Technion.

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