A Numerical Study of Resonance/Antiresonance Line Shape for Transmission in Quantum Waveguides with Resonantly-Coupled Cavities

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Abstract

We investigate the line shape of the transmission probability in quantum waveguides with resonantly-coupled cavities. The lifetime of the quasi-bound states is extracted from the asymmetrical transmission amplitude on the real-energy axis. The resonance/antiresonance feature in the vicinity of each quasi-bound state is characterized by a zero-pole pair in the complex-energy plane. We develop a generalization of the familiar symmetrical Lorentzian line shape, and discuss it in terms of Fano resonances.

I. Introduction

A common computational problem in quantum transport is to find the lifetimes of quasi-bound states from the transmission peaks. The underlying theory is that each quasi-bound state leads to a pole of the propagator (and the transmission amplitude) in the complex-energy plane. If this pole is sufficiently close to the real-energy axis, it will result in a resonance maximum of the observed transmission coefficient. A well understood problem is double-barrier resonant tunneling, where the lifetimes of the quantum well states may be extracted from the width of Lorentzian-shaped transmission peaks. A less understood problem is electronic transport in quantum waveguides with resonantly-coupled cavities [1]. It is known for these structures that the resonator states lead to resonance/antiresonance features [2, 3], but their detailed line shape has not been investigated so far. In this paper, we present a theory of the line shape for transmission in resonantly-coupled quantum waveguide, and we provide a computational method to extract the lifetimes of the corresponding quasi-bound states.

II. Poles and Zeros

For double-barrier resonant tunneling (DBRT), it is well known that the resonant transmission phenomena are related to the quasi-bound states in the quantum well region. Based on the Breit-Wigner formalism, a quasi-bound state at energy E_P and decay time $\tau = \hbar/2\Gamma$ yields a simple pole in the transmission amplitude $t(z)$ at the complex-energy $z = E_P - i\Gamma$ [4],

$$t(z) \sim \frac{1}{z-(E_P - i\Gamma)}. \tag{1}$$

If this pole is sufficiently close to the real-energy axis such that the effect of other poles can be neglected, the transmission probability, $T(E) = |t(E)|^2$, for a physical energy on the real-energy axis, E, is given by,

$$T(E) = \frac{\Gamma^2}{(E - E_0)^2 + \Gamma^2}, \tag{2}$$

which gives rise to a transmission resonance with a Lorentzian shape. It is an easy matter to extract the lifetime of the quantum well states from the width of the observed transmission peak.

An example of the transmission amplitude for DBRT is presented in Figs. 1(a) and (c), where the double-barrier structure and the transmission channnel are schematically shown in the inset of Fig. 1(a). In this example, the barrier is 0.2 eV high and $3nm$ thick, the separation of the barrier is 20 nm. We see the poles in the complex-energy plane are clearly visible in the contour plot of the absolute value of $t(z)$ in Fig. 1(c). The Lorentzian line shape of the transmission probability is shown in Fig. 1(a).

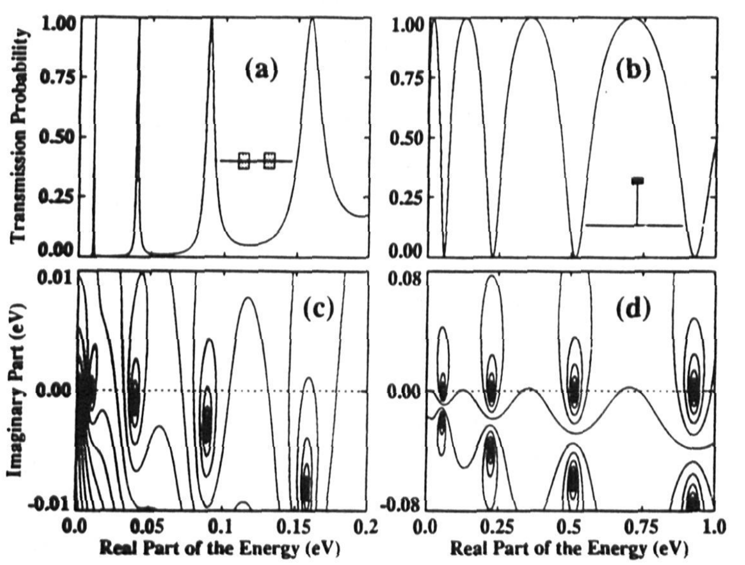

Figure 1. Comparison of the structure of the transmission amplitude in the complex energy plane for double-barrier resonant tunneling (poles) and t-stubs (zero-pole pairs). For DBRT, (a) shows the transmission probability on the real-energy axis, and (c) gives a contour plot of the absolute value of the transmission amplitude in the complex energy plane. For the t-stub structure, the corresponding plots are shown in (b) and (d), respectively.

Recently, much work has been done on transmission in resonantly-coupled quantum waveguide systems, and rich features of the transmission coefficient have been found (resonance/antiresonance) [5]. We have shown that the transmission amplitude exhibits zero-pole pairs in the complex-energy plane for this kind of the structure [6]. As a consquence, zero-pole pairs lead to asymmetrical transmission resonance/antiresonance features on the real-energy axis. As an example, we show the behavior for a t-stub structure, which is schematically shown in the inset of Fig. 1(b). It consists of a main transmission channel and a dangling wire of length $L = 10$ nm. Zero-pole pairs are clearly visible from the contour plot of the absolute value of $t(z)$ in Fig. 1(d).

III. Line Shape

Based on the zero-pole pair nature of the resonances in quantum waveguide structures, we make the following *ansatz* for the transmission amplitude in the vicinity of each quasi-bound state,

$$t(z) \sim \frac{(z - E_0)}{z - (E_P - i\Gamma)} . \tag{3}$$

Here, E_0 and $(E_P - i\Gamma)$ are the positions of the transmission zero and the pole, respectively. The lifetime of the quasi-bound state is given by $\tau = \hbar/(2\Gamma)$, as for the case of double-barrier resonant tunneling. Again, the transmission probability on the real-energy axis is given by $\mathcal{T}(E) = |t(E)|^2$, and the proportionality constant in eqn. (3) is determined by assuming peaks with unity transmission which are known to occur in symmetrical waveguide systems [6]. A unity transmission peak at energy E_1 provides two constraints for $\mathcal{T}(E)$, namely $\mathcal{T}(E_1) = 1$ and $\frac{d}{dE}\mathcal{T}\,|_{E_1} = 0$. It is an easy matter to show that,

$$\mathcal{T}(E) = \left[\frac{\Gamma^2}{(E_P - E_0)^2 + \Gamma^2}\right]\left[\frac{(E - E_0)^2}{(E - E_P)^2 + \Gamma^2}\right] . \tag{4}$$

The above expression gives the line shape of the transmission probability for resonantly-coupled quantum waveguides in terms of three parameters, namely the energy of the transmission zero, E_0, the energy of the resonant state, E_P (the real part of the pole energy), and the inverse lifetime of the state, Γ (the imaginary part of the pole energy). Note that (4) produces an asymmetrical line with a resonance/antiresonance behavior. Such asymmetrical line shapes have previously been noted in atomic and molecular physics [7]. These so-called Fano resonances are know to occur when a bound state is coupled to a continuum of states, thereby leading to resonance phenomena [8].

In his original paper [7], Fano, after somewhat lengthy derivations, found that the autoionization cross section could be parameterized by $(q+\epsilon)^2/(1+\epsilon^2)$, where ϵ is a reduced energy (it is defined as $\epsilon = (E - E_{Res})/\Gamma$, where E_{Res} is the energy of the resonant state) and q is treated as a parameter (it is a complicated expression involving matrix elements). We note that this is the same line shape as our eqn. (4) by making the following substitutions, $\epsilon = (E - E_P)/\Gamma$ and $q = (E_P - E_0)/\Gamma$. Comparing our approach to Fano's [7], we note that ϵ has a similar meaning where E_P, the real-part of the pole energy, corresponds to E_{Res}, the energy of the resonant state. For the parameter q, our approach yields a simple expression which could not have been inferred from Ref. [7]. Apparently, Fano's line shape corresponds to a zero-pole structure in the complex-energy plane, a fact which has not been noted before.

Given a certain transmission curve, we now can fit each resonance/antiresonance feature to obtain the lifetime of the corresponding quasi-bound state. Using the known energies of the transmission zero, E_0, and transmission one, E_1, we can find,

$$E_P = \frac{(E_0 + E_1)}{2} \pm \frac{\sqrt{(E_0 - E_1)^2 - 4\Gamma^2}}{2} , \tag{5}$$

The choice of the sign in the above equation determines whether $E_P > E_0$ or $E_P < E_0$. With this, the only unknown parameter is Γ which may be used to obtain the best fit of the theoretical line shape (4) to the given transmission curve. We seek the best fit in the sense of the least mean square error.

IV. Results

We now present several examples to fit the lineshapes of resonance and antiresonance pairs. Figure 2 presents fits of the resonance/antiresonace line shapes for a family of so-called weakly coupled t-stubs [6], which are schematically shown in the insets. In Figs. 2(a), (b), and (c), the resonant stubs are separated from the main transmission channel by a tunneling barrier of length $\ell = 1.0\ nm$ and height $V_0 = 0.5\ eV$, $V_0 = 1.0\ eV$, and $V_0 = 2.0\ eV$, respectively. In each case, we show 3 quasi-bound states which lead to zero-one features in the transmission probability, and which are labeled in the plots. Figures 2(α), (β), and (γ), show the fitted line shape for the resonance numbered 3 of cases (a), (b), and (c), respectively. The fit is shown by the dotted line, and the curve to be fitted by the solid line.

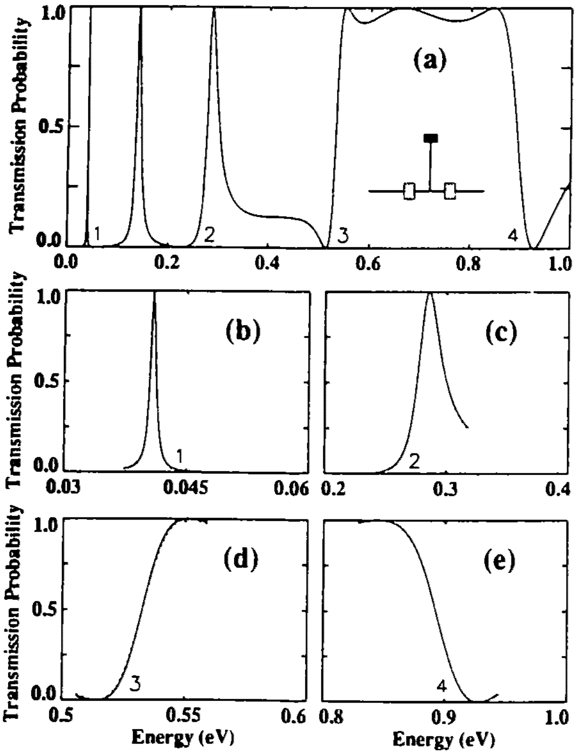

Figure 3. Example of fits using the line shape (4) for a t-stub with a double barrier structure on the transmission channel shown in the inset to (a). The fits of resonances 1 - 4 are shown in (b) - (e), respectively.

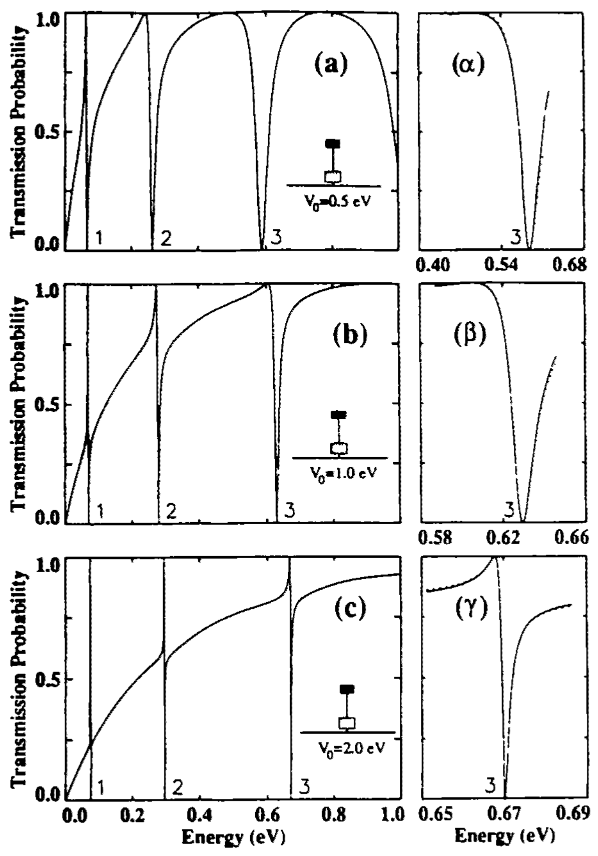

Figure 2. Examples of fits using the line shape (4) for the weakly-coupled t-stub structures shown in the insets. The fits to the third resonant state of (a), (b), and (c) are given in (α), (β), and (γ), respectively. The fits are shown by the dotted line, and the curve to be fitted by the solid line.

In figure 3, we present another example which shows transmission for a t-stub in addition to double-barrier resonant tunneling on the main transmission channel. A schematic drawing of this waveguide structure is displayed in the inset, and the two tunneling barriers have a thickness of 1 nm, height of 0.5 eV, and separation of 4 nm. Figure 3(a) shows the transmission probability on the real-energy axis. Figures 3(b) - (e) display the fits according to our *ansatz*, eqn. (3), for resonances 1 - 4, respectively. Again, the fit is shown by the dotted line, and the curve to be fitted by the solid line. It appears that the zero-pole character of each quasi-bound state, leads to extremely good fits of the transmission probability in the vicinity of each resonance.

In general, the locations of the poles and the zeros on the real-energy axis are not the same, i.e. $E_P \neq E_0$. It is this fact that gives rise to the asymmetric line shape, eqn. (4). Note that from eqn. (5), the position of the pole, E_P, is always between the positions of the transmission zero and one, E_0 and E_1. If the pole and the zero occur at the same real energy, i.e. $E_P = E_0$, then eqn. (4) yields a symmetric line shape,

$$\mathcal{T} \mid_{E_P=E_0} \;=\; \frac{(E-E_P)^2}{(E-E_P)^2+\Gamma^2} \,. \tag{6}$$

The above expression describes a Lorentzian-shaped reflection line.

In recent work [3], Price has pointed out that a resonant quasi-bound state can give rise to either Lorentzian-shaped transmission or reflection peaks, and he terms these peaks resonances of the first and the second kind, respectively. We see that the reflection peaks in general will not have a Lorentzian shape, and that Price's resonances of the second kind are recovered when $E_P = E_0$.

In summary, we have investigated the detailed line shape of the transmission probability in quantum waveguides with resonantly-coupled cavities. The resonance/antiresonance features in the vicinity of each quasi-bound states can be characterized by a zero-pole pair in the complex-energy plane. We have found a generalization of the familiar symmetrical Lorentzian resonance peaks. Using several examples, we have demonstrated the utility of our line shape (4) to extract the lifetime of the quasi-bound state by a fit to the data. We also discussed the asymmetrical line shapes in the context of Fano resonances.

Acknowledgement: This work was supported in part by AFOSR, ARPA, and ONR.

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