# A NUMERICAL STUDY OF TRANSMISSION RESONANCES AND ZEROS IN QUANTUM WAVEGUIDE STRUCTURES

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**Abstract**

It is well known that transmission resonances exist in double-barrier resonant tunneling structures. In this paper, we study transmission in quantum waveguide systems with attached resonators. We find that these quantum wire systems exhibit a rich structure in the transmission amplitude. In addition to transmission resonances, these systems also possess transmission zeros. In order to elucidate these differences, we present a numerical study of the transmission amplitude in the complex-energy plane for both double-barrier resonant tunneling and resonant quantum wire structures.

## Introduction

Transmission in quantum waveguide systems has been studied because of their potential application in nano-scale devices. Sols and co-workers [1] investigated transmission in quantum channels with attached t-stub resonators. They found that resonant states in the t-stubs led to a strong variation in the transmission coefficient, and they proposed to exploit this behavior as a switching mechanism in devices. Lent [2] studied transmission in the so-called "quantum whistle" which is a channel with an attached circular resonator. He also found rich structure in the transmission coefficient as a function of energy, which apparently is related to quasi-bound states in the resonant cavity. Similar features were also seen in the loop structures [3, 4]. In a recent study, Price [5] shed light on the relationship between the transmission coefficient and quasi-bound states for quantum waveguides with attached resonators. Using a scattering matrix approach, he demonstrated that resonant states may lead to both maxima or minima in the transmission coefficient. This rich behavior is in marked contrast to transmission in the much-studied double barrier resonant tunneling structures, where only Breit-Wigner-type resonances are observed.

Here, we present a numerical study of the transmission amplitude in the complex-energy plane for both double-barrier resonant tunneling and quantum wire structures. For both systems, we find that the transmission amplitude has poles in the complex-energy plane [6]. In addition, quantum wire systems (but not double-barrier resonant tunneling structures) possess zeros of the transmission amplitude on the real-energy axis. A pole and a zero in close proximity lead to the sharp variation of the transmission coefficient as a function of energy, which was noted in the previous studies. In the following, we elucidate this behavior by presenting several examples.

## Approach

We solve the time-independent Schrödinger equation to obtain the transmission amplitude in the complex-energy plane for double-barrier resonant tunneling and quantum wire systems. The finite element method is used to discretize the problem domain, and the quantum transmitting boundary method is employed for the current-carrying boundary conditions [7]. The waveguide structures are assumed to consist of thin wires such that only one transverse mode has to be considered. At each branch point in the network, we use matching conditions for the wavefunctions and their derivatives. The resulting system of linear equations is solved utilizing standard routines.

## Results

Double-barrier resonant tunneling has been studied extensively [8-10]. It is well known that the transmission amplitude possesses poles in the complex-energy plane, which correspond to the quasi-bound states in the quantum well region. The real part of the pole locations gives the energy of each resonant state, and the imaginary part determines their lifetime. Figure 1 presents an example of the transmission amplitude in the complex-energy plane for the double-barrier structure shown in the inset (L=30 nm, b=5 nm, $V_0$=0.2 eV, and $V_W$=0.1 eV). The top panel displays the absolute value of the transmission amplitude on the real-energy axis. The bottom panel shows a contour plot of the absolute value of the transmission amplitude in the complex-energy plane. The poles in the lower half (negative imaginary part) of the complex plane are clearly visible. Furthermore, it is evident from this figure that the poles result in transmission resonances on the real-energy axis. Each resonance is centered (Lorentzian shape) around the energy of a quasi-bound state (real-part of a pole).

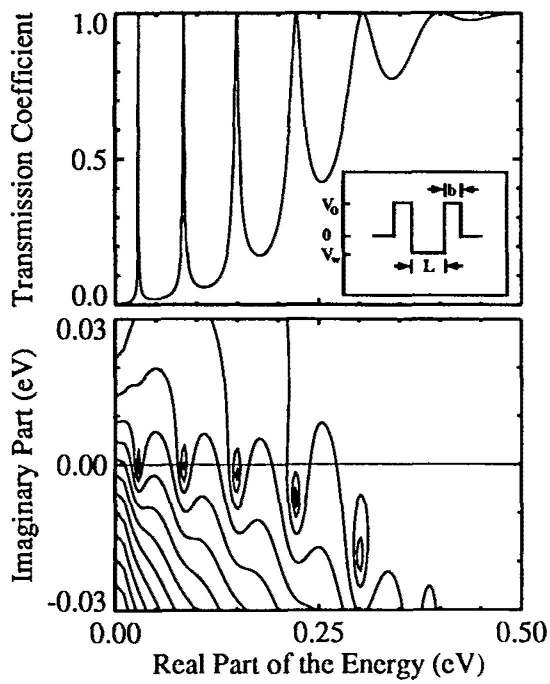


Figure 1: Transmission amplitude in the complex-energy plane for double-barrier resonant tunneling.

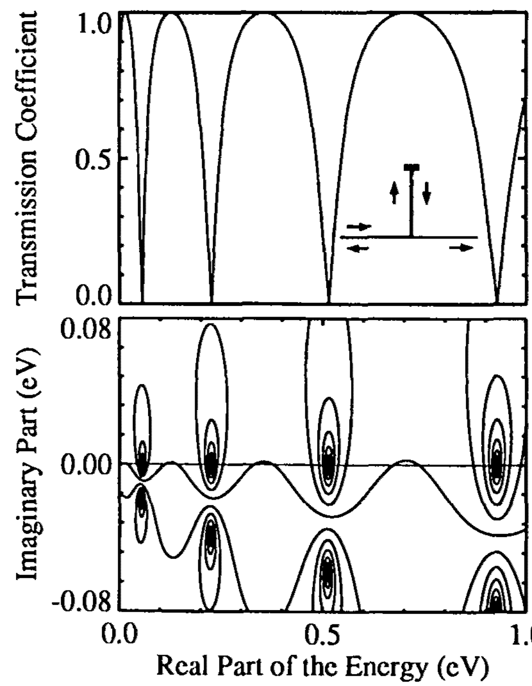


Figure 2: Transmission amplitude in the complex-energy plane for a strongly-coupled t-stub resonator.

Figure 2 displays the transmission amplitude in the complex-energy plane for a strongly-coupled stub. The inset shows the wire structure which consists of a transmission channel and an attached resonator of length L=10 nm. Again, the top panel displays the transmission coefficient on the real-energy axis, and the bottom panel shows the contour plot in the complex-energy plane. Note the existence of transmission zeros on the real-energy axis. In contrast to double-barrier resonant tunneling, the transmission maxima do not occur at the same energies as the poles. Rather, they occur at some intermediate energy between two zeros which is determined by the proximity of the poles to the real-energy axis.

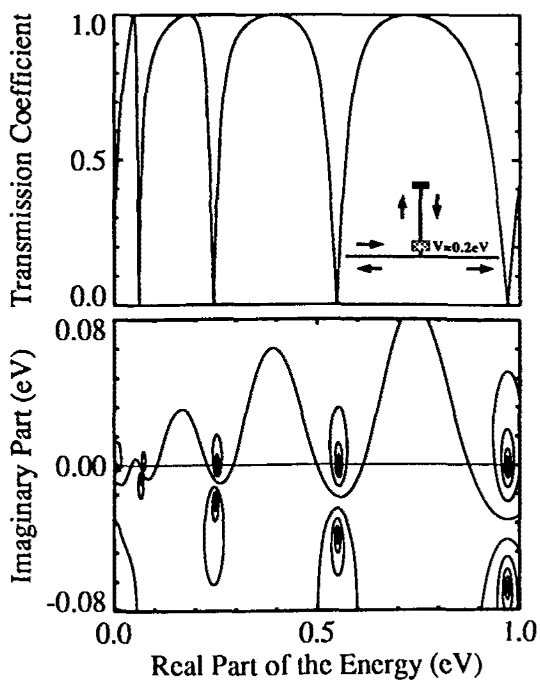


Figure 3: Transmission amplitude in the complex-energy plane for a weakly-coupled t-stub resonator.

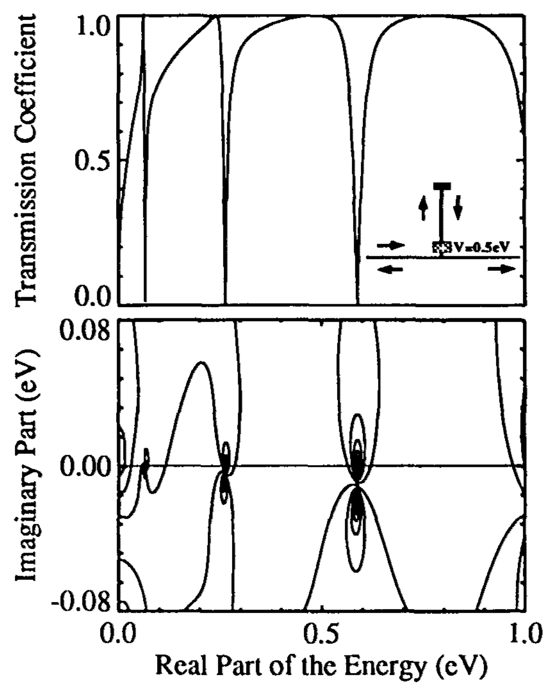


Figure 4: Transmission amplitude in the complex-energy plane for a weakly-coupled t-stub resonator.

A potential barrier may also be used to weakly couple the resonator to the transmission channel. Figures 3 and 4 show the transmission amplitude in the complex-energy plane for two such weakly-coupled t-stubs with barrier heights of 0.2 eV and 0.5 eV, respectively. The insets in these figures schematically show such potential barriers (thickness d=1 nm) which are placed in the side-arm close to the branch point. The main effect of the barriers is to increase the lifetimes of the quasi-bound resonant states in the stub. As can be seen, the longer-lived states for the larger barrier height possess poles which move closer to the real-energy axis. The closer proximity of zeros and poles in Fig. 4 (compared to Fig. 3) leads to a sharper variation of the transmission coefficient on the real-energy axis. In the limit of an infinitely high barrier, the poles and zeros lie on top of each other and the transmission coefficient becomes unity and independent of energy, corresponding to perfect transmission in a completely decoupled transmission channel.

The electronic states in the resonator are standing waves, where the wavenumber $k$ is related to the energy $E$ by the usual free-electron-like dispersion relation, $E = \hbar^2 k^2 / 2m^*$. Transmission zeros and ones occur whenever the wavefunction in the resonator matches a zero or one in the transmission channel, respectively. For the strongly-coupled stub, the zeros and poles are separated by a quarter-wavelength which has to fit into the side arm. For the weakly-coupled stubs, the exponential decay of the wavefunction in the barrier region forces the zeros and ones closer in energy. For each additional quasi-bound state, the matching conditions for an additional transmission zero and one are satisfied. Each resonant state, thus, results in a zero-pole pair in the complex-energy plane.

We also investigated transmission in loop structures. Figures 5 and 6 show the transmission amplitude in the complex-energy plane for a symmetrical ($L_1$=$L_2$=10.5 nm) and an asymmetrical ($L_1$=10.5 nm and $L_2$=12 nm) loop. The symmetrical loop is particularly interesting since it contains true bound states. The associated zero-pole pairs lie right on top of each other which cancels the zero in the transmission coefficient. Any slight asymmetry in the side arms of the loop will separate the zero-pole pairs, as can be seen in Fig. 6, thus resulting in very sharp features in the transmission coefficient on the real-energy axis.

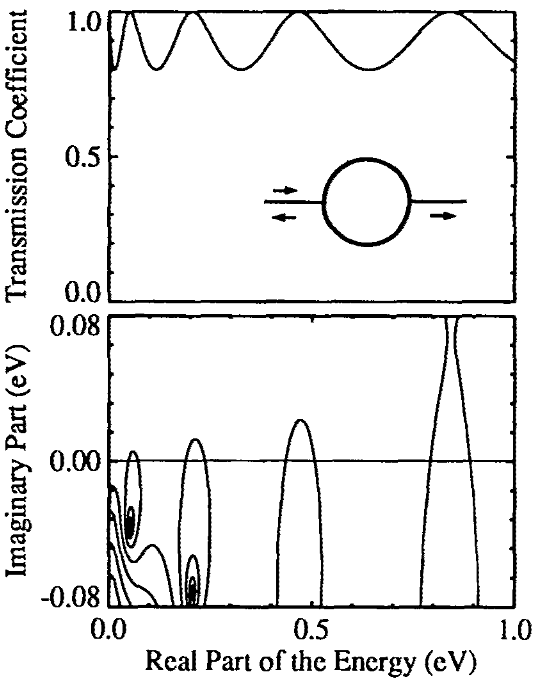


Figure 5: Transmission amplitude in the complex-energy plane for a symmetric loop.

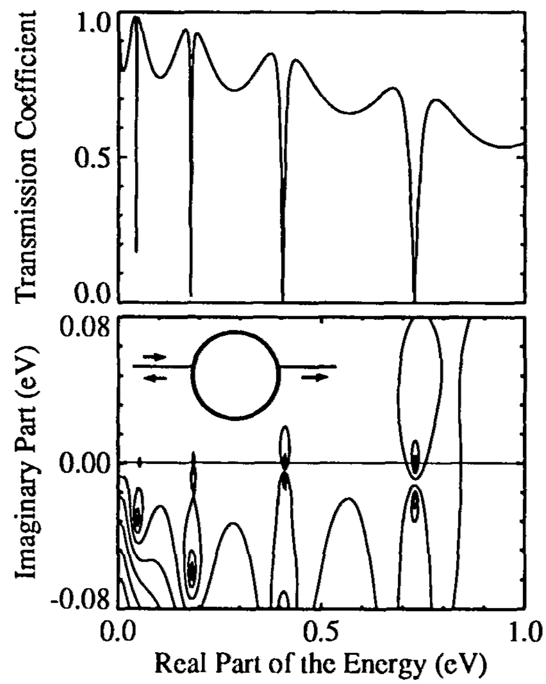


Figure 6: Transmission amplitude in the complex-energy plane for an asymmetric loop.

## Summary

We demonstrated that the transmission amplitude for quantum waveguide systems possesses a richer structure than for the much-studied case of double-barrier resonant tunneling. The interference of the standing wave in the resonator with the wave in the waveguide results in transmission ones and zeros. These are a consequence of a zero-pole pair which each quasi-bound state produces in the complex-energy plane. In contrast, the transmission amplitude for double-barrier resonant tunneling solely possesses poles which lead to the well-known Breit-Wigner resonances.

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