A LINEAR EIGENVALUE METHOD FOR CALCULATING THE POSITIONS OF TRANSMISSION POLES AND ZEROS IN RESONATOR STRUCTURES

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Abstract

We present a numerical technique which yields, as the solutions of a linear eigenvalue problem, the positions of transmission poles and zeros in resonator structures with arbitrary potential profiles. We present several examples to demonstrate the utility of this numerical technique.

I. INTRODUCTION

A common computational problem is to find the quasi-bound states of resonant transmitting systems. For an isolated bound system, because of the zero wavefunction boundary conditions, the Hamiltonian of the system is Hermitian, hence the system has only bound states. However, for an open unbound system, because the wavefunctions at the boundary are non-zero, the complex boundary condition may lead the Hamiltonian of the system non-Hermitian, hence the system possesses quasi-bound states for resonant transmission [1]. In general, to find the quasi-bound states of a given system with scattering boundary conditions requires to search for the zeros of an energy-dependent matrix determinant [2, 3].

In this paper, we use another approach to solve this problem. Based on the quantum transmitting boundary method (QTBM) and a finite element discretization [4], we present an eigenvalue algorithm which yields the positions of the transmission poles. We can also use this algorithm to calculate the positions of transmission zeros in quantum waveguide systems [5].

II. APPROACH

In general, a transmission problem shown in Figs. 1(a) and 2(a) may be formulated as an inhomogeneous problem, $Au=\alpha P$. Here, A is an energy-dependent coefficient matrix, u is the unknown wavefunction, and αP is the source flux. Specifically, α can be either the incoming amplitude, i(E) in figure 1(a), or the transmission amplitude, t(E) in figure 2(a), and P is an energy-dependent vector. For a given source flux αP, the solution of the inhomogeneous system is uniquely determined. We can also force the source flux $\alpha P=0$, as shown in figures 1(b) and 2(b), which results in a homogeneous problem, $Au=0$. This is, in general, a nonlinear eigenvalue problem. Using the finite element discretization, furthermore, results in a linear eigenvalue problem.

For the transmission problem, shown in Fig. 1(a), Schrödinger's equation can be written as the following inhomogeneous system, where all matrices are constant and the energy dependence is shown explicitly,

$$(\mathbf{H} - E\,\mathbf{Q} + k_L\,\mathbf{B_L} + k_R\,\mathbf{B_R})\,\psi = i(E)\,k_L\,\mathbf{p} \ . \tag{1}$$

Here, i(E) is the amplitude of the forcing incoming flux at energy E. The wavenumbers at the left and right boundaries of the system are k_L and k_R, respectively, which are related through the external bias V_{bias} by, $k_R^2-k_L^2 = (2m^*eV_{bias})/\hbar^2$; all symbols have their usual meaning. The bound state problem is contained in the above system as $(\mathbf{H} - E\,\mathbf{Q})\,\psi = 0$, and the matrices $\mathbf{B_L}$, $\mathbf{B_R}$, and $\mathbf{p}$ arise due to the open boundaries.

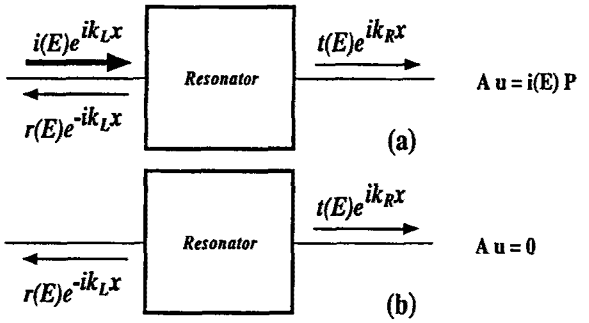

Figure 1. Schematic diagram of a resonant structure with a forcing incoming flux (thick arrow). (a) shows an incident wave from the left (source) with its transmitted and reflected components, which results in an inhomogeneous problem; (b) setting the incident wave (source) to zero, leads to an eigenvalue problem. Its solutions give us the quasi-bound states of the system, or the positions of the transmission poles.

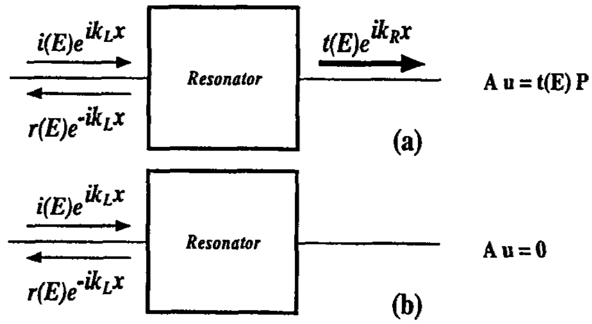

Figure 2. Schematic diagram of a resonant structure with a forcing transmitted flux (thick arrow). (a) shows an incident wave from the left with its transmitted (source) and reflected components, which results in an inhomogeneous problem; (b) setting the transmitted wave (source) to zero, leads to an eigenvalue problem. Its solutions give us the positions of the transmission zeros.

Forcing the incoming flux to zero, i(E)=0 as shown in Fig. 1(b), produces the decaying quasi-bound states of the system. Equation (1) becomes a polynomial eigenvalue problem of degree p=2 for an unbiased system ($V_{bias} = 0$ and $k_L = k_R$) and of degree p=4 for a biased system. In the latter case, we perform the following transformations, $k_R = \bar{k} + \Delta$ and $k_L = \bar{k} - \Delta$, with $\Delta = (m^* eV_{bias})/(2\hbar^2 \bar{k})$. This leads to a fourth-order polynomial eigenvalue problem in $\bar{k}$,

$$(A_0 + \bar{k} A_1 + \bar{k}^2 A_2 + \bar{k}^3 A_3 + \bar{k}^4 A_4) \psi = 0 \ , \tag{2}$$

where the above A's are related to the matrices in equation (1). The polynomial eigenvalue problems of degree p can be rearranged into linear eigenvalue problems with p times the original matrix size. Since the resulting matrix is not Hermitian in this case, the eigenvalues are located in the complex-energy plane. The real and imaginary parts of these eigenvalues correspond to the energies and lifetimes of the quasi-bound states of the resonant transmission system.

The transmission problem may also be viewed as one in which the resonant structure is forced to yield a certain transmitted amplitude t(E), as schematically shown in Fig. 2(a). In this case, the required incident and reflected amplitudes are the unknowns. Using the boundary condition $\psi(x_R) = t(E) \exp(ik_R x_R)$ at the right edge x_R of the system, we may re-write equation (1) in a form where only terms proportional to t(E) appear on the right-hand-side. Terms proportional to the incident amplitude i(E) appear on the left-hand-side, and i(E) now is part of the solution vector ψ which contains the unknowns.

Forcing the transmitted flux to zero, t(E)=0 as shown in figure 2(b), produces the transmission zeros. It can be shown that the corresponding eigenvalue problem is linear in the energy, and has the form,

$$(\mathbf{H'} - E\,\mathbf{Q'}) \psi' = 0 \ , \tag{3}$$

where the matrices **H'** and **Q'** are related to the corresponding ones in (1). For t-stub systems, furthermore, it can be shown that **H'** is also Hermitian. As a consequence, the eigenvalues in this case, which are the energies of the transmission zeros, always occur on the real-energy axis. This result is consistent with our previous scattering matrix investigations, where we also proved that transmission zeros always occur on the real-energy axis [5].

III. EXAMPLES

We now present several examples to demonstrate the utility of our approach. First, we apply our method to a multi-barrier resonant-tunneling structure with applied external bias. Next, we locate the positions of transmission poles and zeros in quantum waveguide systems, which include t-stub and loop structures. We compare the results of our direct eigenvalue method to the more conventional method of searching in the complex-energy plane for the zero of the system determinant.

1. Multi-Barrier Resonant-Tunneling Structure with Applied Bias

As our model system, we consider a 10-barrier resonant-tunneling structure in a uniform electric field of $\mathcal{E}$=150 kV/cm. The barrier width and height are 1.4 nm and 5.0 eV, respectively, and the well width is 4.9 nm. For the finite element discretization, we use an average mesh size of 0.7 nm for the numerical calculation, which yields matrices of dimension 92 in equation (1). We choose the middle of the structure as the zero point of the potential.

Applying our eigenvalue method to this structure, we obtained the energies of the quasi-bound states, which are the poles of the transmission amplitude in the complex-energy plane. It is well known that no transmission zeros exist in this case. It is an easy matter to numerically obtain the eigenvalues of the linear system (2) with dimension 368. The results are plotted in Fig. 3, and the numerical values for the real and imaginary parts of the poles are given in tabular form. The horizontal lines indicate the computed spatial electron densities in each quasi-bound state. The formation of minibands is evident, which are derived from the individual states in each well. The imaginary part of each pole gives the inverse of the lifetime for the corresponding quasi-bound state. As one would expect, the longest-lived states are concentrated in the middle of the structure, and states toward the edges are more "leaky." Note that the imaginary parts vary by many orders of magnitude. This makes a direct search for the locations of the poles in the complex-energy plane very costly since a very fine mesh has to be used in order to avoid missing poles. In contrast, our direct method yields the energies of all poles, without any search, as the solutions of a linear eigenvalue problem.

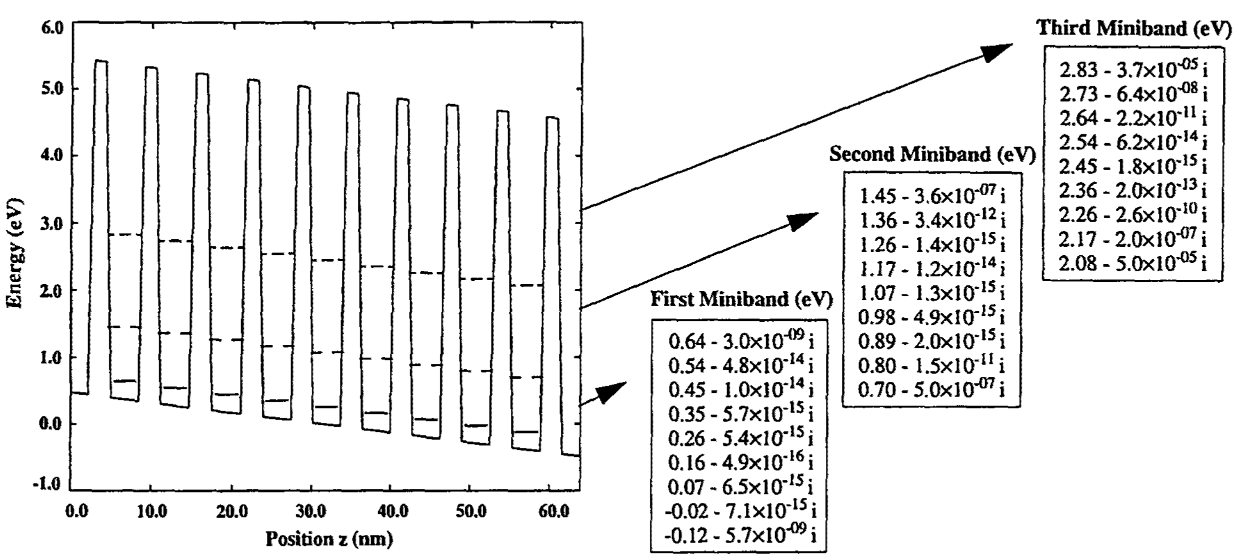

Figure 3. The quasi-bound states of a multi-barrier resonant tunneling structure in a uniform electric field. The states are plotted as horizontal lines at the real energy of the resonance, and the lines are drawn for those positions at which the absolute value of the wavefunction is larger than a threshold value. The real- and imaginary-parts of the resonances in each miniband are also given.

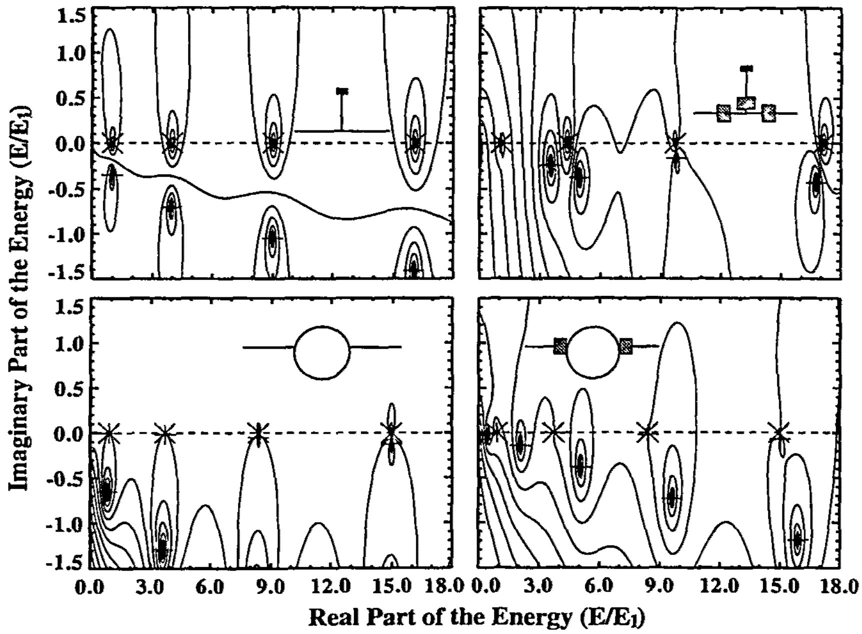

Figure 4. Shown are contour plots of the absolute value of the transmission amplitude for t-stub and loop structures, which are schematically shown in the insets. The '+' and 'X' symbols represent the positions of transmission poles and zeros, respectively, which were calculated by our direct eigenvalue method. The energy of the first standing wave in the stub (E_1=56.2 meV) is used as the unit of energy. The results obtained by both methods agree very well.

2. Quantum Waveguide Structures

We choose t-stub and loop structures as our model systems, which are schematically shown in the insets of Fig. 4. The solid lines represent the waveguides which are transmission channels. The shaded boxes represent tunneling barriers (0.5 eV high and 1 nm thick) and the full filled box terminates the stub. For the t-stub structures, the length of the stub is 10 nm and the distance between two tunneling barriers on the main transmission channel is 4 nm. For the asymmetrical loops shown here, the lengths of the two arms are 10 and 11 nm, respectively. Spatial mesh dimensions of 0.2 nm are used in the numerical calculations.

It is well known that these systems possess both transmission poles and zeros [5]. The contour lines in Fig. 4 represent the absolute value of the transmission amplitude in the complex-energy plane, which is obtained from a solution of the inhomogenoues problem (1). Poles and zeros, which occur on the real-energy axis, are easily discerned. Using the appropriate eigenvalue problem, we also show the directly calculated locations of the transmission poles and zeros which are indicated by the symbols '+' and 'X', respectively. Note the perfect agreement between the two methods. Again, our technique directly yields poles and zeros without a need to search for them in the complex-energy plane.

IV. SUMMARY

We presented a new approach for directly calculating the positions of transmission poles and zeros in resonant transmission structures. In general, a transmission problem is an inhomogeneous problem. Forcing the source flux to zero, for either the incoming wave or the transmitted wave, results in a non-linear eigenvalue problem. Using the finite element method, furthermore, these eigenvalue problems become linear. It is then an easy matter to directly calculate the energies of the transmission poles and zeros.

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