QUANTUM DEVICE SIMULATION: OPEN BOUNDARY CONDITIONS FOR THE SCHRÖDINGER EQUATION

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ABSTRACT

We discuss the problem of solving the Schrödinger equation on a finite domain for the current-carrying "scattering states" that are frequently of interest from a device viewpoint. We compare approaches based on the finite difference approximation with finite element and green function methods.

I. INTRODUCTION

In exploring theoretically the properties of mesoscopic structures it is frequently of interest to be able to calculate current densities and transmission coefficients for the case of purely ballistic transport with no inelastic scattering in the structure. In a typical idealized structure, current carrying leads with constant width are connected to a device region in which scattering from geometrical features of the potential landscape occurs. A straight-forward approach to the problem is to discretized the device region on a real-space mesh and numerically solve the equations which result from discretizing the Schrödinger equation for the wavefunction in that region. The desired current densities and transmission coefficients can then readily be obtained from the wavefunction directly. A difficulty which occurs is to express boundary conditions for the wavefunction at the interface between the leads and the device region. The wavefunction at the input is the sum of the incident and scattered wave, but the reflection (and transmission) coefficients are unknown at the beginning of the calculation. We have used a boundary-condition method, the Quantum Transmitting Boundary Method [1], and employed it in a finite element (FEM) discretization useful in many two-dimensional problems [2]. Here we compare the implementation of these boundary conditions in the finite difference method (FD) and FEM, and also compare with a recently developed Green function approach. We will restrict ourselves to one-dimensional problems for simplicity. The generalizations to higher dimensions have either been treated elsewhere in detail or are straight-forward.

II. BOUNDARY CONDITIONS ON THE WAVE FUNCTION

We examine first the problem of expressing the condition on the boundaries as a constraint on the wavefunction and its derivative. Figure 1 shows the geometry schematically. An arbitrary scattering potential in the device region from $x=0$ to $x=L$ results in scattered and transmitted plane waves. We

(1)

FIGURE 1. Schematic of 1D Schrödinger scattering problem.

assume a plane wave of unit amplitude is incident from the left. In the lead to the left of the device region the wavefunction has the form

$$\psi(x) = e^{ikx} + re^{-ikx}, \tag{1}$$

while in the right lead the wavefunction is,

$$\psi(x) = te^{ikx}. \tag{2}$$

Evaluating the derivative at the left boundary we have,

$$\psi'(0) = ik(1-r) = 2ik - ik\psi(0) \tag{3}$$

Similarly in the right lead we have

$$\psi(x) = te^{ikx}, \tag{4}$$

so that at the boundary with the right lead we have,

$$\psi'(L) = ik\psi(L). \tag{5}$$

The conditions at the boundaries of the discrete domain can therefore be expressed as follows:

$$\psi'(0) + ik\psi(0) = 2ik \tag{6}$$

$$\psi'(L) - ik\psi(L) = 0 \quad . \tag{7}$$

Equations (6) and (7) are the fundamental boundary conditions for open boundaries in one dimension. The inhomogeneous source term on the right-hand-side of equation (6) results in an incoming plane wave of unit amplitude. The generalization to higher dimensions must include the projection of the normal derivatives onto the various transverse mode of the leads and the existence of evanescent, exponentially decaying, modes.

II. FINITE DIFFERENCE FORMULATION

The boundary conditions in (6) and (7) can readily be expressed in terms of finite difference approximations to the derivatives at the boundaries. If the nodal points are numbered from 0 to N in the device region, the difference equations become

$$(ik - \frac{1}{h})\psi_0 + (\frac{1}{h})\psi_1 = 2ik \qquad\qquad (-ik + \frac{1}{h})\psi_N - (\frac{1}{h})\psi_{N-1} = 0 \tag{8}$$

where h is the distance between nodal points. The resulting FD equations can be expressed in terms of an a hopping energy parameter,

$$\Delta = \frac{\hbar^2}{2m^*}(\frac{1}{h^2}). \tag{9}$$

The resulting equations form a linear system with the term $2ik$ from (6) giving the right-hand-side vector. The equations can be written in the form

$$(H - EI)u = p, \tag{10}$$

where u is the column vector of the values of the wavefunctions at the nodal points. If we assume that at the boundaries the potential is zero, this equation becomes,

(11)

$$\begin{bmatrix} (ik-\frac{1}{h}) & (\frac{1}{h}) & & & & & & \\ -\Delta & (2\Delta-E+V_1) & -\Delta & & & & & \\ & -\Delta & (2\Delta-E+V_2) & -\Delta & & & & \\ & & -\Delta & (2\Delta-E+V_3) & \cdots & & & \\ & & & \cdots & \cdots & -\Delta & & \\ & & & & -\Delta & (2\Delta-E+V_{N-1}) & -\Delta & \\ & & & & & -\frac{1}{h} & -ik+\frac{1}{h} & \end{bmatrix} u = \begin{bmatrix} 2ik \\ 0 \\ 0 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

The relationship between the wavevector, k, and the energy, E, bears some attention. For free (effective mass) electrons the dispersion is given by

$$E = \frac{\hbar^2 k^2}{2m^*}. \tag{12}$$

The finite difference approximation is equivalent to a tight-binding model and the dispersion is quadratic only in the limit when $h \rightarrow 0$. At any finite mesh size, the numerical dispersion is given by,

$$E_{FD}(k) = 2\Delta\left[1 - \cos(kh)\right] \tag{13}$$

III. FINITE ELEMENT FORMULATION

A finite element formulation begins by developing the weak form of the Schrödinger equation (S.E.). This is done by multiplying the original S.E. by an arbitrary test function $\overline{\psi}$ which obeys the same essential boundary conditions as the wavefunction, and integrating over the interval.

$$-(\frac{\hbar^2}{2m^*})\int_0^L dx\ \overline{\psi}(x)\psi''(x) + \int_0^L dx\ \overline{\psi}(x)V(x)\psi(x) = E\int_0^L dx\ \overline{\psi}(x)\psi(x) \tag{14}$$

Integrating by parts we obtain the weak form of the S.E.:

$$(\frac{\hbar^2}{2m^*})\int_0^L dx\ \overline{\psi}'(x)\psi'(x) + (\frac{\hbar^2}{2m^*})\left[\overline{\psi}(0)\psi'(0) - \overline{\psi}(L)\psi'(L)\right] + \int_0^L dx\ \overline{\psi}(x)V(x)\psi(x)$$

$$= E\int_0^L dx\ \overline{\psi}(x)\psi(x)$$

Notice that the derivative of the wavefunction at the boundary occurs naturally here. The constraint equations (6) and (7) can now be applied. When both the wavefunction and the test function are expanded in the basis of finite element shape functions (here we use linear functions), we obtain the matrix equation

$$(T + C + V - EM)\,u = p. \tag{15}$$

The matrices T and V represent the kinetic and potential energy operators in this basis. The "mass" matrix M results from the non-orthogonality of the FEM basis functions. The transmitting boundaries are represented by the matrix C. The structure of the FEM matrices is displayed below.

$$T = (h)\begin{bmatrix} \Delta & -\Delta & & & & & \\ -\Delta & 2\Delta & -\Delta & & & & \\ & -\Delta & 2\Delta & -\Delta & & & \\ & & -\Delta & 2\Delta & \dots & & \\ & & & \dots & \dots & -\Delta & \\ & & & & -\Delta & 2\Delta & -\Delta \\ & & & & & -\Delta & \Delta \end{bmatrix} \qquad M = \left(\frac{h}{6}\right)\begin{bmatrix} 2 & 1 & & & & & \\ 1 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ & & 1 & 4 & \dots & & \\ & & & \dots & \dots & 1 & \\ & & & & 1 & 4 & 1 \\ & & & & & 1 & 2 \end{bmatrix}$$

$$p = \left(\frac{h^2}{2m^*}\right)\begin{bmatrix} -2ik \\ 0 \\ 0 \\ 0 \\ \dots \\ 0 \\ 0 \end{bmatrix} \qquad C = (h^2)\begin{bmatrix} -ik\Delta & & & & & & \\ & 0 & & & & & \\ & & 0 & & & & \\ & & & 0 & & & \\ & & & & \dots & & \\ & & & & & 0 & \\ & & & & & & -ik\Delta \end{bmatrix} \tag{16}$$

The Green function operator for the S.E. can be expressed in terms of the FEM matrices.

$$G = (EM - T - C(k) - V)^{-1} \tag{17}$$

The wavefunction is then obtained by operating with the green function on the inhomogeneous "source" term, $u = G(-p)$.

The numerical dispersion relation for the FEM mesh is given by,

$$E_{FEM}(k) = 6\Delta\left[\frac{1-\cos(kh)}{2+\cos(kh)}\right] \tag{18}$$

A comparison between the dispersion relations for the continuum, FD, and FEM meshes is given in Figure 2.

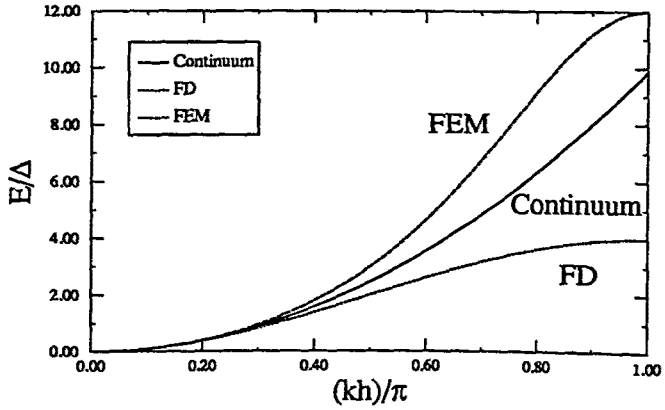

FIGURE 2. Comparison of dispersion relations for the continuum free electron model, the finite difference (FD) model, and the finite element (FEM) model.

IV. GREEN FUNCTION METHOD

An alternative to applying the conditions (6) and (7) on the wavefunction is to apply boundary conditions to the Green function. Let H_0 represent the Hamiltonian for the device isolated from the leads. Let V represent the interaction which couples the 0^{th} and N^{th} nodes in the device to the leads. The leads are assumed to be tight-binding (FD) chains of nodes with the same hopping parameter as in the device, but no potential energy. We can write the Green function as follows:

$$G = \frac{1}{(E - H_0 - V)} = \frac{1}{(G_0^{-1} - V)} \tag{19}$$

The Green function for the uncoupled system can be calculated easily, making use of the known solutions for the Green function of a semi-infinite lead. Because V couples only to nodes *-1* and *N+1* in the lead, we can perform the inversion shown in (19) using only our knowledge of the on-site Green function for the left and right leads:

$$g_L(-1,-1) = g_L(N+1,N+1) = \frac{-e^{kh}}{\Delta}. \tag{20}$$

The green function for the coupled system can the be calculated by performing the matrix inversion shown below.

$$G = \begin{bmatrix} -\Delta e^{-ikh} & \Delta & & & & & & & \\ \Delta & (E-2\Delta-V_0) & \Delta & & & & & & \\ & \Delta & (E-2\Delta-V_1) & \Delta & & & & & \\ & & \Delta & (E-2\Delta-V_2) & \cdots & & & & \\ & & & \cdots & \cdots & \Delta & & & \\ & & & & \Delta & (E-2\Delta-V_N) & \Delta & & \\ & & & & & \Delta & -\Delta e^{-ikh} & & \end{bmatrix}^{-1} \tag{21}$$

Since only the value of the Green function, G(N,0), is required to find the transmission coefficient, one can solve a simple linear system rather than actually calculating the full inverse of the matrix. The transmission coefficient can then be calculated using the relation

$$T = \left(\frac{1}{h^2}\right)(\hbar v)^2 |G(N,0)|^2. \tag{22}$$

Generalization to higher dimension requires only the block-tridiagonal nature of the Hamiltonian.

V. ERROR ANALYSIS

Figure 3 shows an error analysis for each of the techniques discussed here. The transmission coefficient through a single barrier, for which exact results are available, was calculated for a range of energies from 0 to twice the barrier height. The error was calculated using the expression below.

$$error = \sqrt{\left(\frac{1}{N_E}\right)\sum_{i}^{N_E}\left(\frac{T(E_i) - T_{exact}(E_i)}{T_{exact}(E_i)}\right)^2} \tag{23}$$

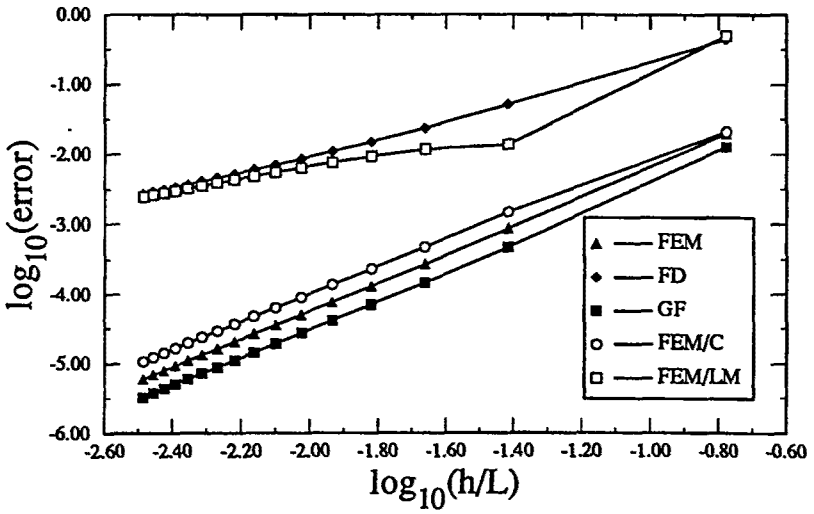

FIGURE 2. Comparison of the error in calculating the transmission coefficient using various numerical approximation. The comparison is made for the case of transmission through a single barrier.

For both FEM, Green function (GF), and FD techniques, the numerical dispersion relations were used. The curve labeled FEM/C employed the continuum dispersion for comparison. The curve labeled FEM/LM used the so-called "lumped mass" approximation for which the FEM matrices V and M are approximated by diagonal matrices. The results show that the GF method slightly improves on the FEM approach. One can see comparing (16) and (21) that the FEM matrix results actually is the second order expansion of the exponential in (20).

The GF and FEM approaches are sufficiently similar in performance that the choice of method will often be dictated by other strengths. The FEM is particularly well suited to complicated boundary shapes in higher dimensions and has been generalized to include applied magnetic fields [3]. The GF method is useful in small problems because analytical results for the matrix inversion can be obtained. Further, it can be used with Keldysh Green function to handle non-equilibrium and dissipative problems [4].

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