Quantum Waveguides Discontinuities Analysis

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***Abstract* –A finite-element bidirectional beam propagation method based on Blocked Schur (BS-FE-BiBPM) is presented for the solution of quantum waveguides discontinuities. By using BS-FE-BiBPM, scattering properties of electron waveguide discontinuities could be accurately calculated based on the 1-D time-independent Schrödinger equation avoiding the use of modal solution stage without affecting the accuracy of the results. As will be shown through the analysis of a quantum resonant cavity, a quantum directional coupler, and a quantum waveguide transistor, the suggested BS-FE-BiBPM is very accurate, versatile, efficient, fast and stable.**

I. Introduction

Many research efforts have been paid to take advantage of wave nature of electrons to investigate high-density low-power high-speed nanoscale systems. One of challenges is the communications between the nanoscale components in the system, such as transistors [1], nanosensors, antennas [2], tunneling structures, and nanowires or quantum waveguides. In order to develop quantum interference between devices, it is vital to investigate the scattering properties of electron waveguide discontinuities. Several analysis methods have been proposed in the literature to simulate these devices which can be classified into time- [3]-[5] and frequency-domain techniques [6],[7].

Time-domain techniques, which could introduce the high speed response of recent quantum interference devices, suffer from being very expensive in terms of computational resources since very large memory and simulation running time are required. On the other hand, the accuracy of the frequency-domain techniques based on the mode-matching method (MMM) [7] depends highly on the number of guided and radiation modes. Furthermore, many difficulties arise in dealing with radiation modes which should be included to conserve the power balance condition at interfaces. Other frequency-domain techniques based on 2-D finite-element method (FEM) [6] rely on dividing the whole computational region into 2-D elements. Of course, solving 2-D problem with fine resolution puts an addition of computational effort.

In this paper, we introduce, for the first time to the best of our knowledge, the use of BiBPM [8] for the solution of quantum waveguides discontinuities based on the 1-D time-independent Schrödinger equation. It is well known that the electrons in the heterostructure devices start behaving more like waves than particles so that the transport of electrons through the nanoscale structure is similar to the propagation of electromagnetic waves in dielectric. On the other hand, BiBPMs are widely used in the study of guided-wave optics owing to its numerical speed, simplicity and efficiency. Moreover, the proposed BS-FE-BiBPM is relying on the Blocked Schur algorithm [9] which could accurately compute the square root operators of the characteristic matrices at the discontinuity section in a very stable way with reducing the execution time. Therefore, the use of BS-FE-BiBPM for quantum waveguides discontinuities will be considered as a very efficient method, as will be shown through the results section.

II. Analysis

Under the effective-mass approximation, the 1-D time-independent Schrödinger equation is given by

$$\left(\frac{d}{dy}\frac{1}{m^*(y)}\frac{d}{dx}+\frac{2}{\hbar^2}[E-U(y)]\right)\psi(y)=\beta^2\frac{1}{m^*(y)}\psi(y) \qquad (1)$$

where ψ is electron wave function, E is the electron's total energy, U is the potential energy, m^* is the effective mass, β is the longitudinal propagation constant, and $\hbar$ is the reduced Plank constant. A characteristic matrix $[A]$ could be produced by using the standard Galerkin's finite element procedure as optical waveguide analysis [10]. Then, the fast and noniterative Blocked Schur algorithm [9] has been applied to compute the square root of the characteristic matrix $[A]$. Then, the stable and noniterative BiBPM based on the scattering operators [8] has been applied.

III. Numerical Results

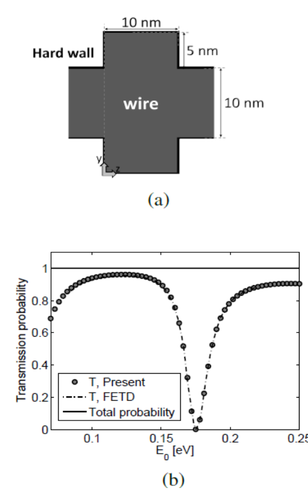

Fig. 1. (a) Quantum resonant cavity; (b) Transmission and total probabilities.

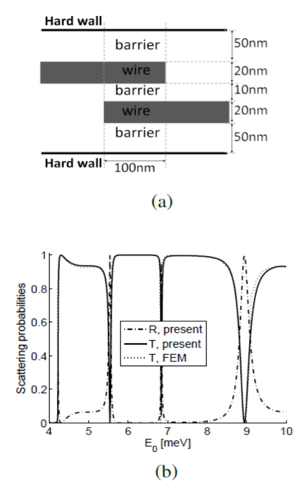

Fig. 2. (a) Quantum field effect directional coupler (QFED) geometry; (b) Scattering probabilities.

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A. *Quantum resonant cavity*

To ensure the accuracy and stability of the proposed BS-FE-BiBPM, a quantum resonant cavity [4] of Fig. 1(a) is simulated, where the electron's potential energy of the wire is assumed to be zero. The boundaries in y direction are considered as hard walls. The effective mass m^* is normalized by the rest mass of electron m_0 is taken as 0.067.

For the fundamental mode of the wire, Fig. 1b shows the transmission probabilities T as a function of electron's total energy E_0. Our results are in excellent agreement with those obtained through finite element time domain method (FETD) [4]. However, it took less than 0.4 s to calculate the transmission probability with excellent observed stability represented by the total probability in Fig. 1(b).

B. *Quantum field effect directional coupler*

Next example considered is a Quantum field effect directional coupler (QFED), which consists of two parallel identical electron waveguides, separated by narrow barrier with finite coupling length $l=100nm$, as shown in Fig. 2(a). The electron's potential energies of the wire and the barrier regions are assumed to be 0 and 10meV with hard walls considered as the boundary condition. The effective mass also normalized by the rest mass of electron is taken as 0.067. The same structure was studied in [6] with 2-D finite element method (FEM).

Fig. 2(b) shows the transmission T and reflection R probabilities of the fundamental mode as a function of the electron's total energy E_0. Our presented results exhibited excellent correspondence with the results simulated by FEM [6].

C. *Quantum waveguide transistor*

Next, a quantum waveguide transistor is simulated based on a GaAs-waveguide with the T-shaped geometry and hard walls considered as the boundary conditions in y direction, as shown in Fig. (3). The effective electron mass is $m^*=0.069m_0$ corresponding to GaAs. The incident wave is the fundamental mode of the electron's total energy $E_0=29.9meV$ excited from left to propagate in z direction. The same structure was studied in [5] using the 2-D time-dependent Schrödinger equation discretized with the Crank-Nicolson finite difference scheme (FDTD) without external potential (V=0).

The main interest here is to ensure the validity of our proposed BS-FE-BiBPM to introduce the same switching performance(OFF/ON-states) of this quantum waveguide transistor reported in [5]. So, there is no need now to have a coupling to Poisson equation for the current simulation of the MOSFET-channels. The absolute values of the wave functions are calculated here based on the time-independent Schrödinger equation for two stub lengths (L) in order to control the current through the channel. First, for the stub length of 32nm, the incident mode is almost completely reflected as shown in Fig. 4a representing the (OFF-state) of the transistor. Second, for the stub length of 42.5nm, Fig. 4(b) shows that the incident mode is almost completely transmitted to the output waveguide representing the (ON-state) of the transistor.

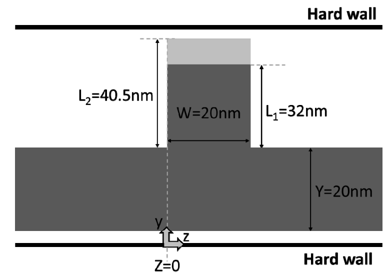

Fig. 3. Quantum waveguide transistor geometry.

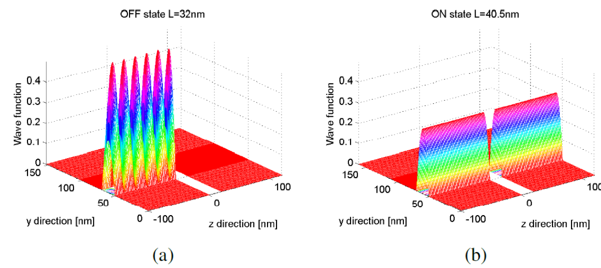

Fig. 4. The wave function distributions at $E_0 = 29.9meV$ for two stub lengths: (a) $L_1 = 32nm$; (b) $L_2 = 42.5nm$.

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