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A Generalized Stationary Algorithm for Resonant Tunneling: Multi-Mode Approximation and High Dimension

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Abstract. The multi-mode approximation is presented to compute the interior wave function of Schrödinger equation. This idea is necessary to handle the multi-barrier and high dimensional resonant tunneling problems where multiple eigenvalues are considered. The accuracy and efficiency of this algorithm is demonstrated via several numerical examples.

AMS subject classifications: 35C99, 65N99, 81Q05

Key words: Schrödinger equation, numerical scheme, resonant tunneling, multi-mode approximation, high dimension.

1 Introduction

The resonant tunneling diode(RTD) is a diode with a resonant tunneling structure in which electrons can tunnel through some resonant states at certain energy levels. It has been widely studied both theoretically and experimentally [7, 8, 10] for its important role in constituting different functions of the nanoscale semiconductor devices, e.g. integrated circuit, microprocessor, memory devices, wide-band wired and wireless communications [21, 27]. The RTD is made up of two large reservoirs and an active region. The reservoirs, which are highly conducting, can be used for exchanging electrons with external electrical circuit. The active region (see Fig. 1) can be a double barrier, triple barrier, quantum well, quantum wire, quantum dot, etc.

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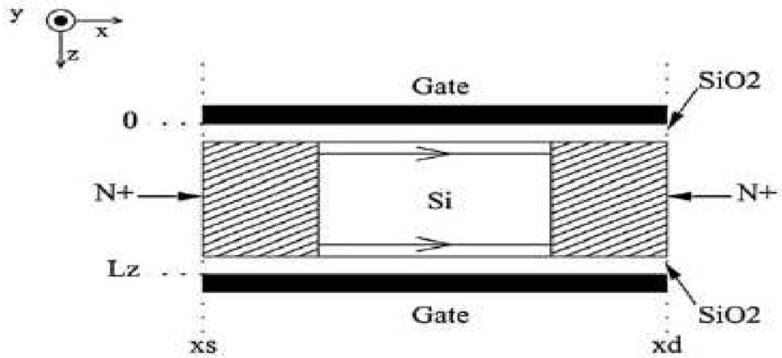

Figure 1: The picture of two dimensional device for the active region of RTD. This figure is copied from [24].

Since the length scale is small in RTD, quantum effects should be considered. Therefore a general approach to model such device is through the Schrödinger equation for wave function coupled to Poisson equation for the electric potential [20].

There are two primary issues in the numerical simulation. One is the numerical integration of the Schrödinger equation, e.g. finite difference method [18, 19], spectral type method [5, 6, 22], the WKB-scheme [3, 4], and the Gaussian beam method [14, 15]. The other is the reduction of energy grid points [4,9,23]. Besides these, the artificial boundary conditions [1, 2, 17], the dimensionality reduction [3, 24], the Gummel iteration [11, 23], the Green function's method [12, 13, 26] and many other related topics are investigated.

The well known numerical difficult in RTD is that the curve of transmission coefficient versus energy tends to be singular in the vicinity of resonant energies. Therefore, a very fine energy mesh is needed to capture the correct integral of the density, which results a large supplementary numerical cost for computing these Schrödinger equations. In order to deal with this problem, an adaptive energy mesh method was developed in [23]. But it still consume lots of computational resource since the mesh should be very fine near the resonant energies. Moreover, it doesn't work for the time dependent case because the resonances move.

Lately, the one mode approximation [4, 16, 25] was proposed to compute the density. The method decompose the wave function into an exterior part and an interior part. The exterior part is smooth in energy mesh and thus does not require a fine energy mesh. The interior part can be well approximated by its projection on the resonant state. The one-mode approximation does save the computational cost, but this approximation may not work for some applications, e.g. multiple barrier problem and high dimensional problem.

In this paper, we present the multi-mode approximation to overcome these difficulties. The one dimensional problem is discussed in Section 2. In Section 3, it is extended for high dimensions. We conduct numerical examples in Section 4 to verify the accuracy of the numerical methods. In Section 5, we give some discussions on the algorithm efficiency. Finally, we make the conclusive remarks in Section 6.