An accelerated algorithm for 2D simulations of the quantum ballistic transport in nanoscale MOSFETs

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Abstract

An accelerated algorithm for the resolution of the coupled Schrödinger/Poisson system, with open boundary conditions, is presented. This method improves the sub-band decomposition method (SDM) introduced in [N. Ben Abdallah, E. Polizzi, Subband decomposition approach for the simulation of quantum electron transport in nanostructures, J. Comput. Phys. 202 (1) (2005) 150–180]. The principal feature of the here presented model consists in an inexpensive and fast resolution of the Schrödinger equation in the transport direction, due to the application of WKB techniques. Oscillating WKB basis elements are constructed and replace the piecewise polynomial interpolation functions used in SDM. This procedure is shown to reduce considerably the computational time, while keeping a good accuracy.
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Keywords: Schrödinger–Poisson equation; Open boundary conditions; Subband model; WKB approximation; Confinement effects; Quantum tunneling

1. Introduction

MOSFET size dimensions continue to decrease rapidly towards the sub-10 nm range. The interest for such a scaling is multiple: more functionality, higher operating speeds, reduced power consumption. To support this effort, it is of primary importance to develop modeling and simulation tools that are adequate for the description of ultra small devices. The objective of this paper is the presentation of a very efficient and inexpensive method for the simulation of nanoscale MOSFET devices. This method was previously introduced by the authors in a condensed form in [20].

The scaling of devices beyond a certain limit enhances the importance of some physical phenomena, with correlated consequences on device modeling techniques. The electron transport becomes near-ballistic and quantum effects, as interferences, tunneling and confinements, can no more be neglected. Quantum ballistic transport models are thus adequate to describe what can be ultimately expected in these devices. The interested

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reader can find more physical details in [1,3,10,12]. There is a great amount of work dedicated to semiconductor device simulations, either by the non-equilibrium Green's function formalism [11,16,17,26,27] or by a finite element/difference resolution of the Schrödinger–Poisson system [4,5,8,13,18,22]. The approach presented in this paper is based on the resolution of the self-consistent Schrödinger–Poisson equation with open boundary conditions, which enable the current flow.

In previous works of Ben Abdallah and Polizzi [8], respectively Laux et al. [18], the Schrödinger–Poisson equation is solved self-consistently via standard variational formulations in the whole definition/simulation domain. The first approach uses the original QTBM boundary conditions [19], whereas the second one extends these boundary conditions to simulate devices far from equilibrium. The disadvantage of these approaches is that they are very time consuming due to the expensive resolution of the 3D or 2D Schrödinger equation. In a recent work of Ben Abdallah and Polizzi [7], a sub-band decomposition method (SDM) was proposed to reduce the numerical cost for the resolution of the 2D Schrödinger equation. The SDM method is based on the fact that in modern devices the electron gas is confined in one or more directions and that consequently the dimension of the propagation space is reduced. Hence the resolution of the Schrödinger equation in the whole 2D domain is replaced by 1D eigenvalue problems in the confined (or transversal) direction and a system of coupled 1D Schrödinger equations projected on the transport (or longitudinal) direction. It is important to remark that the SDM method retains the coupling effects in both directions of space.

The goal of the present paper is to propose a new powerful model, further named SDM/WKB, which develops the SDM method to provide a relatively inexpensive way to solve the 2D Schrödinger equation. This new method reduces once again considerably the simulation time by accelerating the resolution of the longitudinal coupled 1D Schrödinger system through the use of WKB techniques. The WKB approximation, often called also semi-classical approximation, is a powerful technique to treat problems involving two different scales. It is used in [9] for the Helmholtz equation and in [15,25] for the Schrödinger equation with the objective to investigate the high frequency asymptotics ($\hbar \to 0$) of the just mentioned equations. In the present work, however, we are interested in an approximation method for the Schrödinger equation, suitable for fixed, arbitrary wavelengths and equally accurate independently on the Planck constant $\hbar$ and the electron energy E (see [23] for the Helmholtz equation). Indeed, for slowly varying potentials this approximation is good not only for high frequencies. In [6] the WKB approximation is used in this manner by Ben Abdallah and Pinaud for the 1D simulation of a resonant tunneling diode (RTD). The present paper combines the two methods, SDM and WKB, with the objective to lower the numerical burden for two dimensional applications, as the MOSFET devices.

The principal idea is the following. The SDM method uses the conventional finite element approach to solve the 1D Schrödinger equation in the transport direction. The ''10 degrees of freedom per wavelength''-rule requires thus a refined mesh size in this direction to accurately approximate the highly oscillating wave functions, which correspond to high injection energies. The original contribution of the SDM/WKB method consists in replacing the linear or polynomial interpolation functions by more elaborated, oscillating interpolation functions. These oscillating basis functions are determined by means of the WKB plane-wave Ansatz and posses a frequency close to that of the unknown wave-function. Therefore, accurate results can be obtained with much coarser grids, leading for this reason to a highly reduced simulation time.

The outline of this paper is the following. Section 2 starts by briefly presenting the SDM method, in order to introduce afterwards the new SDM/WKB method, which is the core of this work. Section 3 compares numerically (simulation time, accuracy) the two methods with a standard variational resolution method for the Schrödinger equation. Moreover, it enumerates some interesting points concerning the implementation of the SDM/WKB method. Finally, Section 4 is devoted to the discussion of the simulation results obtained with the SDM/WKB method for several devices in order to validate the results from a physical point of view. To keep this paper simple, we preferred to present the extensive mathematical and numerical analysis of this model in a separate future work [2,21].

2. Description of the SDM/WKB model

The purpose of this section is to introduce the original 3D SDM/WKB transport model, developed for the simulation of the ballistic quantum electron transport in nanoscale MOSFETs. This paper deals with the stationary problem.