Journal of Computational Physics 230 (2011) 2031–2044

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Accuracy of the Frensley inflow boundary condition for Wigner equations in simulating resonant tunneling diodes

Haiyan Jiang [a,b], Wei Cai [b,*], Raphael Tsu [c]

[a] Department of Applied Mathematics, Beijing Institute of Technology, Beijing 100081, China
[b] Department of Mathematics and Statistics, University of North Carolina at Charlotte, Charlotte, NC 28223-0001, USA
[c] Department of Electrical and Computer Engineering, University of North Carolina at Charlotte, Charlotte, NC 28223-0001, USA

ARTICLE INFO

Article history:
Received 19 July 2010
Received in revised form 10 November 2010
Accepted 1 December 2010
Available online 7 December 2010

Keywords:
Frensley inflow boundary condition
Wigner function
Resonant tunneling diode

ABSTRACT

In this paper, the accuracy of the Frensley inflow boundary condition of the Wigner equation is analyzed in computing the *I–V* characteristics of a resonant tunneling diode (RTD). It is found that the Frensley inflow boundary condition for incoming electrons holds only exactly infinite away from the active device region and its accuracy depends on the length of contacts included in the simulation. For this study, the non-equilibrium Green's function (NEGF) with a Dirichlet to Neumann mapping boundary condition is used for comparison. The *I–V* characteristics of the RTD are found to agree between self-consistent NEGF and Wigner methods at low bias potentials with sufficiently large GaAs contact lengths. Finally, the relation between the negative differential conductance (NDC) of the RTD and the sizes of contact and buffer in the RTD is investigated using both methods.

1. Introduction

The impressive progress of semiconductor fabrication technology pushes the devices to the scale where out of equilibrium quantum effects play an important role. To clearly understand the dynamic characteristics of nano-scale devices, quantum transport models should be considered. The Schrödinger equation is the fundamental equation for describing quantum phenomena, which dictates how the quantum state (i.e. wave function) of a given physical system evolves in time and space. All classical dynamic quantities of electrons (such as density distribution, current distribution, etc.) can be obtained by computing the expectation of relevant dynamic operators with given wave functions. In modeling quantum transport of open systems, two approaches based on the wave mechanics are commonly used: the non-equilibrium Green's function (NEGF) method and the Wigner distribution method, which will be studied and compared in this paper.

For transport in an open system, it is necessary to provide a physically justifiable boundary condition to produce realistic numerical solutions for finite devices. The usual zero boundary condition or the periodic boundary condition for Schrödinger wave equations in band structure calculations can not describe transport when the terminals of the devices are at different chemical potentials (due to an external driving bias), namely, devices in a non-equilibrium environment. In the quantum kinetic approach, Wigner equations are used to treat quantum transport, similar to the Boltzmann kinetic theory for classical particles. In fact, the Wigner equation was derived by Wigner in 1932 as a correction to the semi-classical Boltzmann distribution for low temperature systems [1]. In order to solve the Wigner equation in a finite region containing the quantum devices, boundary conditions are used for numerical calculations. The most popular boundary condition is the inflow

* Corresponding author. Tel.: +1 704 687 4581; fax: +1 704 687 6415.
E-mail address: wcai@uncc.edu (W. Cai).

0021-9991/$ - see front matter © 2010 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2010.12.002

boundary condition proposed by Frensley in 1987 [2], which ensures the incoming electron waves along the semi-infinite contact toward a quantum device will not be reflected. In [2], Frensley used a finite difference method (FDM) for the Wigner equation with the proposed inflow boundary condition for a resonant tunneling diode (RTD), which is considered the prototype device for studying quantum models due to its negative differential resistance (NDR), and reproduced successfully the NDR of the device. On the other hand, the NEGF formulism also provides a sound framework for quantum transport models in open systems [5,7]. Here, in order to describe the effects of the semi-infinite contacts to the device, a self-energy is introduced as the boundary condition for the Green's function. The self energy is a mathematical construct – a Dirichlet to Neumann mapping [8], whose role is to make sure that the electron leaving the active device region will not experience reflection at the simulation boundary. All physical properties of the device can be expressed in terms of device Green's function and the self-energy. However, the application of the NEGF method involves large computation if the bodily scattering effects inside the device are considered.

There have been much work using both approaches in modeling quantum devices. First of all, self-consistent Wigner–Poisson equations were used in [3] [4] to clarify the origin of the hysteresis and a plateau-like structure of the *I–V* curve of the RTD by identifying two triangular quantum wells formed outside the double barriers of the RTD and the resulting energy coupling with the quantum well between the double barriers [4]. In other works, the Wigner equations with a FDM have been used to analyze the effect of spatially varying effective mass on the *I–V* characteristics in the RTDs [9,10] and the influence of the channel thickness on the *I–V* characteristics in the double-gate Metal-Oxide-Silicon Field Effect Transistors (DG-MOSFETs)[11]. The Monte Carlo (MC) method was also used to solve the Wigner equation recently exploiting its similarity to the classical dynamic formulism with a Boltzmann-like scattering treatment [12–18]. Meanwhile, the NEGF method has gained popularity for the simulation of MOSFETs, RTDs, Carbon Nano-tubes, Quantum Dots (QDs) [5]. The 1D NEMO is a simulator based on the NEGF method for the RTDs [19]. The NEGF method can be applied with both mode space and real space methods to study double gate MOSFETs [20,21]. Meanwhile, finite element methods has been used with the NEGF for devices with arbitrary boundaries [22].

Recent work on the comparison between the Wigner equation and the NEGF for double gate MOSFETs [18] and the RTDs [13] [14] has produced qualitatively similar results. However, these results also show that the transport current calculated by the Wigner equation method with the Frensley inflow boundary condition is higher than that by the NEGF method. This fact was noted in our work [23] with some possible causes discussed. In this paper, we will conduct a systematic study on the accuracy of the Frensley inflow boundary condition for the Wigner distribution in the ballistic transport simulation of the RTD. Specifically, we will investigate how the accuracy of the inflow boundary condition is affected by the size of contact regions included in the simulation domain of the RTD. For comparison, the NEGF with its analytical self-energy boundary condition will be used for validations. Consistent results between the two approaches are achieved for low bias potentials as the size of the contact region is increased.

The paper is organized as follows: In Section 2, the NEGF method and its boundary condition are introduced, together with the Green's function representation of the electron density and the current density. Section 3 describes the Wigner equation, its inflow boundary condition, a FDM discretization, and the conservation condition for the FDM. Self-consistent algorithms of the quantum transport models via a Poisson equation are presented in Section 4. Section 5 contains the analysis of the boundary conditions of the Wigner distribution method and the NEGF method, numerical convergence studies of the two methods, and self-consistent simulations of the RTDs by the two methods. Also, the relation between the negative differential conductance (NDC) of the RTD and the sizes of contact and buffer in the RTD is investigated using both methods. Finally, a conclusion is given in Section 6.

2. Non-equilibrium Green's function (NEGF) method

2.1. Green's function and electron density

The Schrödinger equation in 3D provides the fundamental description of a quantum state as:

$$\mathbf{H}\Psi(x,y,z) = E\Psi(x,y,z), \tag{1}$$

where **H** is the Hamiltonian operator

$$\mathbf{H} = -\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2} + V(x,y,z). \tag{2}$$

As the scales of the device in y and z directions are assumed to be large, the effective potential energy $V(x,y,z)$ can be assumed to be constant in y and z directions and the 3D Schrödinger Eq. (1) is reduced to an 1D Schrödinger equation

$$-\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2}\psi(x) + v(x)\psi(x) = E\psi(x). \tag{3}$$

The effective potential energy $v(x)$ splits into two parts: $v(x) = v_s(x) + v_e(x)$, where $v_e(x)$ is the conduction band structure and $v_s(x)$ is the self-consistent potential energy calculated via a Poisson equation. For a device with two contacts, the effective energy $v(x)$ assumes constant values inside the contacts with the following form: