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A device adaptive inflow boundary condition for Wigner equations of quantum transport

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ABSTRACT

In this paper, an improved inflow boundary condition is proposed for Wigner equations in simulating a resonant tunneling diode (RTD), which takes into consideration the band structure of the device. The original Frensley inflow boundary condition prescribes the Wigner distribution function at the device boundary to be the semi-classical Fermi–Dirac distribution for free electrons in the device contacts without considering the effect of the quantum interaction inside the quantum device. The proposed device adaptive inflow boundary condition includes this effect by assigning the Wigner distribution to the value obtained from the Wigner transform of wave functions inside the device at zero external bias voltage, thus including the dominant effect on the electron distribution in the contacts due to the device internal band energy profile. Numerical results on computing the electron density inside the RTD under various incident waves and non-zero bias conditions show much improvement by the new boundary condition over the traditional Frensley inflow boundary condition.

1. Introduction

As semiconductor devices are being scaled down to nanometer dimensions, the quantum effects, such as size quantization and tunneling, become important in studying the properties of the devices [1–3]. The non-equilibrium Green function (NEGF) formalism and the Wigner equation are two popular simulation methods in quantum transport of nano-scale devices as open systems. For ballistic transport, the NEGF formalism is equivalent to solving the Schrödinger equation [4,5] while using self-energies for treating device contacts attached to the active device region [6], and a phenomenological treatment of the bodily scattering effects [7,8]. On the other hand, the Wigner distribution, defined via a Wigner–Weyl transform of the density correlation function of the quantum device, was introduced by E. Wigner in 1932 as an analog of the classical Boltzmann distribution for the quantum system [9]. Being a quantum kinetic analog of the classical Boltzmann equation, the Wigner equation has advantages over the NEGF method in two aspects [10,11]. One is that the Wigner framework allows the modeling of scattering phenomena for the quantum kinetic equation. The other is that its phase space formulation makes it easier to impose boundary conditions for the Wigner distribution at the device contacts, using the knowledge of the semi-classical distribution such as the Fermi–Dirac distribution for electrons in the device contacts [12].

In the last decades, the Wigner equation has received much attention in simulating quantum transport of nano-scale devices [12–14]. It was originally used for studying the current–voltage characteristics of RTDs by Frensley [12]. Frensley

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successfully reproduced the negative differential resistance by using an upwind finite difference method for the Wigner equation with an inflow boundary condition. This work motivated later work on Wigner equation based numerical simulations of nano-scale devices [14–23]. Furthermore, self-consistent Wigner–Poisson equations were used in [24,25] to clarify the origin of the hysteresis and a plateau-like structure of the I–V curve of RTDs. Works on the comparison between the Wigner equation and the NEGF for double gate MOSFETs [5,23] and for RTDs [18,19] have 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 [5]. Recently, Jiang et al. [26] investigated how the accuracy of the inflow boundary condition is affected by the size of contact regions included in the simulation domain of the RTD. In [26], it was found that the Frensley inflow boundary condition for incoming electrons holds exactly only infinite away from the active device region and its accuracy depends on the length of the contacts included in the simulation. This result implies that, in order to get more accurate results, larger regions of the contacts should be included, which would lead to higher computational cost. Therefore, it is necessary to design a better inflow boundary condition using smaller contact regions to reduce the computational cost while still preserving numerical accuracy.

The Frensley inflow boundary condition specifies the distribution function at the contacts to be some given function, most often in practice, the Fermi–Dirac distribution. Electrons entering the device will interact with the intrinsic band structure of the active device region, resulting in reflection and transmission electrons into the incoming and opposite sides of the device, respectively. For RTDs, electrons tunnel through the band structure profile through resonant coupling, in addition to interacting with other electrons through quantum interference and collisions. These quantum effects will influence the Wigner distribution function at the boundary as the Wigner function by definition is constructed through a global Wigner transform of the density correlation function [9]. In Frensley's original paper [12], the band structure profile inside the device is totally ignored when setting the boundary condition. In this paper, we will propose a device adaptive boundary condition which reflects the dominant effect of the device internal band structure in prescribing the values of the Wigner distributions at the device boundaries. In general, the electron wave functions inside a quantum device for non-zero bias will be hard to predict a prior. Therefore, our strategy will only consider the dominant quantum interaction inside the device, namely, the states of the electrons inside the device at zero bias during the impact of incident free electrons, so called scattering states of the electrons [27,28]. We then compute the corresponding Wigner distribution of these scattering states and the resulting distributions will be used as the boundary data for the Wigner distribution function for general non-zero bias situations. This new boundary condition will be called the device adaptive boundary condition (DABC) as the internal band structure is indirectly used in the prescription of the Wigner distribution in the contacts. We expect, as validated by our numerical tests, the new DABC will improve the density profile inside the device for a reasonably wide range of applied external biases.

The rest of the paper is organized as follows. The Wigner function and its truncated version and their governing equations are introduced in Section 2. Section 3 gives the original Frensley inflow boundary condition and then the improved device adaptive inflow boundary condition. An upwind finite difference method for the Wigner equation is described in Section 4 and the numerical studies of the DABC are presented in Section 5. Finally, Section 6 gives the conclusion of the paper and some discussion on future work.

2. Wigner function and its truncated version using the correlation length $L_{\mathbf{coh}}$

In this paper, the stationary and linear Wigner equation will be used for finding better inflow boundary condition for the Wigner distribution functions. The Wigner equation is a quantum kinetic equation derived from the Schrödinger equation as a quantum mechanical analog to the Boltzmann equation [9,29]. In the following the key idea of the derivation of the Wigner equation for pure states is sketched.

The stationary Schrödinger equation for an electron of effective mass m in a potential energy $V(x)$ reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x), \tag{1}$$

where $\hbar$ is the reduced Planck constant, $\psi(x)$ is the eigen-wavefunction and E is the eigen-energy. If the state of a quantum system can be described completely with a given wave function $\psi(x)$, we will consider the quantum system in a pure state. Otherwise, if the quantum system can be found in states described in multiple wave functions with a specific probability, then we consider the quantum system in a mixed state. The density matrix $\rho(x,x')$ for a pure state system is defined simply as

$$\rho(x,x')=\psi(x)\psi^*(x'), \tag{2}$$

which satisfies the von Neumann equation

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x'^2}\right]\rho(x,x')+\left[V(x)-V(x')\right]\rho(x,x')=0. \tag{3}$$

The von Neumann equation (3) is equivalent to the Schrödinger equation (1) in the sense that either can be derived from the other, but the former holds advantage over the latter in describing quantum systems in mixed states [30].