A Particle Model for Wigner Transport through Tunneling Structures

H. Kosina, M. Nedjalkov, and S. Selberherr

Institute for Microelectronics
Technical University Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria

Abstract: – The Wigner equation taking into account both the non-local potential operator and a scattering operator represents a suitable physical model for carrier transport in nano structures. In this paper a new Monte Carlo method is proposed for the solution of the stationary Wigner equation. Scattering can be included at the level of the semi-classical Boltzmann scattering operator, whereas coherent effects are treated without simplifying approximations. As opposed to the Monte Carlo method for semi-classical transport, in the quantum case the weight of a particle can take on positive and negative values.

Key-Words: particle model, Wigner equation, nano structures, Monte Carlo method, scattering, tunnel effect

1 Introduction

Description of quantum phenomena by means of a particle picture is a promising approach to the modeling of transport in nanoscale electronic devices. A single particle Wigner equation has been derived which accounts for coherent effects via the Wigner potential operator and for dissipation processes via the Boltzmann collision operator.

With deterministic methods using finite difference discretization one usually considers the coherent Wigner equation, or includes dissipation in the relaxation time approximation. A one-dimensional momentum space is assumed. Stochastic methods using particles are motivated by the Monte Carlo (MC) method for device simulation, where the dissipation operator is treated in an exact manner but the coherent part is presented by its classical limit. This limit transforms the Wigner potential operator into a classical force term, and hence the Wigner equation into the semi-classical Boltzmann equation.

The treatment of the Wigner potential operator is the main concern of the particle approach. In [1] it has been interpreted as a quantum force giving rise to dynamic particle trajectories. They nicely explain the tunneling process but yet cannot solve the Wigner equation: the quantum force itself depends on the solution f_w. Recently the coherent Wigner equation has been solved numerically by using particles [2] which cross the device by collisionless drift over classical trajectories. The information about the Wigner potential is retained as particle weight. The physical observables are obtained as weighted ensemble averages.

2 The Particle Model

In this work we consider the Wigner equation which accounts for the coherent part of the transport via the Wigner potential V_w and for dissipation processes due to the electron-phonon interaction. The equation can be derived from the generalized electron-phonon Wigner equation by a hierarchy of approximations [3]. The approximations concern only the phonon interaction, while the coherent part is treated at a rigorous quantum level. The classical limit of the dissipation part gives rise to the common Boltzmann collision operator. For

one dimensional devices the equation reads:

$$\left(\frac{\partial}{\partial t}+\frac{\hbar k_x}{m}\frac{\partial}{\partial x}\right) f_w(x,\mathbf{k},t) = \int dk_x{}' V_w(x,k_x{}'-k_x) f_w(x,k_x',\mathbf{k}_{yz},t) + \int d\mathbf{k}' f_w(x,\mathbf{k}',t) S(\mathbf{k}',\mathbf{k}) - f_w(x,\mathbf{k},t)\lambda(\mathbf{k}). \quad (1)$$

We propose a stochastic method which treats the entire right hand side of the stationary equation (1) as a scattering term. The method retains the basic features of the weighted Single Particle MC method [4]. All three dimensions of the momentum space are included. The algorithms for injection from the boundary distribution, the build up of the trajectory by consecutive drift and scattering events, and the record of the physical averages remain unchanged. In addition to phonon scattering the potential V_w is also a source of scattering. This scattering source gives rise to sign changes of the particle weights. The method is based on the separation into two positive functions.

$$V_w(k_x) = V_w^+(k_x) - V_w^-(k_x)$$
$$V_w^+ = V_w H(V_w), \quad V_w^-(k_x) = -V_w H(-V_w)$$

Here H denotes the Heavyside function. Because of $\int dk_x V_w(x,k_x) = 0$, a unique function

$$\gamma(x) = \int dk_x V_w^{\pm}(x,k_x) \quad (2)$$

can be introduced, which is interpreted as the out-scattering rate of the potential operator in strict analogy with the phonon out-scattering rate λ. The free-flight time is selected as in the classical MC scheme, however, with an out-scattering rate given by the sum $(\gamma+\lambda)$. The quantum character of the transport affects mainly the scheme for the after-scattering state selection. The conditional probability densities for a transition from the free-flight end state $(x,\mathbf{k})$ to the after scattering state $(x,\mathbf{k}')$ are given in the following table.

transition density	**scattering source**
$\frac{\gamma(x)}{\mu(x,\mathbf{k})}\frac{V_w^+(x,k_x{}'-k_x)\delta(\mathbf{k}'_{yz}-\mathbf{k}_{yz})}{\gamma(x)}$	potential V^+
$\frac{\gamma(x)}{\mu(x,\mathbf{k})}\frac{V_w^-(x,k_x{}'-k_x)\delta(\mathbf{k}'_{yz}-\mathbf{k}_{yz})}{\gamma(x)}$	potential V^-
$\frac{\gamma(x)}{\mu(x,\mathbf{k})}\frac{\gamma(x)\delta(\mathbf{k}'-\mathbf{k})}{\gamma(x)}$	self-scattering
$\frac{\lambda(\mathbf{k})}{\mu(x,\mathbf{k})}\frac{S(\mathbf{k}',\mathbf{k})}{\lambda(\mathbf{k})}$	phonons

where $\mu(x,\mathbf{k}) = 3\gamma(x)+\lambda(\mathbf{k})$ and $\nu(x,\mathbf{k}) = \gamma(x)+\lambda(\mathbf{k})$.

Particles enter the device from the contacts with unit weight. The weight is updated after each scattering by factor $\frac{\mu(x,\mathbf{k})}{\nu(x,\mathbf{k})}$. It becomes negative, $-\frac{\mu(x,\mathbf{k})}{\nu(x,\mathbf{k})}$, in the case when the scattering source is V_w^-. When $\gamma \simeq 0$, e.g. far from the quantum region, the weight remains unity. In this case the method simplifies to the classical Single Particle MC method. The practical application of the method includes a discretization of the x and k_x coordinates. The discretization satisfies $\Delta x \Delta k_x = \pi/N$, where N is the number of points of the discrete Fourier transform used to calculate V_w.

3 Results and Discussion

To study the MC method it is applied to a coherent tunneling process ($\lambda = 0$). In the simulated experiment particles are injected between the two 1nm thin, 0.05eV high barriers of an unbiased resonant-tunneling device (RTD). The injected particles are evenly distributed in the middle 2nm part inside the 4nm wide potential well and have a Maxwell-Boltzmann distribution in energy. Material parameters for $GaAs$ at 300K temperature are assumed. The chosen energies are such that the injected particles can cross the barriers only by tunneling. The tunneled particles leave the device through the left to right absorbing contacts. On contrary classical particles will accumulate with the time inside the well - there is no stationary classical solution. The method provides the stationary solution which consistently characterizes the quantum nature of the transport process. The current and density distributions in Fig. 1 reflect the symmetry of the task. Out-

side the injection region the current densities to the left and right contacts are constant and equal in magnitude. In the injection region the particle density is constant in space and time. The density drops outside the injection region well before the physical location of the barriers, which shows the nonlocal character of the potential scattering. Indeed the potential out-scattering rate γ is remarkably high around the barriers on a distance determined by the coherence length $L_c = N\Delta x$. As shown in Fig. 2, γ assumes even higher values outside the barriers than inside. A clear demonstration of the tunneling process is given by the mean kinetic energy distribution. It becomes negative in the barriers, where the wave vector of the tunneling particles is imaginary.

The above experiment gives an insight to the conventional modes of operation of the RTD's. Under moderate bias conditions, when the I-V curve is simulated, the dominant transport mechanism through the first barrier is tunneling. The transport mechanism through the second barrier becomes classical when the mean kinetic energy becomes positive.

Acknowledgment

This work has been supported by the IST-Program, Project NANOTCAD, IST-1999-10828

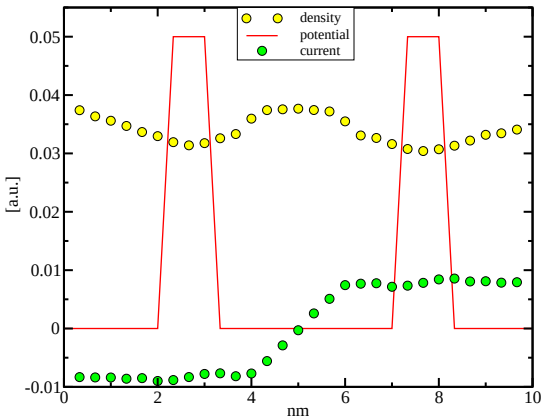

Fig. 1. Device potential, current and particle density distribution in the device.

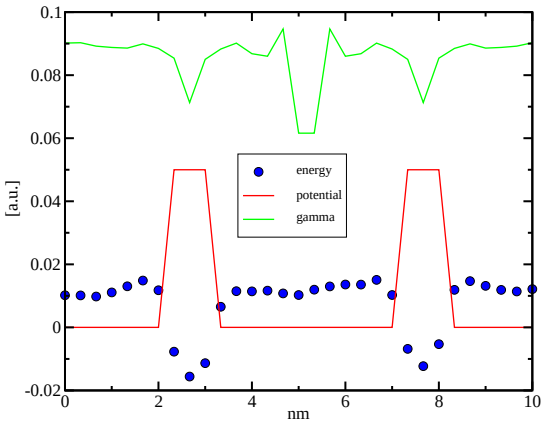

Fig. 2. Device potential, out-scattering rate γ and kinetic energy distribution in the device.

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