Wigner Transport through Tunneling Structures - Scattering Interpretation of the Potential Operator

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

Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, Vienna, Austria
Email: Nedjalkov@iue.tuwien.ac.at

Abstract – A stochastic method for simulation of quantum transport in nanoscale electronic devices is proposed. The interaction with the Wigner potential is interpreted as a scattering mechanism, which is a counterpart to the scattering mechanisms due to the lattice imperfections. The derived quantum Monte Carlo algorithm retains the basic features of the Single Particle Monte Carlo method used for simulation of classical devices. The method is applied for simulation of tunneling process through energy barriers.

I. INTRODUCTION

Description of quantum phenomena in terms of particle trajectories is a promising approach for understanding and modeling the transport in nanoscale electronic devices. Considered is the Wigner equation which accounts for the coherent part of the transport via the Wigner potential V_w and for dissipation processes via the Boltzmann collision operator B. For one-dimensional devices the equation reads:

$$\left(\frac{\partial}{\partial t} + \frac{\hbar k_x}{m}\frac{\partial}{\partial x}\right) f_w(x, \mathbf{k}, t) = (Bf_w)(x, \mathbf{k}, t) \tag{1}$$

$$+ \int dk_x' V_w(x, k_x' - k_x) f_w(x, k_x', \mathbf{k}_{yz}, t)$$

The Wigner potential is defined by the Fourier transform:

$$V_w(x, k_x) = \int ds e^{-ik_x s}\frac{1}{i2\pi\hbar}\left(V(x - \frac{s}{2}) - V(x + \frac{s}{2})\right) \tag{2}$$

The Boltzmann collision operator is defined by the scattering rate S:

$$(Bf_w)(x, \mathbf{k}, t) =$$

$$\int d\mathbf{k}' f_w(x, \mathbf{k}', t)S(\mathbf{k}', \mathbf{k}) - f_w(x, \mathbf{k}, t)\lambda(\mathbf{k})$$

$S(\mathbf{k}', \mathbf{k})$ is the probability density per unit time for scattering from state $(x, \mathbf{k}')$ to state $(x, \mathbf{k})$. S is a cumulative quantity which accounts for different scattering sources such as phonons and impurities. The total out-scattering rate λ is defined by the integral over all after-scattering states:

$$\lambda(\mathbf{k}) = \int S(\mathbf{k}, \mathbf{k}')d\mathbf{k}' \tag{3}$$

Deterministic methods consider the momentum space also as one-dimensional and can solve the coherent Wigner equation or include dissipation in a relaxation time approximation [1].

The particle approach is motivated by the Monte Carlo (MC) method for device simulation, where the dissipation operator is treated exactly, but the coherent part is presented by its classical limit. This limit leads to a classical force term transforming (1) into the Boltzmann equation. How to account for the complete potential term is the main concern of the particle approach.

In [2] the potential term has been interpreted as a quantum force giving rise to dynamic particle trajectories. They nicely explain the tunneling process but yet cannot solve (1): the quantum force itself depends on the solution f_w.

In [3] a particle approach to the coherent Wigner equation has been proposed. The Wigner potential has been treated exactly by the iteration series of the equation. The convergence of the obtained backward Monte Carlo method has been theoretically investigated.

Recently the coherent equation (1) has been solved numerically by using particles [4] which cross the device by collisionless drift over classical trajectories. The information about V_w is retained as particle affinity.

We propose a forward stochastic method which treats the entire right hand side of the stationary equation (1) as a scattering term. All three dimensions of the momentum space are considered. The method retains the basic features of the weighted Single Particle MC method [5].

II. THE QUANTUM MC METHOD

The forward method is designed to evaluate the mean value

$$\langle A \rangle = \int_\Omega A(x,\mathbf{k}) f_w(x,\mathbf{k}) dx d\mathbf{k}$$

of a generic physical quantity A such as carrier density, velocity, energy, current. Ω is a given domain of the phase space.

A mean value $\langle A \rangle$ can be calculated either by solving (1) or alternatively by using the conjugate equation. To obtain the latter, a separation of the antisymmetric function V_w into two complementary positive functions

$$V_w(x,k_x) = V_w^+(x,k_x) - V_w^-(x,k_x)$$

is used. A unique function

$$\gamma(x) = \int V_w^\pm(x,k_x) dk_x$$

can be introduced. γ is interpreted as the out-scattering rate of the Wigner potential in strict analogy with the phonon out-scattering rate λ, given by equation (3). The potential out-scattering rate γ is added to the both sides of (1) and the steps used to derive the the equation conjugate to the Boltzmann equation [6] are applied. The Neumann expansion of the conjugate equation allows to express $\langle A \rangle$ as an infinite series.

The probabilities of the quantum MC (QMC) algorithm are derived from the consecutively repeated term of the series:

$$\int_0^\infty dt \int d\mathbf{k}' \left\{ (\nu(x(t),\mathbf{k}(t)) e^{-\int_0^t (\nu(x(t)\mathbf{k}(y))) dy} \right\}$$

$$\times \frac{\Gamma(x(t),\mathbf{k}(t),\mathbf{k}')}{\nu(x(t),\mathbf{k}(t))}$$

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

The term in the curly brackets determines the distribution of the free-flight time t. A particle with coordinates $x,\mathbf{k}$ at time 0 drifts over Newton's trajectory:

$$x(\tau) = x + v_x(\mathbf{k})\tau; \qquad \mathbf{k}(\tau) = \mathbf{k} \qquad (4)$$

At time t the particle reaches the point $x(t), \mathbf{k}(t)$ where the next scattering occurs. The selection of the free-flight time follows the classical MC scheme but with an out-scattering rate ν. The term becomes the classical distribution for the free-flight duration when γ approaches zero.

The after-scattering state $\mathbf{k}'$ is selected from the function

$$\Gamma(x,\mathbf{k},\mathbf{k}') = S(\mathbf{k},\mathbf{k}') + \gamma(x)\delta(\mathbf{k}' - \mathbf{k})$$
$$+ \left(V_w^+(x,k_x' - k_x) - V_w^-(x,k_x' - k_x) \right) \delta(k_{yz}' - k_{yz})$$

To become a probability density Γ must be properly normalized. Normalization factors are introduced for the components of Γ. The conditional probability density for a transition from the free-flight end state $(x,\mathbf{k})$ to the after scattering state $(x,\mathbf{k}')$ is presented in the following table, where $\mu(x,\mathbf{k}) = 3\gamma(\mathbf{k}) + \lambda(x)$.

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

Particles enter the device from the contacts with unit weight. The weight is multiplied at each scattering event by the inverse of the corresponding normalization factor give in the following table:

weight factor	scattering source
$\dfrac{\mu(x,\mathbf{k})}{\gamma(x)}$	potential V^+, self-scattering γ and phonons S
$-\dfrac{\mu(x,\mathbf{k})}{\gamma(x)}$	potential V^-

The basic feature of the presented approach is that the quantum potential is treated in the same way as the phonon scattering. Accordingly the derived algorithm retains the basic features of the weighted Single Particle Monte Carlo method. The rules for injection from the boundary distribution, the build up of the trajectory by consecutive drift and scattering events, the accumulation of the weight over the trajectory and the recording of the physical averages remain unchanged.

Two limiting cases can be considered. When the quantum nature of the transport is negligible, the quantities V_w^+, V_w^- and γ become zero. Accordingly the weight becomes unity. In this case the QMC method turns into the classical MC method.

When coherent transport is considered, the Boltzmann scattering operator is switched off by setting S to zero. Then the weight factors become simple numbers:

188

weight factor	scattering source
3	potential V^+, self-scattering γ
-3	potential V^-

In Section IV. the method is examined for a coherent transport problem. A numerical property is observed, which is related to the accumulated weight. With each scattering event the absolute value of the weight increases by factor of 3. As large is the simulated domain and/or as frequent are the scattering events, as much weight is accumulated per trajectory. This leads to a rapid increase of the variance of the method. Intensive computations and application of the trajectory split technique characterize the numerical aspects of the method.

The application of the method includes a discretization of the x and k_x coordinates. The discretization follows the requirements for completeness of the deterministic approach for solving the Wigner equation [7]. In particular the values of Δx and N, where N is the number of points of the discrete Fourier transform, are free parameters. The product $N\Delta x$ gives the coherence length used to calculate V_w. The momentum interval obeys the relation $\Delta k_x = \pi/N$.

III. INCLUSION OF THE ELECTRIC FIELD

The explicit appearance of the electric filed in the transport equation can be convenient for several reasons. Augmented by the classical force term $\dfrac{eE(x)}{\hbar}\dfrac{\partial}{\partial x}$ the left hand side of (1) becomes equivalent to the free streaming operator of the Boltzmann equation. The field gives rise to a accelerating force in (4) which drives the particles throughout the device as in the classical MC method. Furthermore particles stay less time in the quantum region which reduces the number of the scattering events per trajectory and thus the accumulated weight.

In the present formulation the potential V is a sum of the barrier potential V_b and the electrostatic potential V_e, $V = V_b + V_e$. A separation of these potentials can be first addressed. Particularly the idea is to use V_b in equation (2) to obtain the Wigner potential, while the derivative of V_e to give the electric field E. Such separation appears to be an approximation if the electric field is not a constant in the domain of the Fourier transform. It can be shown that equation (2) gives rise to a field term only in the case where V is up to a quadratic function of the position [8].

A rigorous reformulation of (1) is as follows:

$$\left(\frac{\partial}{\partial t} + \frac{\hbar k_x}{m}\frac{\partial}{\partial x} + \frac{eE(x)}{\hbar}\frac{\partial}{\partial x}\right) f_w(x, \mathbf{k}, t) = (Bf_w)(x, \mathbf{k}, t)$$
$$+ \int dk_x' V_w(x, k_x' - k_x) f_w(x, k_x', \mathbf{k}_{yz}, t) \quad (5)$$

$$\tilde{V}_w(x, k_x) =$$

$$\frac{1}{i2\pi\hbar}\int \left(V(x - \frac{s}{2}) - V(x + \frac{s}{2}) - eE(x)s\right) e^{-ik_x s}\, ds$$

It can be shown that the Fourier transform of the term $eE(x)s$ compensates exactly the inclusion of the force term in the left hand side of (5)

IV. APPLICATION OF THE METHOD

We examine the method as applied to a tunneling process. In the simulated experiment particles are injected between the two 1nm thin, 50meV 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, the tail of which is truncated at 50 meV such that the injected particles can overcome the barriers only by tunneling. Material parameters for $GaAs$ at 300K temperature are assumed. Particles crossing the barriers can leave the device through the left or right absorbing contacts.
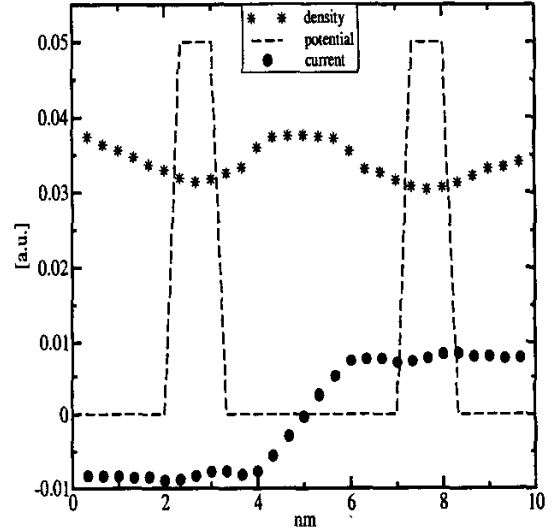

Figure 1: Device potential, current and particle density as depending on the position in the device.

The experiment is especially designed for comparison with a classical system. Under the assumed conditions classical particles have a simple behavior which will be used as a reference for evaluation of the QMC results. Classical particles cannot overcome the barriers. The particle density would grow with the time inside the well and no stationary solution exists for this case. The current density outside the well would be zero because no particles leave the well region. It would be zero also inside the well, due to the fact that the injection region is centered in the well and that the reflection from the barrier walls does not destroy the equilibrium distribution.

The QMC method provides the stationary solution which consistently characterizes the quantum nature of the transport process. The electron density plotted in Figure 1 remains independent of the simulation time. The density remains constant in the region of injection (middle part of the quantum well). It decreases outside the injection region well before the physical location of the barriers, because of the nonlocal character of the quantum potential. 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 Figure 2, γ which is on the order of $10^{-14}s^{-1}$ assumes even higher values outside the barriers than inside.

The current density in Figure 1 clearly demonstrates the tunneling process. The density is nonzero in contrast with the classical case. Particles tunneling through the left barrier give rise to negative current, as opposite to those leaving through the right barrier. Outside the injection region the current densities to the left and right contacts are space-independent because of the current continuity.
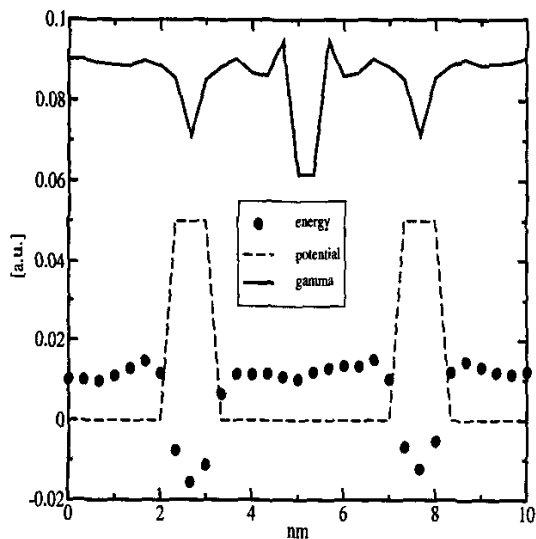

Figure 2: Device potential, out-scattering rate γ and kinetic energy distribution in the device.

A quantitative characterization of the tunneling process is given by the mean kinetic energy, Figure 2. As proportional to the square of the wave vector, the kinetic energy becomes negative in the barriers. This is the place where the wave vector of the tunneling particles transforms from real to imaginary quantity. The particles are injected in the well with mean energy corresponding to the equilibrium value $\simeq 13meV$ for one direction. Each individual scattering by the quantum potential changes the energy of the particle. In this experiment particles can gain energy well above $1eV$. Despite that scattering

occurs in the whole device, the equilibrium value is maintained in the regions with zero potential energy. Conservation of the total energy is demonstrated.

V. CONCLUSION

A stochastic method for simulation of quantum transport in nanoscale electronic devices has been proposed. The interaction with the quantum potential is interpreted as an additional scattering mechanism. An advantage of the presented approach is that the quantum algorithm gradually turns into the classical MC algorithm when $V_w \rightarrow 0$. In this way the artificial separation of the simulated device into quantum and classical domain, inherent for the standard approaches, can be avoided. There is no need from boundary conditions linking the two domains. Moreover, the existing classical MC routines can be reused and extended for quantum simulations.

REFERENCES

[1] J. Sun, G. Haddad, P. Mazumder, and J. Schulman, Proceedings of IEEE 86, 641 (1998).

[2] H. Tsuchiya and T. Miyoshi, Computational Electronics 156 (1998).

[3] M.Nedjalkov, I.Dimov, F.Rossi, and C.Jacoboni, Journal of Mathematical and Computer Modelling 23, 159 (1996).

[4] L. Shifren and D. Ferry, Physics Letters A285, 217 (2001).

[5] H. Kosina, M. Nedjalkov, and S. Selberherr, in Proc. Modeling and Simulation of Microsystems, MSM 2001, edited by M. Laudon and B. Romanowicz (Computational Publications, 2001), pp. 11–14.

[6] H. Kosina, M. Nedjalkov, and S. Selberherr, IEEE Trans.Electron Devices 47, 1898 (2000).

[7] W. Frensley, Reviews of Modern Physics 62, 745 (1990).

[8] C. Jacoboni, A. Bertoni, P. Bordone, and R. Brunetti, Mathematics and Computers in Simulations 55, 67 (2001).