Quantum Monte Carlo Simulation of a Resonant Tunneling Diode Including Phonon Scattering

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ABSTRACT

A Quantum Monte Carlo method taking into account both interference and dissipation effects is presented. The method solves the space-dependent Wigner equation which includes semi-classical scattering via the Boltzmann collision operator. The classical force term is separated from the Wigner potential and included in the Liouville operator on the left hand side. The Wigner potential is treated as an additional scattering source. To permit a probabilistic interpretation, the Wigner potential is expressed as a difference of two positive functions. Scattering from the negative part of the Wigner potential results in a sign change of the particle's weight. A resonant tunneling diode has been simulated using the new Monte Carlo method. The results clearly demonstrate that both semi-classical and quantum transport features are well treated by the method.

Keywords: quantum transport, Wigner equation, Monte Carlo method, resonant tunneling diode

1 INTRODUCTION

At room temperature the electrical characteristics of nanoelectronic and highly down-scaled microelectronic devices are influenced simultaneously by semiclassical and quantum mechanical effects. A kinetic equation suitable for describing this mixed transport regime is given by the Wigner equation. This equation can be formulated in such a way that it simplifies to the semiclassical Boltzmann equation in those device regions where quantum effects are negligible. The Monte Carlo (MC) method has proven to be a reliable and accurate numerical method for solving the Boltzmann equation. Therefore, it appears very promising to devise MC techniques also for the solution of the Wigner equation. The advantage of a particle method is that semiclassical scattering from various sources can be included in a straightforward way. The major problem to be overcome originates from the scattering kernel of the Wigner equation, which is, as opposed to the semiclassical case, no longer positive. A solution to this so-called negative-sign problem is presented in the framework of stationary transport, and the feasibility of the resulting MC method is demonstrated.

2 WIGNER EQUATION

We consider the space-dependent Wigner equation, including semiclassical scattering via the Boltzmann collision operator $Q[f_w]$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + q\mathbf{E}\cdot\nabla_k\right) f_w = Q[f_w] + \Theta_w[f_w]\,, \quad (1)$$

$$\Theta_w[f_w](\mathbf{k},\mathbf{r},t) = \int V_w(\mathbf{r},\mathbf{k}-\mathbf{k}')f_w(\mathbf{k}',\mathbf{r},t)d\mathbf{k}'\,. \quad (2)$$

The classical force term $q\mathbf{E}$ is separated from the Wigner potential [1]

$$V_w(\mathbf{r},\mathbf{k}) = \frac{1}{2\pi i\hbar}\int \left(V(\mathbf{r}+\frac{\mathbf{s}}{2}) - V(\mathbf{r}-\frac{\mathbf{s}}{2}) + q\mathbf{s}\cdot\mathbf{E}\right) e^{-i\mathbf{k}\cdot\mathbf{s}}\,d\mathbf{s}\,, \quad (3)$$

and thus appears in the Liouville operator on the left hand side of (1). The kinetic equation (1) has now the form of a Boltzmann equation with an additional term caused by the Wigner potential. Whether the collision operator or the potential operator is dominant depends on the device under consideration. The chosen formulation of the Wigner equation ensures that in the classical limit the Boltzmann equation is obtained. Consequently, the MC method presented below simplifies gradually to the classical MC method when the Wigner potential vanishes. Therefore, an artificial separation of the simulation domain into a quantum and classical region and application of different numerical methods is avoided.

3 PARTICLE MODEL

Because the Wigner potential assumes positive and negative values, it cannot be used directly as a scattering probability. To permit a probabilistic interpretation, V_w is expressed as a difference of two positive functions. Introducing the truncated Wigner potential

$$V_w^+(\mathbf{k}) = \begin{cases} V_w(\mathbf{k}), & V_w(\mathbf{k}) \geq 0 \\ 0, & V_w(\mathbf{k}) < 0 \end{cases} \quad (4)$$

and accounting for the antisymmetry of V_w with respect to $\mathbf{k}$, the potential operator can be expressed as

$$\Theta_w[f_w](\mathbf{k}) = \int V^+(\mathbf{q})[f_w(\mathbf{k}-\mathbf{q}) - f_w(\mathbf{k}+\mathbf{q})]\,d\mathbf{q}\,. \quad (5)$$

In terms of a particle model, the positive and negative terms of the integrand might be interpreted as in-scattering and out-scattering terms, respectively. However, the out-scattering operator is non-local in **k**-space, whereas, for comparison, the semiclassical out-scattering operator is local. Therefore, (5) does not describe a scattering in the sense that an initial state is annihilated and a final state is created. Instead, (5) describes the creation of two new states, $\mathbf{k}-\mathbf{q}$ and $\mathbf{k}+\mathbf{q}$. When generating the second state, the sign of the statistical weight is changed.

$$\gamma(\mathbf{r}) = \int V_w^+(\mathbf{r},\mathbf{k})\, d\mathbf{k}\,. \tag{6}$$

It should be noted that the Wigner equation strictly conserves charge, as can be seen by taking the zero-order moment of (1)

$$\frac{\partial n}{\partial t} + \operatorname{div} \mathbf{J} = 0\,.$$

Looking at the number of particles regardless of their statistical weight, that is, counting each particle as positive, another potential operator needs to be considered.

$$\Theta_w^*[f_w](\mathbf{k}) = \int V^+(\mathbf{q})[f_w(\mathbf{k}-\mathbf{q}) + f_w(\mathbf{k}+\mathbf{q})]\, d\mathbf{q} \tag{7}$$

Using (7), a continuity equation for numerical particles is obtained.

$$\frac{\partial n^*}{\partial t} + \operatorname{div} \mathbf{J}^* = 2\gamma(\mathbf{r}) n^* \tag{8}$$

The high generation rate in this equation is a direct consequence of the negative-sign problem. Not only can we expect cancellation effects in the estimators due to the positive and negative statistical weights, but also an exponential growth in time of certain quantities, such as particle number, particle weight or variance.

4 MONTE CARLO METHOD

The particle model described in the previous sections provides a guideline for the development of new and the characterization of existing MC algorithms for solving the Wigner equation. Applying a formal approach, which employs the Neumann series expansion of the underlying transport equation [2], leads to a MC algorithm with two significant properties: the number of numerical particles is conserved, and the particle weights increase exponentially in time. Using this algorithm it has been demonstrated that tunneling can be treated numerically by means of a particle model [3]. However, because of the exponential increase of the absolute value of the particle weight at the very short time scale $(2\gamma)^{-1}$ (see (8)), application of this algorithm turned out to be restricted to single-barrier tunneling and small barrier heights only.

For the simulation of double-barrier structures a similar MC algorithm has been designed, which now conserves the statistical weight, $|w_i(t)| = 1$, where $w_i(t)$ denotes the weight of the i-th particle at time t. In return, particles are generated at the rate of 2γ. Variance reduction is accomplished by continuously removing numerical particles. Those particles which have opposite weight and a sufficiently small distance in phase space can be assumed to annihilate each other.

This algorithm has been implemented for the steady state. To apply well-posed boundary conditions, parts of the highly doped contact regions are included in the simulation domain. In these regions the non-local potential vanishes and conditions are near-equilibrium. Therefore, particles can be injected from a classical distribution at the domain boundaries. As in the semi-classical MC method, particles undergo a sequence of accelerated free flights and scattering. In regions where V_w is non-zero pairs of numerical particles are generated according to the generation term (5). After each scattering event one has to deal with three states, namely the generated ones, $\mathbf{k}-\mathbf{q}$, $\mathbf{k}+\mathbf{q}$, and the initial state **k**, which is not affected by (5) and thus has to be retained. In the stationary MC algorithm developed the weights of two out of the three states are stored on a phase space grid, and the trajectory is continued from the remaining state. In the course of a simulation the weights on the grid cancel to a large extent. The goal of the algorithm is to minimize the residual weight on the grid, which is an indicator for the numerical error of the method.

5 RESULTS AND DISCUSSION

A resonant tunneling diode (RTD) has been investigated, assuming a barrier height of $E_b = 0.3$eV, a barrier width of 3nm, and a well width of 5nm (Fig. 1). The Wigner potential is discretized using $N_k = 640$ equidistant k_x points and $\Delta x = 0.5$nm spacing in x-direction. Assuming a coherence length of $L_c = 80$nm one would require at least $N_k = L_c/\Delta x = 160$. This minium value is often used in finite difference methods for the Wigner equation. However, since other numerical methods based on the Schödinger equation use typically much finer grids in order to resolve the resonances properly we believe that also for the Wigner equation a fine k-grid is required.

The annihilation mesh is three-dimensional. In x-direction the grid covers the region where the Wigner potential is non-zero. Because of the cylindrical symmetry of the Wigner function only two momentum coordinates have to be considered. The mesh extends to an energy of 6eV in both axial and radial k-direction.

The semiclassical scattering model includes polar optical and acoustic deformation potential scattering, assuming parameter values for GaAs.

The Wigner generation rate (5) is on the order of

$10^{15}s^{-1}$ for the structure considered (Fig. 2). Comparing this rate with the much smaller semiclassical scattering rate is a quantitative measure of the fact that quantum interference effects are dominant. The zero-field contact regions have been chosen sufficiently large, such that the Wigner potential drops to zero within these regions. The temperature dependence of the current-voltage characteristics of the RTD is shown in Fig. 3. The resonance current is higher at low temperature due to the smaller spreading of the energy distribution. On the other hand, the valley current increases with temperature. Fig. 4 shows the electron concentration in the device at voltages below the resonance voltage. A classical behavior is found before and after the double barrier, whereas in the quantum well the behavior of the solution is non-classical. In front of the barrier an accumulation layer forms, with its maximum concentration increasing with the band bending. In the quantum well the concentration increases as the resonance is approached. After the barrier a depletion layer forms, which grows with applied voltage. In this region the concentration at 0.15V varies exponentially in response to the linear potential (Fig. 1), which is again a classical property.

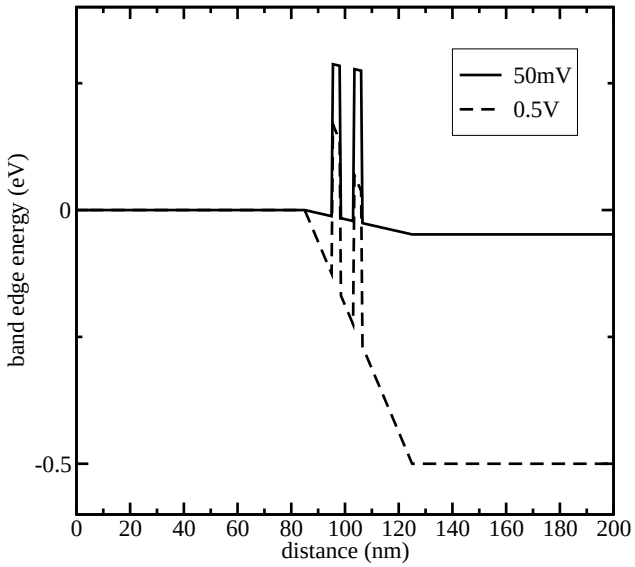

Figure 1: Conduction band edge of the RTD for different voltages. A linear voltage drop is assumed over a distance of 40 nm.

For voltages above the resonance voltage, the concentration in the well drops, whereas the depletion layer continues to grow. The mean kinetic energy of the electrons is depicted in Fig. 6. In the zero-field regions an energy close to the equilibrium energy is obtained, which demonstrates that the energy conservation property of the Wigner potential operator is also satisfied by the numerical MC procedure. One has to keep in mind that the Wigner potential can produce a rather large momentum transfer. For the chosen x-discretization the related energy transfer can reach values as large as 5eV, which shows that a large degree of cancellation occurs in the estimator for the mean energy. In the barrier the mean energy assumes a minimum. At lower temperature even negative mean energies can be obtained, which can be expected for tunneling states. Electrons injected from

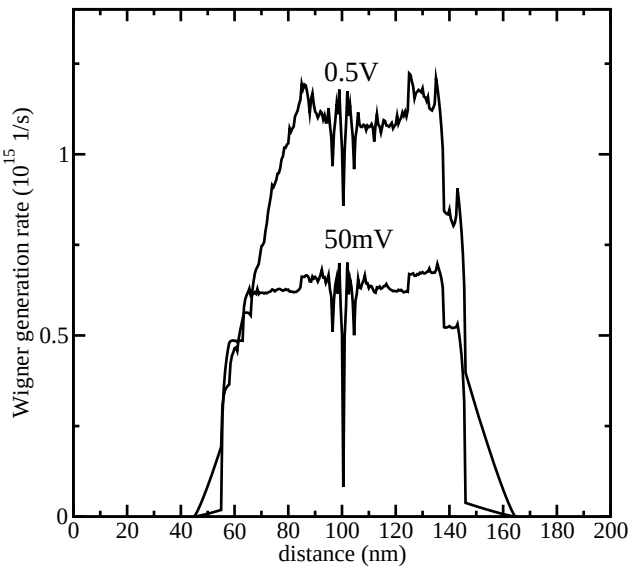

Figure 2: Pair generation rate $\gamma(x)$ caused by the Wigner potential for two different voltages.

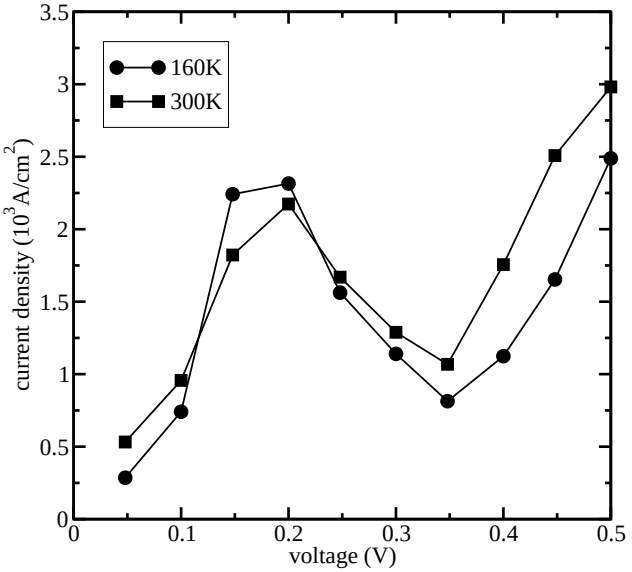

Figure 3: IV-characteristics of the RTD for two different temperatures.

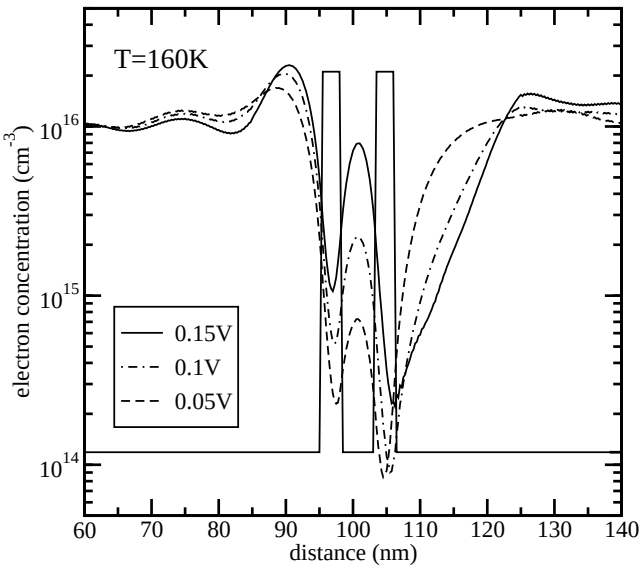

Figure 4: Electron concentration in the RTD for voltages less than the resonance voltage.

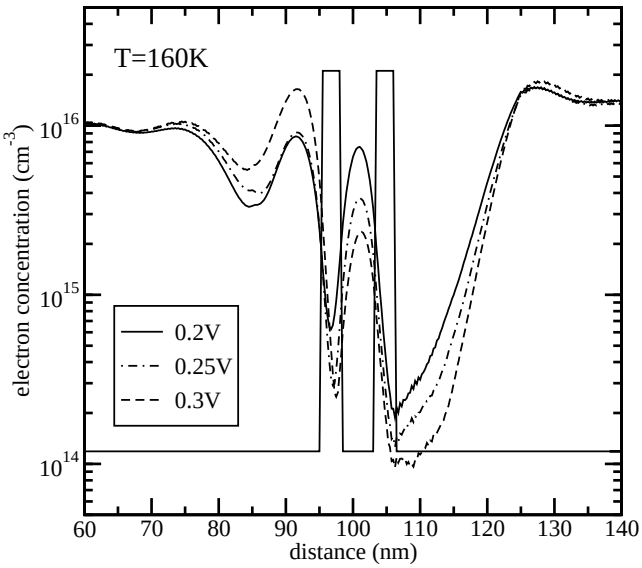

Figure 5: Electron concentration in the RTD for voltages greater than the resonance voltage.

the second barrier into the collector space charge region show initially a high kinetic energy.

6 CONCLUSION

A Monte Carlo method for the simulation of far-from-equilibrium transport in nanostructures has been presented. The method solves the Wigner equation including the Boltzmann scattering operator. Scattering

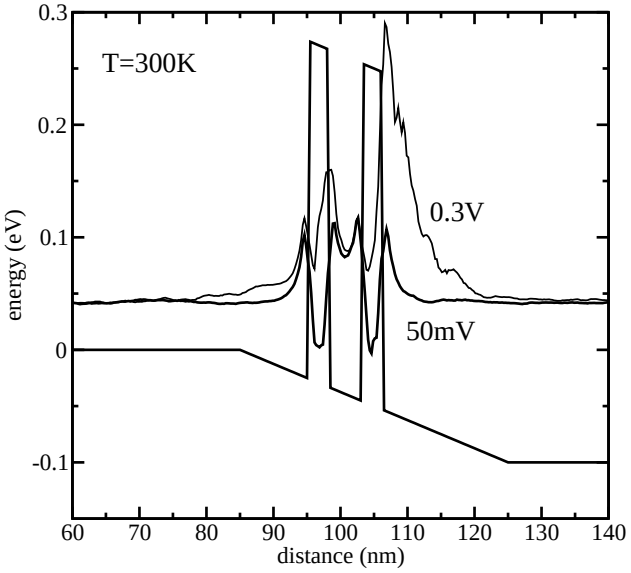

Figure 6: Mean kinetic energy for two different voltages.

from the Wigner potential is complicated by the so-called negative sign problem. The latter would lead to a run-away of variance, unless a proper variance reduction technique is used. In the presented approach variance reduction is accomplished by annihilation of numerical particles at the same rate as they are generated. Simulation results for a resonant tunneling diode demonstrate that the solution of the non-coherent Wigner equation exhibits a mixed semiclassical and quantum behavior.

7 ACKNOWLEDGMENT

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