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A Monte Carlo Method Seamlessly Linking Quantum and Classical Transport Calculations

H. KOSINA, M. NEDJALKOV AND S. SELBERHERR
Institute for Microelectronics, TU Vienna, Gusshausstr 27–29, A-1040 Vienna, Austria
kosina@iue.tuwien.ac.at

Abstract. A Monte Carlo method for carrier transport is presented, which simultaneously takes into account quantum interference and dissipation effects. The method solves the space-dependent Wigner equation including semi-classical scattering through the Boltzmann collision operator. To this equation a particle model is assigned, which interprets the non-local potential operator as a generation term for numerical particles of positive and negative statistical weight. A numerical technique to control the avalanche of numerical particles is discussed. Since the Wigner equation simplifies to the Boltzmann equation in classical device regions, the solutions of the quantum kinetic equation and the classical one are linked in a natural way. This approach allows the simulation of a quantum region embedded in an extended classical region. Results of this approach are demonstrated for a resonant tunneling diode.

Keywords: Wigner equation, quantum transport, Monte Carlo method, device simulation

1. Introduction

At room temperature the electrical characteristics of nanoelectronic and highly down-scaled microelectronic devices are influenced simultaneously by classical and quantum transport effects. A kinetic equation suitable for describing this mixed transport regime is given by the Wigner equation. It can be be formulated in a way to give the Boltzmann equation in the classical limit. The Monte Carlo (MC) method is nowadays a well established, reliable and accurate numerical method for solving the Boltzmann equation. Because of the similarity of both equations it appears very promising to develop a MC method also for the solution of the Wigner equation. Such approaches have been reported recently [1–4]. The major problem to overcome is that the Wigner potential does not represent a positive definite function. This so-called negative sign problem generally calls for the introduction of particles of negative statistical weight.

A consequence of the negative sign problem is that even for a system of non-interacting particles the MC method has to include inter-particle interactions, allowing a transfer of, for example, the negative weight of one particle to the positive weight of another particle in order to achieve weight cancellation.

Otherwise, if such a mechanism is not included, the MC method can be shown to be instable [4]. The particle weights of either sign grow exponentially at a very high rate, and because of the large degree of cancellation in the estimators the variance would also grow exponentially.

2. The Particle Model

The quantum transport model is based on the generalized Wigner equation describing one electron interacting with a many-phonon system. Assuming the weak scattering limit, an equilibrium phonon system, and the mean phonon number approximation gives a system of three equations, which determines the reduced Wigner function and two auxiliary functions [5]. This model still includes effects such as collisional broadening and the intra-collisional field effect. To obtain a model more suitable for device simulation, the classical

limit is introduced in the electron-phonon interaction, which results in a Wigner equation with a Boltzmann scattering operator of the following form:

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

In this equation, f_w denotes the reduced electron Wigner function, and $Q[f_w]$ and $\Theta_w[f_w]$ are the Boltzmann scattering and the Wigner potential operators, respectively. The classical force term $q\mathbf{E}$ is separated from the Wigner potential

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

and thus appears on the left hand side of (1) [2]. Because the Wigner potential assumes positive and negative values, it cannot directly be used as a probability density. However, the antisymmetry of V_w with respect to $\mathbf{k}$ allows the potential operator to be expressed solely in terms of the function $V_w^+(\mathbf{k}) = \mathrm{Max}(0, V_w(\mathbf{k}))$, which is positive definite and thus amenable to a probabilistic interpretation [4]. Expressing the Liouville operator in (1) as a total time derivative and writing the operators on the right hand side explicitly gives

$$\begin{aligned}\left[\frac{\mathrm{d}}{\mathrm{d}t} + \underbrace{(\lambda+\alpha)}_{\text{out-scatt.}}\right] f_w(\mathbf{k},\mathbf{r},t) &= \int f_w(\mathbf{k}',\mathbf{r},t)\,\underbrace{[S(\mathbf{k}',\mathbf{k}) + \alpha\delta(\mathbf{k}'-\mathbf{k})]}_{\text{in-scatt.}}\, d\mathbf{k}' \\ &+ \int \underbrace{V_w^+(\mathbf{q},\mathbf{r}) f_w(\mathbf{k}-\mathbf{q},\mathbf{r},t)}_{\text{gen. pos. part.}}\, d\mathbf{q} \\ &- \int \underbrace{V_w^+(\mathbf{q},\mathbf{r}) f_w(\mathbf{k}+\mathbf{q},\mathbf{r},t)}_{\text{gen. neg. part.}}\, d\mathbf{q}.\end{aligned} \tag{3}$$

The three characteristic rates in this equation are the semiclassical scattering rate, $\lambda(\mathbf{k}) = \int S(\mathbf{k},\mathbf{k}')d\mathbf{k}'$, a self-scattering rate to be determined later, $\alpha(\mathbf{k},\mathbf{r}) \geq 0$, and a rate associated with the Wigner potential, $\gamma(\mathbf{r}) = \int V_w^+(\mathbf{r},\mathbf{k})d\mathbf{k}$. Equation (3) is now interpreted as a Boltzmann equation, where in- and out-scattering processes are exactly balanced, augmented by a generation term for positive particles and one for negative particles. Note that an interpretation of the very last integral in (3) as an out-scattering term is ruled out by its non-locality in momentum space.

3. The Monte Carlo Method

In the same way as for the Boltzmann equation, a formal integration in time gives a path-integral equation for the Wigner function f_w. From the adjoint integral equation one can then derive forward MC algorithms. Various probabilities and probability densities employed in the MC algorithm can be directly identified from the integral-differential form (3). Introducing the rate $\mu = \lambda + \alpha$, which will determine the free-flight duration, and the normalized distributions $S(\mathbf{k}',\mathbf{k})/\lambda(\mathbf{k}')$ and $V^+(\mathbf{q},\mathbf{r})/\gamma(\mathbf{r})$, (3) is reformulated as

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + \mu\right] f_w(\mathbf{k},\mathbf{r},t) = \int d\mathbf{k}'\, f_w(\mathbf{k}',\mathbf{r},t)\mu(\mathbf{k}')\Gamma(\mathbf{k}',\mathbf{k},\mathbf{r}), \tag{4}$$

with the integral kernel

$$\begin{aligned}&\Gamma(\mathbf{k}',\mathbf{k},\mathbf{r}) \\ &= \left\{\frac{\lambda}{\mu}\right\}\left\{\frac{S(\mathbf{k}',\mathbf{k})}{\lambda(\mathbf{k}')}\right\} + \left\{\frac{\alpha}{\mu}\right\}\{\delta(\mathbf{k}'-\mathbf{k})\} \\ &\quad + \left\{\frac{\gamma}{\mu}\right\}\left(\left\{\frac{V_w^+(\mathbf{k}-\mathbf{k}')}{\gamma(\mathbf{r})}\right\} - \left\{\frac{V_w^+(\mathbf{k}'-\mathbf{k})}{\gamma(\mathbf{r})}\right\}\right).\end{aligned} \tag{5}$$

In this equation all probabilities and probability distributions are enclosed in curly brackets. The kernel satisfies the normalization $\int \Gamma(\mathbf{k}',\mathbf{k},\mathbf{r})d\mathbf{k} = 1$. The self-scattering rate α has to be chosen such that $\mu \geq \gamma$. Typical choices are $\mu = \lambda + \gamma$ or $\mu = \mathrm{Max}(\lambda, \gamma)$.

3.1. Free Flight and Scattering

As in the classical MC method, the distribution of the free flight duration is given by an exponential distribution with the total scattering rate μ as parameter. At the end of a free flight the complementary probabilities $p_1 = \lambda/\mu$ and $1 - p_1 = \alpha/\mu$ are considered. With probability p_1 one selects the semiclassical scattering mechanism and generates for the given initial state $\mathbf{k}'$ the final state $\mathbf{k}$, employing the normalized distribution $S(\mathbf{k}',\mathbf{k})/\lambda(\mathbf{k}')$. The alternative event having a probability of $1 - p_1$ is the selection of self-scattering. In that

case the normalized distribution $\delta(\mathbf{k}' - \mathbf{k})$ determines the final state simply as $\mathbf{k} = \mathbf{k}'$.

3.2. *Particle Generation and Annihilation*

At the end of a free flight, a pair of particles is generated with probability $p_2 = \gamma/\mu$. The particle states are $\mathbf{k}' + \mathbf{q}$ and $\mathbf{k}' - \mathbf{q}$, where $\mathbf{q}$ is selected from the normalized distribution $V_w^+(\mathbf{q}, \mathbf{r})/\gamma(\mathbf{r})$. The statistical weights of the particles have opposite sign. In the present algorithm particle weights take on only the integer values ± 1.

Because repeating this generation step will lead to an exponential increase in particle number, an additional procedure has to be introduced to control the particle number. One can assume that two particles of opposite weight and a sufficiently small distance in phase space annihilate each other.

It should be noted that the particle model and the associated probability distributions describe the general, time and space-dependent case. In the following we restrict ourselves to the stationary transport problem. In the steady state a phase space grid can be utilized, on which particle states can be temporarily stored. Due to stationarity a particle stored in a cell at some time can be annihilated by a particle of opposite sign visiting the same cell at any other time. In the present algorithm this idea is realized as follows.

After each generation event one has to deal with three particle states, namely the after-scattering state $\mathbf{k}$ and the two generated states, $\mathbf{k}' + \mathbf{q}$ and $\mathbf{k}' - \mathbf{q}$. In a first step the grid cells corresponding to these three states are located. The weight of each particle is assigned to the respective cell. In a second step the total weights in the three cells are compared. The cell with the largest absolute weight is selected and the corresponding particle state is used to continue the trajectory. In the third step the sign of the continuing particle is selected such that the weight in the cell is reduced. The method of selecting the continuing particle aims at compensating the weight locally stored on the grid as much as possible. The residual weight on the grid has to be minimized as it is an indicator for the numerical error of the method. Simulations show that the weights on the grid cancel to a large extent.

The procedure described gives a single-particle MC method. Particle trajectories are constructed sequentially in a simulation. Apparently, for $\gamma = 0$ no particles need to be generated and the classical MC method is regained.

3.3. *Boundary Conditions*

Assuming that extended contact regions with high doping concentration are included in the simulation domain, one can safely neglect quantum effects in these regions and apply a classical distribution at the metal/semiconductor contacts. As in the classical MC method, a particle is injected at a contact from a classical distribution and undergoes a sequence of accelerated free flights and scattering events. In regions where the Wigner potential and hence the pair generation rate are non-zero, pairs of numerical particles are generated as described in the previous section. Since there is only one transport equation applied in the whole device, there is no particular interface condition needed at the interfaces between classical and quantum regions. The particle model ensures continuity of the various macroscopic fluxes at these interfaces.

4. 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 3 nm, and a well width of 5 nm. The Wigner potential is discretized using $N_k = 640$ equidistant k_x points and $\Delta x = 1$ nm spacing in x-direction. A coherence length of $L_c = 80$ nm is assumed.

By means of the Wigner generation rate γ the simulation domain can be decomposed into quantum regions ($\gamma > 0$) and classical regions ($\gamma \simeq 0$), as shown in Fig. 1. In Fig. 2 it is demonstrated that the electron concentration and the mean energy are smooth in the

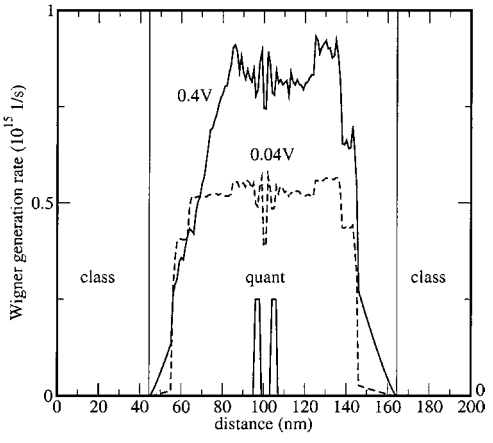

Figure 1. Pair generation rate $\gamma(x)$ caused by the Wigner potential.

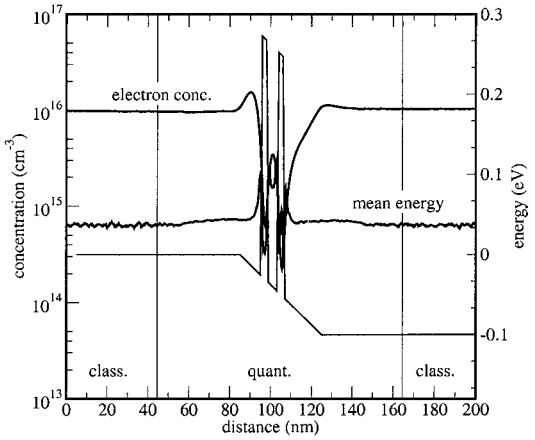

Figure 2. Electron concentration and mean electron energy in the RTD at $T = 300$ K and 0.1 V bias.

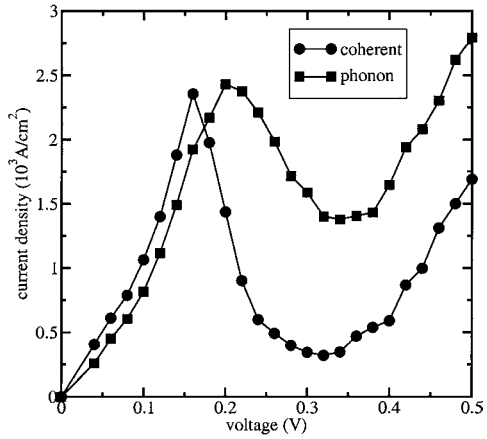

Figure 3. Influence of phonon scattering on the IV-characteristics of the RTD.

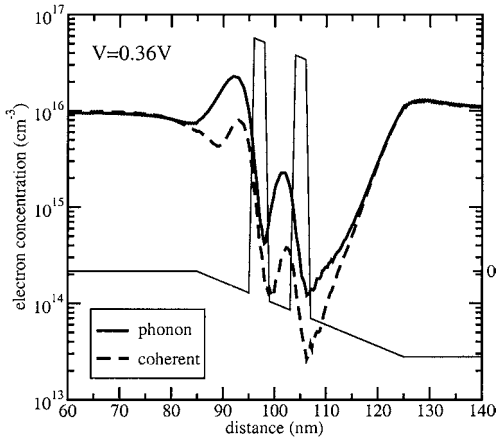

Figure 4. Electron concentration in the RTD in off-resonance condition.

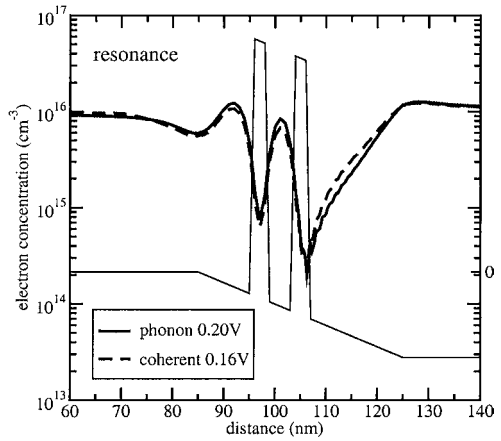

Figure 5. Electron concentration in the RTD in resonance condition.

extended contact regions and not affected by the strong onset of the Wigner generation rate.

Phonon scattering strongly affects the current/voltage characteristic (Fig. 3). As compared to the coherent case, phonon scattering leads to an increase in the valley current and a resonance voltage shift. The large difference in valley current can be explained by the electron concentration in off-resonance condition (Fig. 4). With phonon scattering included a significantly higher concentration forms in the emitter notch, and injection in the double barrier is increased. This indicates that a quasi bound state forms in the emitter notch. The population of this state increases when scattering is switched on. On the other hand, in resonance condition where the applied voltage is lower such a bound state does not form and very similar electron concentrations are observed for the coherent and non-coherent case (Fig. 5).

5. Conclusion

A MC method for the simulation of non-equilibrium transport in nanostructures has been presented. The method solves the Wigner equation including the Boltzmann scattering operator. The non-local potential operator is interpreted as a generation term of numerical particles of opposite sign. A runaway in particle number is avoided by annihilating numerical particles at the same rate as they are generated. In this way a single-particle method is obtained. The MC method turns gradually into the classical MC method when the classical limit is

approached. Therefore, non-equilibrium transport can be simulated throughout a device formed by a central quantum region embedded in extended classical regions. A resonant tunneling diode has been simulated and the effect of phonon scattering on the device characteristics is discussed.

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