Stochastic interpretation of the Wigner transport in nanostructures

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Abstract

A stochastic interpretation of the quantum transport in nanoscale electronic devices is proposed. The Wigner potential is treated as a scattering source which determines the electron–potential interaction. A particle picture where each scattering event generates positive and negative particles is associated to the transport process.
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1. Introduction

The numerical theory of the Monte Carlo (MC) method is used to propose a particle picture of the quantum transport in nanoscale devices. The approach is just opposite to the classical case, where the transport picture is used to devise the MC method. The Wigner equation is considered which accounts for the coherent part of the transport via the Wigner potential V_w and for dissipation processes introduced by phonons via the Boltzmann collision operator B [1]. For one-dimensional devices the equation reads

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

$$= (Bf_w)(x, \mathbf{k}, t) + \int dk'_x V_w(x, k'_x - k_x)f_w(x, k'_x, \mathbf{k}_{yz}, t) \quad (1)$$

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

where V is the device potential. The Boltzmann operator is defined in the standard way by the scattering rate $S(\mathbf{k}', \mathbf{k})$ which is the probability density per unit time for scattering from state $(\mathbf{k}')$ to state $(\mathbf{k})$. S determines the total out-scattering rate λ as the integral over all after-scattering states: $\lambda(\mathbf{k}) = \int S(\mathbf{k}, \mathbf{k}')d\mathbf{k}'$. From a mathematical point of view, Eq. (1) is very similar to the Boltzmann equation. Without V_w Eq. (1) is the zero field Boltzmann equation (BE). The classical limit of V_w leads to a force term converting Eq. (1) into the standard BE. This similarity

allows to reformulate Eq. (1) using the steps applied to the BE in the formal theory of the MC method [2]. First the integral form of Eq. (1) is obtained for the case of stationary transport

$$f_w(x, \mathbf{k}) = \phi(x, \mathbf{k}) + \int_{t_b}^0 dt' \int d\mathbf{k}' f_w(x(t'), \mathbf{k}')\Gamma(x(t'), \mathbf{k}, \mathbf{k}')$$

$$\times e^{-\int_{t'}^0 \mu(x(y), \mathbf{k})dy} \quad (2)$$

where the boundary condition $\phi(x, \mathbf{k})$ determines the device characteristics. $x(t) = x + v_x(\mathbf{k})t$ is the backward Newton's trajectory ($t < 0$) initialized at $t = 0$ by the initial phase point $(x, \mathbf{k})$ and t_b is the time of intersection of the trajectory with the boundary. In the sum $\mu = \lambda + \nu$ an arbitrary function ν is introduced which will be determined later. In Eq. (2) Γ is defined by

$$\Gamma(x, \mathbf{k}, \mathbf{k}') = V_w(x, k'_x - k_x)\delta(\mathbf{k}'_{yz} - \mathbf{k}_{yz}) + \nu(x, \mathbf{k})\delta(\mathbf{k}' - \mathbf{k})$$

$$+ S(\mathbf{k}', \mathbf{k})$$

The negative time scale characterizes the backward evolution of the trajectory. A particle interpretation of the equation requires forward evolution and positive times which are introduced by the conjugate equation to Eq. (2).

It is shown that the mean value (A, f_w) of any physical quantity A can be expressed by the series

$$\int Af_w\, d\mathbf{k}dx = (A, f_w) = \left(\phi, \sum_i K^i A\right) \quad (3)$$

where $K^i A$ denotes the ith iteration of the conjugate kernel K on A: $K^i A = (K, K^{i-1}A)$.

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A Monte Carlo algorithm which evaluates Eq. (3) has been derived. In the framework of the weighted single particle MC method [2], the quantum potential is included as a scattering source. The algorithm retains the basic features of the classical counterpart. A particle injected into the device propagates over a numerical trajectory built up by consecutive iterations of K. When the trajectory leaves the device a new particle is injected. Each trajectory provides an independent MC experiment, which contributes to the statistics collected for the mean value (3). The injection from the boundary distribution, the accumulation of the weight over the trajectory and the recording of the physical averages follow the classical prescriptions.

The rules for building the trajectories, imposed by the structure of K are discussed in Section 2. It is shown that the number of simulated trajectories must be huge for reasonable nanoscale devices. Aiming at variance reduction, in Section 3 a modification of the method is proposed, which gives rise to a particle picture of the quantum process.

2. Stochastic approach

For the sake of transparency the kernel of the coherent equation is discussed

$$\int_0^{t_b} dt \int dk_x' \left\{ \nu(t) e^{-\int_0^t \nu(y)dy} \right\}_1 \left(\left\{ \frac{\nu(t)}{\mu(t)} \right\}_2 \{ \delta(k_x - k_x') \}_3 \right.$$
$$\left. + \left\{ \frac{\gamma(t)}{\mu(t)} \right\}_{2'} \left\{ \frac{|V_w(x(t), k_x - k_x')|}{\gamma(t)} \right\}_{3'} \text{sign}(V_w) \right) \frac{\mu(t)}{\nu(t)}$$

Extra factors are introduced in a way conserving the value of the integrand. They serve for normalization of the probabilities, enclosed in curly brackets, which are used for construction of the particle trajectory. The subscripts denote the order of application of these conditional probabilities. $\{ \}_1$ generates the free flight duration so that the particle drifts between an initial, $(k_x, x, 0)$, and a final state, $(k_x, x(t), t)$, over a classical trajectory. At the final point a scattering occurs. $\{ \}_2$ is the probability to use the first kernel component for selection of the after scattering k_x'. Since $\mu = \gamma + \nu$, the second component is selected according $\{ \}_{2'} = 1 - \{ \}_2$. Thus k_x' is chosen either with the probability density $\{ \}_3$ or with the probability density $\{ \}_{3'}$. The normalization of the latter is ensured by the function γ: $\gamma(x(t)) = \int |V_w(x(t), k)| dk$. Note that this procedure is relevant if ν and γ differ no more than one order of magnitude. The after-scattering state $(k_x', x(t), t)$ is the initial state of a free flight for the next iteration of the kernel.

The remaining term $w_i = \pm(\mu(t)/\nu(t))$, where the sign is given by the sign of V_w, is the weight factor. w_i multiplies the weight accumulated by the trajectory during the previous iterations of the kernel. It can be shown that the mean accumulated weight w per trajectory does not depend on the choice of ν. If T is the mean time particles spend in the device, the number of scattering events n is $n = T\nu$. The mean weight is then $w = \pm(1 + \gamma/\nu)^n = \pm(1 + \gamma T/n)^n$, which is evaluated by $w = \pm e^{\gamma T}$ since n is large. Indeed for a 0.3 eV potential $\gamma \simeq 10^{15}$ s^{-1} while T is commonly greater than picosecond if the device dimensions are above 10 nm. Two conclusions can be done. First ν can be selected in a way to simplify the weight factor w_i. With the choice $\nu = \gamma/2$ the weight factor becomes $w_i = \pm3$. Furthermore, the mean trajectory weight grows exponentially with the V_w and the dwelling time T. This result is in accordance with the exponential growth with time of the variance of the MC evaluations of Feynman path integrals [3]. For the time and potential scales discussed above the weight w becomes huge. Accordingly high must be the number of independent experiments in order to average the weights to the mean (3). The application of the method is restricted to single barrier tunneling and small barrier heights.

3. Particle model

To overcome the problem of growing variance, the method can be modified in the following way. The antisymmetric function V_w is decomposed into two positive functions: $V_w = V_w^+ - V_w^-$. Due to the choice of ν, it holds $\nu = \int V^\pm dk_x$. The kernel can be written as:

$$\int_0^{t_b} dt \int dk_x' \left\{ \nu(t) e^{-\int_0^t \nu(y)dy} \right\}_1 \left(\{ \delta(k_x - k_x') \}_2 \right.$$
$$\left. + \left\{ \frac{V_w^+(x(t), k_x - k_x')|}{\nu(t)} \right\}_2 - \left\{ \frac{V_w^-(x(t), k_x - k_x')|}{\nu(t)} \right\}_2 \right)$$

The three kernel components simultaneously create three after scattering states. These states cannot coincide since the k_x space is complementary decomposed by the probabilities $\{ \}_2$. Each state gives rise of a trajectory and thus presents a separate particle which must be simulated until exiting the device boundary. Two of the particles carry the weight of the initial state, the third one has a weight of opposite sign. The absolute value of the weight remains 1 so that the particles can be marked as positive and negative.

The following picture can be associated to the transport process. With each iteration of the kernel a positive (negative) particle undergoes a free flight and scattering event. After the scattering event the particle survives in the same state with the same weight due to the delta function.
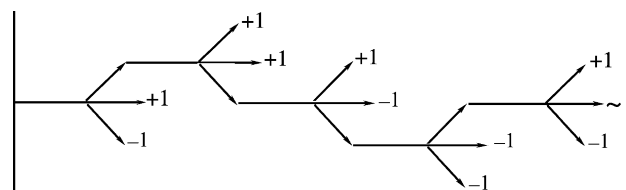
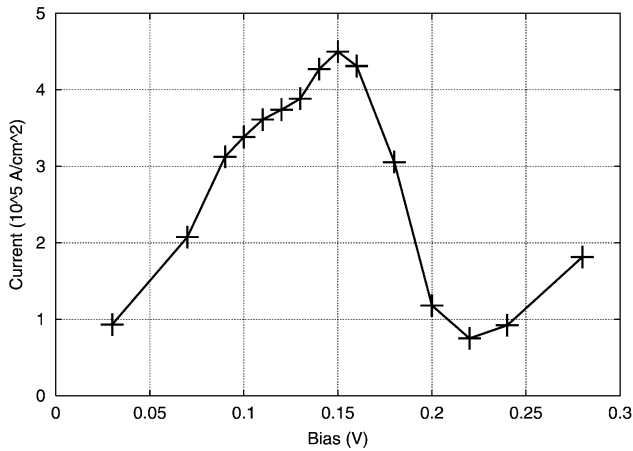

Fig. 1. Trajectory of the randomly selected particle.

Fig. 2. $I-V$ characteristics at temperature 77 K.

Fig. 3. Electron densities at the central part of the device.

Additionally a positive and a negative particles are created by $V_w^\pm$. Fig. 1 shows the evolution of a particle randomly selected after each scattering event. If phonons are included the picture remains similar. The free flights are additionally interrupted by the phonon scattering which only changes the momentum of the particle as in the classical case.

We note that other interpretations conserving the absolute weight are possible. The free flight could be two times longer on the expense that four particles must be created per scattering event. The proposed two-particle picture is the most simple one which shows the idea of the approach. Instead of collecting the weight over a single trajectory, the weight is split in the phase space. Positive and negative particles have opposite contribution to the statistics. They have the same probabilistic future if located close together in the phase space and thus can be canceled. The MC simulation follows the randomly selected particle while remaining particles are stored on a mesh for further processing. The active particle cancellation saves simulation time leading to a variance reduction.

A resonant tunneling diode investigated in Ref. [4] has been simulated for the coherent case. The barriers are 0.3 eV high, 3 nm thin and the well is 5 nm wide. The potential drops linearly in the central 17 nm part of the device.
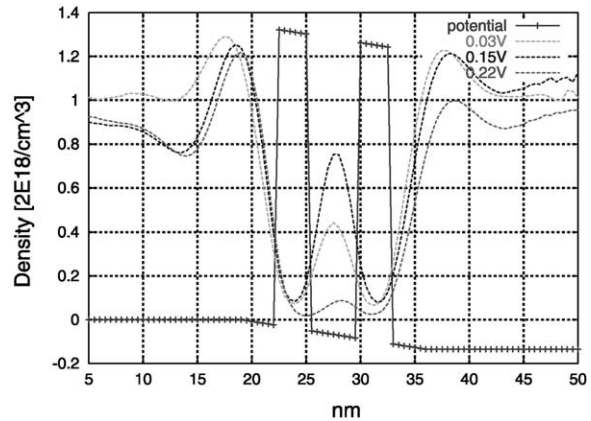
The doping of the 19 nm electrode layers is 2×10^{18} cm^{-3}. The obtained $I-V$ curve is shown in Fig. 2. Fig. 3 shows the electron densities for initial, peak and valley bias points. The results are in good agreement with the characteristics presented in Ref. [4].

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