

A Weight Decomposition Approach to the Sign Problem in Wigner Transport Simulations

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Abstract. A stochastic method for simulation of carrier transport in semiconductor nanostructures is presented. The Wigner formulation of quantum mechanics is used. The method which aims at evaluation of mean values of physical quantities, is obtained by following the rules of the Monte Carlo theory. A particular numerical feature of the method are statistical weights with inverse signs which can achieve large absolute values. They give rise to high variance of the simulation results, the so called sign problem in quantum Monte Carlo simulations. A weight decomposition approach is proposed which limits the value of a weight by storing part of it on a phase space grid. Annihilation of positive and negative stored weights, which occur during the simulation significantly improves the variance of the method.

1 Introduction

The Wigner-function (f_w) formalism has been recognized as a convenient approach to describe electron transport in mesoscopic systems. The formalism combines a rigorous quantum-kinetic level of treatment with the classical concepts for phase space and open boundary conditions. Moreover dissipation processes introduced by phonons can be taken into account by adding the classical Boltzmann collision operator to the Wigner operator V_w [1]. The basic similarity with the classical transport picture motivates a Monte Carlo (MC) method for solving the Wigner equation. For the sake of transparency the method is described for the case of stationary, coherent one-dimensional transport. A generalization for phonon scattering follows the same approach. The corresponding Wigner equation reads:

$$\frac{\hbar k}{m} \frac{\partial}{\partial x} f_w(x, k) = \int dk' V_w(x, k' - k) f_w(x, k') \quad (1)$$
$$V_w(x, k) = \int ds e^{-iks} \frac{1}{i2\pi\hbar} \left(V(x - \frac{s}{2}) - V(x + \frac{s}{2}) \right)$$

where V is the device potential, x is the position, and $\hbar k$ is the momentum.

The proposed method aims at evaluation of the mean value $\langle A \rangle$ of a given physical quantity $A(x, k)$. The basic expression is obtained by a series expansion of $\langle A \rangle$ derived in the next section.

2 The series expansion of $\langle A \rangle$

As a first step an integral form of the Wigner equation is obtained. A non-negative function $\nu(x)$ is introduced, which will be determined later, and $\nu(x)f(x, k)$ is added to both sides of (1). The characteristics of the differential operator are classical Newton's trajectories

$$x(t) = x + v(k)t, \quad k(t) = k; \quad v(k) = \frac{\hbar k}{m}$$

A trajectory $(x(t), k(t))$ is initialized by the phase space point (x, k) at time 0. $v(k)$ is the electron velocity and the parameterization is backward in time, $t < 0$.

Newton's trajectories are used to transform (1) into the following integral equation:

$$\begin{aligned} f_w(x, k) &= \int_{t_b}^0 dt' \int dk' f_w(x(t'), k') \Gamma(x(t'), k(t'), k') e^{-\int_{t'}^0 \nu(x(y)) dy} \\ &+ e^{-\int_{t_b}^0 \nu(x(y)) dy} f_b(x(t_b), k(t_b)) \end{aligned} \quad (2)$$

$$\Gamma(x, k, k') = \nu(x)\delta(k' - k) + V_w(x, k' - k)$$

Here t_b is the time of the trajectory crossing point $x(t_b)$ with the device boundary, where the Wigner function values f_b are known.

The mean value $\langle A \rangle$ is defined by the inner product of A and f_w :

$$\langle A \rangle = \int dx \int dk f(x, k) A(x, k)$$

In this formulation $\langle A \rangle$ is obtained from the solution f_w , which can be evaluated by a backward MC method.

An alternative formulation leads to a forward MC method which directly evaluates the mean value $\langle A \rangle$. Considered is the conjugate equation of (2) with a free term A and solution g . The following relation can be established:

$$\int dx \int dk f(x, k) A(x, k) = \int dx \int dk f_b(x(t_b), k(t_b)) e^{-\int_{t_b}^0 \nu(x(y)) dy} g(x, k) \quad (3)$$

Equation (3) shows that the mean value of A is determined by the inner product of the free term of (2) with the solution g of the conjugate Wigner equation. The latter is obtained from (2) by applying the same steps used to derive the conjugate Boltzmann equation [2].

$$g(x, k) = \int_0^\infty dt \int dk' \Gamma(x, k', k) e^{-\int_0^t \nu(x(y)) dy} \theta_D(x) g(x(t), k'(t)) + A(x, k) \quad (4)$$

Here the indicator $\theta_D(x)$ of the device domain D takes values 1 if $x \in D$ and 0 otherwise. The trajectories are in a forward parameterization, $t > 0$. The last term in (3) is also expressed in a forward parameterization [2]. Then the space

integral gives rise to a time integral and a sum over the left and right boundaries x_l , x_r of the one-dimensional device:

$$\langle A \rangle = \sum_{x_b=x_l, x_r} \int_0^\infty dt_0 \int dk_i |v(k_i)| f_b(x_b, k_i) e^{-\int_0^{t_0} \nu(x(y)) dy} g(x(t_0), k(t_0)) \quad (5)$$

The index i denotes the subspace of wave vectors pointing inside the device.

The iterative expansion of g , obtained from (4), is replaced in (5) which leads to the series expansion:

$$\langle A \rangle = \sum_l \langle A \rangle_l \quad (6)$$

In this way the mean value of any physical quantity is determined by the velocity weighted boundary conditions and the consecutive iterations of the conjugate kernel K on the free term A . The expression for $\langle A \rangle_1$ is shown as an instructive example:

$$\langle A \rangle_1 = \sum_{x_b=x_l, x_r} \int dk_i \int_0^\infty dt_0 \int_0^\infty dt_1 \int dk_1 |v_\perp(k_i)| f_b(x_b, k_i) \theta_D(x_b(t_0)) \times \quad (7)$$

$$e^{-\int_0^{t_0} \nu(x_b(y)) dy} \Gamma(x_b(t_0), k_1, k_b(t_0)) e^{-\int_0^{t_1} \nu(x_1(y)) dy} A(x_1(t_1), k_1(t_1))$$

Due to θ_D only that part of a Newton's trajectory which belongs to D contributes to $\langle A \rangle_1$.

The series (6) is the main entity of the stochastic approach. Following the MC theory, numerical trajectories are constructed which evaluate the consecutive terms of the series. The numerical trajectories are constructed by an initial P and a transition PP probability density chosen for this purpose. P is used to choose the initial points of the numerical trajectories on the device boundary. The initial density P is adopted from the classical single-particle MC method [2], since $|v|f_b$ in (5) resembles the boundary term of the Boltzmann transport case.

The trajectories are built up by consecutive applications of the transition density PP . At each iteration i of the kernel a quantity called statistical weight w is multiplied by the weight factor $w_i = K/PP$. The random variable ξ_{A_i} whose realizations sample $\langle A \rangle_i$ is evaluated from the product of $wA(x_i, k_i)$. The random variable corresponding to $\langle A \rangle$ is given by $\xi_A = \sum_i \xi_{A_i}$.

The choice of the transition density plays an important role for the numerical properties of the MC algorithm. The kernel can be expressed as a product of a weight factor w_i and conditional probability densities which comprise the transition density PP :

$$K = PP_1 PP_2 \dots w_i$$

In the following two possible formulations are discussed. In the first case the numerical trajectories are associated with particles which evolve on parts of Newton's trajectories, linked by scattering processes. The kernel is interpreted

as a scattering operator. In the second case a weight decomposition is proposed. This is achieved by splitting the evolving trajectory in phase space. The kernel is interpreted as an operator which generates particles during the process of evolution.

3 Scattering Interpretation of the Kernel

The kernel of (4) is augmented by extra factors, introduced in a way to conserve the value of the integrand. They ensure the normalization of the conditional probability densities which are enclosed in curly brackets.

$$K = \int_0^\infty dt \int dk' \left\{ \nu(t) e^{-\int_0^t \nu(y) dy} \right\}_1 \theta_D(x(t)) \left(\left\{ \frac{\nu(t)}{\mu(t)} \right\}_2 \{ \delta(k(t) - k') \}_3 \right. \\ \left. + \left\{ \frac{\gamma(t)}{\mu(t)} \right\}_{2'} \left\{ \frac{|V_w(x(t), k(t) - k')|}{\gamma(t)} \right\}_{3'} \text{sign}(V_w) \right) \times \frac{\mu(t)}{\nu(t)}$$

The subscripts denote the order of application of these conditional probabilities. $\{\}_1$ generates a value of t , associated with a free flight time of a particle which drifts over a piece of Newton's trajectory between an initial state (x, k) at time 0, and the final state, $(x(t), k(t))$. The final state is used in the next probability density to select the value k' . The transition between $k(t)$ and k' is interpreted as scattering of the particle. $\{\}_2$ is the probability to use the first kernel component for selection of the after-scattering value of k' . Since $\mu = \gamma + \nu$, the second component is selected according $\{\}_{2'} = 1 - \{\}_2$. Thus k' is chosen either with the probability density $\{\}_3$ or with the probability density $\{\}_{3'}$. The normalization of the latter is ensured by the function $\gamma: \gamma(x(t)) = \int |V_w(x(t), k)| dk$. The after-scattering state $(k', x(t), t)$ is the initial state of a free flight for the next iteration of the kernel.

The weight factor $w_i = \pm \frac{\mu(t)}{\nu(t)}$, where the sign is given by the sign of V_w , multiplies the weight w accumulated by the trajectory. It can be shown that the mean accumulated weight is evaluated by $\bar{w} = \pm e^{\gamma T}$, where T is the dwelling time of the particle in the device. Since the weight \bar{w} does not depend on ν , the latter can be chosen according to some criteria of convenience. A choice $\nu = \gamma/2$ gives rise to a weight factor $w_i = \pm 3$.

For typical nanoscale devices $\gamma \simeq 10^{15} s^{-1}$, $T > 10^{-12} s$ so that \bar{w} and thus the realizations of ξ_A which sample $\langle A \rangle$ become huge positive and negative numbers. The sample variance is orders of magnitude larger than the sample mean, where positive and negative terms cancel each other. This problem, known as the sign problem, exists also in stochastic approaches to alternative formulations of quantum mechanics. For instance MC evaluations of Feynman path integrals demonstrate an exponential growth of the variance with the evolution time [3].

Due to the sign problem, the application of the derived method is restricted to single barrier tunneling and small barrier heights.

4 Weight Decomposition Approach

The following modification of the method is proposed to overcome the problem of the growing variance. The idea is to decompose the weight into a part which continues with the trajectory and a part which is left for future processing. The antisymmetric function V_w is decomposed into two positive functions: $V_w = V_w^+ - V_w^-$. With these functions ν can be expressed as $\nu = \gamma/2 = \int V^\pm dk$. The kernel is written as:

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

The three kernel components simultaneously create three after-scattering states. Each state gives rise of a trajectory which must be simulated until it leaves the simulation domain.

Two of the trajectories carry the weight of the trajectory before the scattering event, the third one changes its sign. Since the initial weight at the boundary is 1, the absolute value of the weight of each trajectory remains 1. 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. Additionally a positive and a negative particle are created by V_w^\pm . A phase space grid $(n\Delta_x, m\Delta_k)$, $n = 1, \dots, N$, $m = -M, \dots, M$ is introduced, where all three particles are stored. The simulated trajectory continues from the grid cell with the highest number of stored particles. It is selected among all k cells with a position index $m = \text{int}(x(t)/\Delta_x)$ where $x(t)$ is the location of the scattering event.

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 active cancellation reduces the simulation time leading to a variance reduction.

If phonon scattering is included the picture remains similar. The free flights are additionally interrupted by the phonon scattering events, which as in the classical case, only change the particle momentum.

5 Results and Discussions

The method has been applied for simulation of a resonant tunneling diode. A double barrier structure from the literature [4] is used as a benchmark device. Physical parameters of GaAs with a uniform 0.067 effective mass and a temperature $T = 77\text{K}$ assumed. The potential drop is linear across the central device, the barriers have a thickness of 2.825nm and a height 0.27eV, the well is 4.52nm wide. The device is shown schematically in Fig.1.

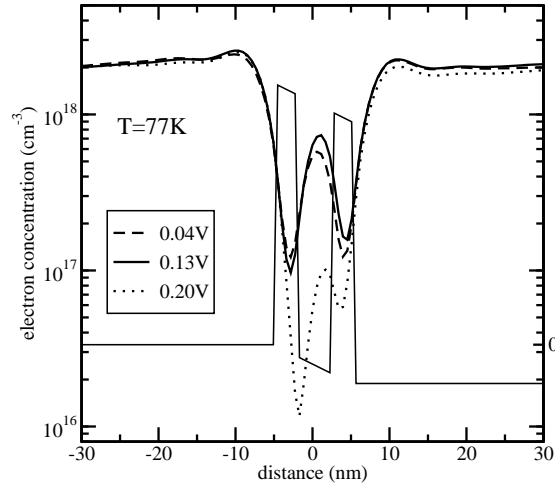


Fig. 1. Electron concentration distribution in the central part of the resonant tunneling diode for three different bias points.

Numerical results for the electron concentration, $A_n(x_0) = \delta(x - x_0)$, are presented for three different values of the applied bias. The values correspond to bias points near equilibrium, and the peak and valley current of the current-voltage characteristics. The accumulation of electrons in the quantum well at the resonance bias 0.13V respectively is well demonstrated. The physical quantity which gives the current is $A_J = qv(k)/L_D$ where q is the electron charge and L_D is the length of the device. The current-voltage characteristics is shown on Fig.2. The peak of the current at 0.13V is followed by a negative differential mobility region, which is a typical feature of the resonant tunneling diodes. The current-voltage characteristics are in good quantitative agreement with the results obtained by other methods [5].

Fig.3. shows the current for the chosen three bias points as a function of the number of scattering events. The latter quantity is an empirical measure of the elapsed simulation time which is independent of the computer platform. 10^{10} scattering events correspond to a 24 hours simulation time on a 1GHz CPU. The three curves illustrate the variations of the $\langle A_J \rangle$ during the simulation. Above $8 \cdot 10^9$ scattering events the variance of the corresponding values becomes negligible.

6 Conclusions

The proposed weight decomposition method significantly improves the numerical properties of the stochastic approach to the Wigner transport equation. Annihilation of positive and negative weights reduces the computational effort of the task. The method has proven suitable for the simulation of nanoelectronic devices.

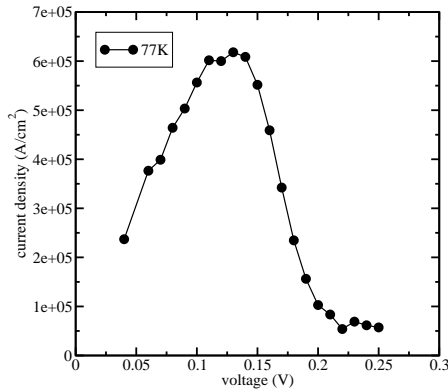


Fig. 2. Current-voltage characteristics of the resonant tunneling diode. The peak is at resonance bias 0.13V.

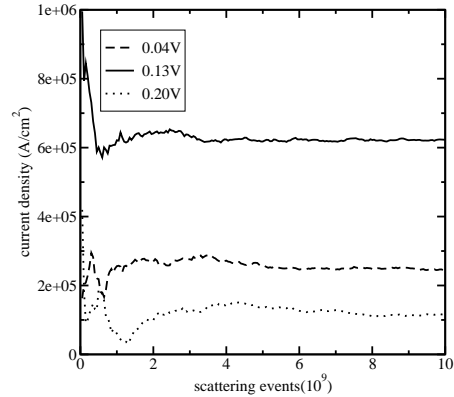


Fig. 3. Electron current for the chosen bias points as a function of the number of scattering events.

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