A Stable Backward Monte Carlo Method for the Solution of the Boltzmann Equation

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Abstract. Backward Monte Carlo methods for solving the Boltzmann equation are investigated. A stable estimator is proposed since a previously published estimator was found to be numerically instable. The principle of detailed balance, which is obeyed by state transitions of a physical system and ensures existence of a stable equilibrium solution, is violated by the transition probability of the unstable method, and is satisfied by construction with the proposed backward transition probability.

1 Introduction

For the numerical study of non-equilibrium charge carrier transport in semiconductors the Monte Carlo (MC) method has found wide spread application. In particular the physically transparent forward MC method is commonly employed, which evaluates functionals of the distribution function. The more abstract backward MC method, however, has found virtually no application in semi-classical transport calculations. This method follows the particle history back in time and allows the distribution function to be evaluated at given points with desired accuracy. The method is particularly appealing in cases where the solution is sought in sparsely populated regions of the phase space only.

In the field of semi-classical transport the backward MC method has been proposed end of the 1980's [1] [2]. One of the roots of this method is in quantum transport [3], a field where also various applications are reported [4][5].

2 Boltzmann Equation

On a semi-classical level the transport of charge carriers in semiconductors is described by the Boltzmann Equation (BE). For the time- and position-dependent transport problem the BE reads

$$\left(\frac{\partial}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} + \mathbf{F}(\mathbf{r},t) \cdot \nabla_{\mathbf{k}}\right) f(\mathbf{k},\mathbf{r},t) = Q[f](\mathbf{k},\mathbf{r},t)\,, \qquad \mathbf{r} \in D\,. \tag{1}$$

This equation is posed in the simulation domain D and has to be supplemented by boundary and initial conditions. The distribution function is commonly normalized as $\int_D \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{k}\, f(\mathbf{k},\mathbf{r},t) = 4\pi^3 N_D(t)$, with N_D denoting the number of carriers contained in the semiconductor domain of volume V_D.

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In (1) the carrier's group velocity $\mathbf{v}$ is related to the band energy $\epsilon(\mathbf{k})$ by $\mathbf{v} = \hbar^{-1}\nabla_k\epsilon(\mathbf{k})$. The force field $\mathbf{F}$ takes into account electric and magnetic fields. If only an electric field $\mathbf{E}$ is present, the force field is given by $\mathbf{F} = q\mathbf{E}/\hbar$, where q is the charge of the carrier. The scattering operator $Q = Q_g - Q_l$ consists of a gain and a loss term, respectively. If many-body effects such as carrier-carrier scattering and degeneracy are neglected, the scattering operator will be linear, an assumption that is crucial for the presented approach. The two components of Q are

$$Q_g[f](\mathbf{k},\mathbf{r},t) = \int f(\mathbf{k}',\mathbf{r},t)S(\mathbf{k}',\mathbf{k},\mathbf{r},t)\,\mathrm{d}\mathbf{k}'\,, \tag{2}$$

$$Q_l[f](\mathbf{k},\mathbf{r},t) = \lambda(\mathbf{k},\mathbf{r},t)f(\mathbf{k},\mathbf{r},t)\,, \tag{3}$$

with $\lambda(\mathbf{k},\mathbf{r},t) = \int S(\mathbf{k},\mathbf{k}',\mathbf{r},t)\,\mathrm{d}\mathbf{k}'$ denoting the total scattering rate.

2.1 Integral Form of the Boltzmann Equation

The BE is now transformed to integral form by a formal integration over a phase space trajectory.

$$\mathbf{K}(\tau) = \mathbf{k}_0 + \int_{t_0}^{\tau} \mathbf{F}\left(\mathbf{R}(y),y\right)\mathrm{d}y\,, \qquad \mathbf{R}(\tau) = \mathbf{r}_0 + \int_{t_0}^{\tau} \mathbf{v}\left(\mathbf{K}(y)\right)\mathrm{d}y \tag{4}$$

This trajectory has the initial condition $\mathbf{K}(t_0) = \mathbf{k}_0$ and $\mathbf{R}(t_0) = \mathbf{r}_0$ and solves the equations of motion in phase space, given by Newton's law and the carrier's group velocity. The following integral form of the BE is obtained [6]:

$$\begin{aligned} f(\mathbf{k},\mathbf{r},t) = \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{k}'\ f(\mathbf{k}',\mathbf{R}(t'),t') \\ \times S(\mathbf{k}',\mathbf{K}(t'),\mathbf{R}(t'),t')\exp\!\left(-\int_{t'}^{t}\lambda(\mathbf{K}(y),\mathbf{R}(y),y)\mathrm{d}y\right) \\ + f_i(\mathbf{K}(0),\mathbf{R}(0))\exp\!\left(-\int_0^t \lambda(\mathbf{K}(y),\mathbf{R}(y),y)\mathrm{d}y\right) \end{aligned} \tag{5}$$

This equation represents the generalized form of Chamber's path integral [7]. The source term contains f_i, a given initial distribution. Augmenting the kernel by a delta-function of the real space coordinate and a unit step function of the time coordinate allows transformation of (5) into an integral equation of the second kind:

$$\begin{aligned} K(\mathbf{k},\mathbf{r},t,\mathbf{k}',\mathbf{r}',t') = S(\mathbf{k}',\mathbf{K}(t'),\mathbf{r}',t')\exp\!\left(-\int_{t'}^{t}\lambda(\mathbf{K}(y),\mathbf{R}(y),y)\mathrm{d}y\right) \\ \times \delta(\mathbf{r}' - \mathbf{R}(t'))H(t-t') \end{aligned} \tag{6}$$

$$f(\mathbf{k},\mathbf{r},t) = \int_0^\infty \mathrm{d}t' \int \mathrm{d}\mathbf{k}' \int \mathrm{d}\mathbf{r}'\ K(\mathbf{k},\mathbf{r},t,\mathbf{k}',\mathbf{r}',t')f(\mathbf{k}',\mathbf{r}',t') + f_0(\mathbf{k},\mathbf{r},t) \quad (7)$$

2.2 The Neumann Series

Substituting (5) recursively into itself gives the Neumann series expansion of the solution f in a given phase space point $\mathbf{k},\mathbf{r}$ at time t.

$$f(\mathbf{k},\mathbf{r},t) = f^{(0)} + f^{(1)} + f^{(2)} + \ldots \quad (8)$$

Convergence of the series has been proven in [8]. MC algorithms for solving an integral equation can be derived by evaluating the terms of the iteration series by MC integration. Each term of the iteration series has the same structure. In the term of order n the integral operator is applied n-times to the source term f_0. As an example we write the term of second order explicitly.

$$\begin{aligned} f^{(2)}(\mathbf{k},\mathbf{r},t) = \int_0^t \mathrm{d}t_1 \int \mathrm{d}\mathbf{k}_1 \int_0^{t_1} \mathrm{d}t_2 \int \mathrm{d}\mathbf{k}_2 \\ f_i(\mathbf{K}_2(0),\mathbf{R}_2(0)) \exp\Big(-\int_0^{t_2} \lambda(\mathbf{K}_2(y),\mathbf{R}_2(y),y)\mathrm{d}y\Big) \\ \times S(\mathbf{k}_2,\mathbf{K}_1(t_2),\mathbf{R}_1(t_2),t_2) \exp\Big(-\int_{t_2}^{t_1} \lambda(\mathbf{K}_1(y),\mathbf{R}_1(y),y)\mathrm{d}y\Big) \\ \times S(\mathbf{k}_1,\mathbf{K}_0(t_1),\mathbf{R}_0(t_1),t_1) \exp\Big(-\int_{t_1}^{t} \lambda(\mathbf{K}_0(y),\mathbf{R}_0(y),y)\mathrm{d}y\Big) \quad (9) \end{aligned}$$

Final conditions for the $\mathbf{k}$-space trajectories are given first by $\mathbf{K}_0(t) = \mathbf{k}$ and then by the before-scattering states $\mathbf{K}_1(t_1) = \mathbf{k}_1$ and $\mathbf{K}_2(t_2) = \mathbf{k}_2$ (See Fig. 1). The real space trajectory ends at final time t in the given point $\mathbf{R}_0(t) = \mathbf{r}$ and is continuous at the time of scattering: $\mathbf{R}_1(t_1) = \mathbf{R}_0(t_1)$, $\mathbf{R}_2(t_2) = \mathbf{R}_1(t_2)$.

The iteration term (9) describes the contribution of all second order trajectories to the solution. On such a trajectory a particle undergoes two scattering events during propagating from time 0 to t and is found on its third free-flight path at time t.

3 Backward Monte Carlo Methods

Backward MC algorithms for the solution of the Boltzmann equation have been proposed in [1] [2]. Given an integral equation $f(x) = \int K(x,x')f(x')dx' + f_0(x)$, the backward estimator of the n-th iteration term is constructed as

$$\nu^{(n)}(x_0) = \frac{K(x_0,x_1)}{p(x_0,x_1)} \ldots \frac{K(x_{n-1},x_n)}{p(x_{n-1},x_n)} f_0(x_n) \quad (10)$$

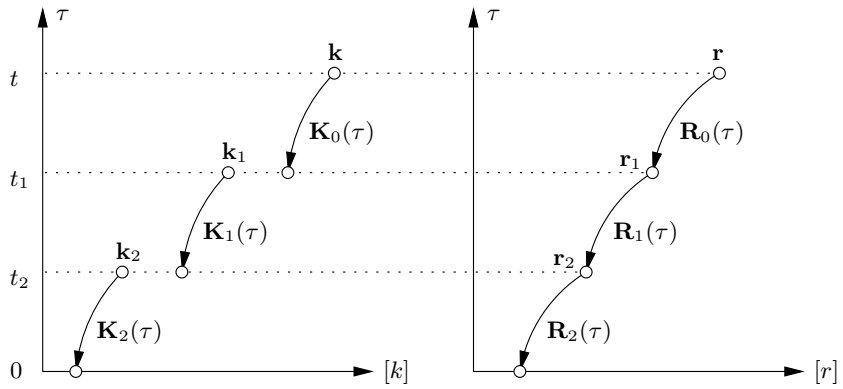

Fig. 1. Sketch of a backward trajectory starting at time t and reaching time 0 after three free flights. The symbols used in (9) are shown.

where p denotes a transition probability density. The set of points $x_0, x_1, \ldots x_n$ is referred to as a numerical trajectory. After generation of N numerical trajectories the n-th iteration term is estimated by the sample mean

$$f^{(n)}(x_0) \simeq \frac{1}{N} \sum_{s=1}^{N} \nu_s^{(n)}(x_0) \tag{11}$$

For the Boltzmann equation considered here the variable x denotes $x = (\mathbf{k}, \mathbf{r}, t)$. In this work we discuss two specific choices of the transition probability p.

3.1 Probability Density Functions

The components of the kernel (6) are used to construct probability density functions (pdf). From the scattering rate S one can define a pdf of the after-scattering states $\mathbf{k}_a$,

$$p_k(\mathbf{k}_a, \mathbf{k}_b) = \frac{S(\mathbf{k}_b, \mathbf{k}_a)}{\lambda(\mathbf{k}_b)}\,, \tag{12}$$

with the total scattering rate $\lambda(\mathbf{k}_b) = \int S(\mathbf{k}_b, \mathbf{k}_a)\,\mathrm{d}\mathbf{k}_a$ as a normalization factor. Conversely, the pdf of the before-scattering states $\mathbf{k}_b$ is defined as

$$p_k^*(\mathbf{k}_b, \mathbf{k}_a) = \frac{S(\mathbf{k}_b, \mathbf{k}_a)}{\lambda^*(\mathbf{k}_a)}. \tag{13}$$

The normalization factor is given by the backward scattering rate, $\lambda^*(\mathbf{k}_a) = \int S(\mathbf{k}_b, \mathbf{k}_a)\,\mathrm{d}\mathbf{k}_b$.

The pdf of the backward free-flight time t_i is given by

$$p_t(t_i, t_j, \mathbf{k}_j) = \lambda(\mathbf{K}_j(t_i)) \exp\left(- \int_{t_i}^{t_j} \lambda(\mathbf{K}_j(y))\,\mathrm{d}y \right), \tag{14}$$

and satisfies the normalization $\int_{-\infty}^{t_j} p_t(t_i, t_j)\mathrm{d}t_i = 1$. Final condition of the trajectory is $\mathbf{K}_j(t_j) = \mathbf{k}_j$.

3.2 The Source Term

In case of the Boltzmann equation the source term is treated in a specific way.

$$f_0(\mathbf{k}, \mathbf{r}, t) = f_i(\mathbf{K}(0), \mathbf{R}(0)) \exp\left(- \int_0^t \lambda(\mathbf{K}(y))\mathrm{d}y \right) \tag{15}$$

The exponential function represents the probability that a particle moves without scattering from 0 to t. This probability is now used as an acceptance probability. The probability is expressed as an integral over the respective pdf, given by (14).

$$\exp\left(- \int_0^t \lambda(\mathbf{K}(y))\mathrm{d}y \right) = \int_{-\infty}^0 p_t(\tau, t, \mathbf{k})\, \mathrm{d}\tau \tag{16}$$

The acceptance probability is checked as follows. For a particle in state $\mathbf{k}$ at time t the backward free flight time τ is generated from p_t. If τ is negative, the estimator is nonzero, otherwise, the estimator evaluates to zero. To obtain a nonzero estimator of the n-th iteration term all the generated times $t_1, \ldots t_n$ must be positive, whereas the next time generated, t_{n+1}, must be negative. For a trajectory of order n all other estimators of order $m \neq n$ evaluate to zero. In this way an estimator for the distribution function f is obtained as

$$f(x_0) = \sum_{n=0}^{\infty} f^{(n)}(x_0) \simeq \frac{1}{N} \sum_{s=1}^{N} \nu_s^{(n(s))}(x_0) \tag{17}$$

Here $n(s)$ denotes the order of the s-th numerical trajectory. The estimator is now defined as

$$\nu^{(n)}(x_0) = \frac{K(x_0, x_1)}{p(x_0, x_1)} \ldots \frac{K(x_{n-1}, x_n)}{p(x_{n-1}, x_n)} f_i(\mathbf{K}_n(0), \mathbf{R}_n(0)) \,. \tag{18}$$

Note that this estimator samples the initial distribution f_i, whereas in (10) the source term f_0 is sampled.

3.3 Transition Probability Densities

In the original work [2] $S(\mathbf{k}_b, \mathbf{k}_a)$ is interpreted as the unnormalized distribution of the before-scattering states $\mathbf{k}_b$, and consequently the normalized pdf (13) is employed. Using the transition density

$$P(\mathbf{k}', \mathbf{r}', t'; \mathbf{k}, \mathbf{r}, t) = p_k^*(\mathbf{k}', \mathbf{K}(t'))\; p_t(t', t, \mathbf{k})\; \delta(\mathbf{r}' - \mathbf{R}(t'))\; H(t - t') \tag{19}$$

the estimator (18) becomes

$$\nu^{(n)}(\mathbf{k},\mathbf{r},t) = \frac{\lambda^*(\mathbf{K}_0(t_1))}{\lambda(\mathbf{K}_0(t_1))} \ldots \frac{\lambda^*(\mathbf{K}_{n-1}(t_n))}{\lambda(\mathbf{K}_{n-1}(t_n))} f_i(\mathbf{K}_n(0),\mathbf{R}_n(0))\,. \tag{20}$$

Although the MC algorithm based on the estimator (20) is consistently derived from the integral form of the BE, computer experiments reveal a stability problem. The particle energy becomes very large when the trajectory is followed backward in time. The initial distribution takes on very small values at high energies, such that many realizations of the estimator will be very small. With small probability, the particle energy will stay low, where the initial distribution is large. These rare events give large contributions to the estimator, resulting in a large variance. The computer experiments show that the variance increases rapidly with time. However, for a given time t the variance of the estimator is finite.

The time evolution of the particle energy can be understood from a property of the scattering rate known as the principle of detailed balance. This property ensures that in any system particles scatter preferably to lower energies. If for trajectory construction the backward transition rate (13) is employed, the principle of detailed balance is inverted in the simulation and scattering to higher energies is preferred.

The principle of detailed balance is reflected by the following symmetry property of the scattering rate:

$$S(\mathbf{k}_i,\mathbf{k}_j) = S(\mathbf{k}_j,\mathbf{k}_i)\exp(\beta(\epsilon(\mathbf{k}_i)-\epsilon(\mathbf{k}_j)))\,, \tag{21}$$

where $\beta = 1/(k_B T)$ and $\epsilon(\mathbf{k})$ denotes the carrier energy. The scattering rate of carriers in a semiconductor contains contributions from various scattering sources and is thus represented by the sum of the corresponding rates.

$$S(\mathbf{k}_i,\mathbf{k}_j) = \sum_l S_l(\mathbf{k}_i,\mathbf{k}_j) \tag{22}$$

The total scattering rate is given by $\lambda(\mathbf{k}) = \sum_l \lambda_l(\mathbf{k})$. A scattering mechanism is either elastic, that is $\epsilon(\mathbf{k}_i) = \epsilon(\mathbf{k}_j)$, or inelastic, $\epsilon(\mathbf{k}_i) \neq \epsilon(\mathbf{k}_j)$. For each inelastic process the sum contains two entries, where one entry describes the inverse process of the other. In the case of phonon scattering these partial processes are caused by absorption and emission of a phonon, respectively. The scattering rates are commonly derived from Fermi's golden rule,

$$S_{\mathrm{ab}}(\mathbf{k}_j,\mathbf{k}_i) = \frac{2\pi}{\hbar}|M|^2\, N_q\, \delta(\epsilon(\mathbf{k}_j)+\hbar\omega-\epsilon(\mathbf{k}_i))\,, \tag{23}$$

$$S_{\mathrm{em}}(\mathbf{k}_j,\mathbf{k}_i) = \frac{2\pi}{\hbar}|M|^2\, (N_q+1)\, \delta(\epsilon(\mathbf{k}_j)-\hbar\omega-\epsilon(\mathbf{k}_i))\,, \tag{24}$$

where M denotes the interaction matrix element, N_q the Bose-Einstein statistics and $\hbar\omega$ the phonon energy. Interchanging $\mathbf{k}_j$ and $\mathbf{k}_i$ and taking into account the relation $(N_q+1) = N_q \exp(\beta\hbar\omega)$ gives the following symmetry property

$$S_{\mathrm{ab}}(\mathbf{k}_i,\mathbf{k}_j) = S_{\mathrm{em}}(\mathbf{k}_j,\mathbf{k}_i)\exp(-\beta\hbar\omega) \tag{25}$$

$$S_{\mathrm{em}}(\mathbf{k}_i,\mathbf{k}_j) = S_{\mathrm{ab}}(\mathbf{k}_j,\mathbf{k}_i)\exp(\beta\hbar\omega) \tag{26}$$

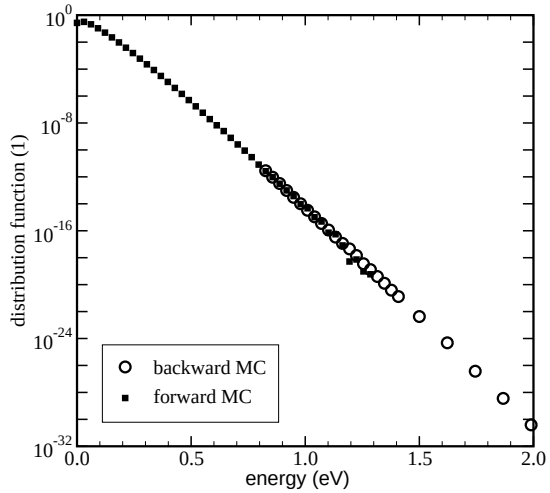

Fig. 2. Electron energy distribution functions obtained by backward and forward MC algorithms.

This formulation shows that the absorption rate in backward direction is proportional to the emission rate in forward direction, and vice versa. From (25) and (26) it follows then that $S = S_{\mathrm{ab}} + S_{\mathrm{em}}$ has the symmetry property (21).

The stability problem can be solved using the forward scattering rate also for the construction of the backward trajectory and changing the estimator accordingly. In the transition density the forward pdf (12) is employed.

$$P(\mathbf{k}', \mathbf{r}', t'; \mathbf{k}, \mathbf{r}, t) = p_k(\mathbf{k}', \mathbf{K}(t'))\; p_t(t', t, \mathbf{k})\; \delta(\mathbf{r}' - \mathbf{R}(t'))\; H(t - t') \tag{27}$$

The estimator (18) becomes

$$\nu^{(n)}(\mathbf{k}, \mathbf{r}, t) = \exp(\beta \Delta\epsilon_1) \ldots \exp(\beta \Delta\epsilon_n) f_i(\mathbf{K}_n(0), \mathbf{R}_n(0))\,. \tag{28}$$

The $\Delta\epsilon_l$ denote the difference in particle energy introduced by the l-th scattering event.

4 Results

MC calculations of electron transport in silicon have been performed. Conditions assumed are $E = 10\,\mathrm{kV/cm}$ and $t = 3\,\mathrm{ps}$ at $T = 300\,\mathrm{K}$. Fig. 2 compares the electron energy distributions as computed by the backward MC method and a forward MC method employing statistical enhancement through event biasing. As initial distribution a Maxwellian distribution is assumed. The backward method is used to evaluate the energy distribution at discrete points above 800 meV. The statistical uncertainty of the result is controlled by the number of numerical trajectories starting from each point. In the simulation 10^7 backward trajectories are computed for each point. The backward method resolves

the high energy tail with high precision as shown in Fig 2. The depicted range of 30 decades is out of reach for the here considered variant of the forward MC method.

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