NEW HIGHLY EFFICIENT METHOD FOR THE ANALYSIS OF CORRELATION FUNCTIONS BASED ON A SPHERICAL HARMONICS EXPANSION OF THE BOLTZMANN TRANSPORT EQUATION'S GREEN'S FUNCTION

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Abstract

A new method for a more efficient calculation of correlation functions for stationary and Markovian processes described by the Boltzmann transport equation is given. The conditional probability representing the dynamics of the system is expanded with spherical harmonics. In the resulting discrete system the evaluation of the correlation functions involves only matrix-vector operations which can be performed very efficiently. The results for different electric and magnetic fields agree very well with standard Monte Carlo results and the cpu time usage is about one order of magnitude smaller.

I. INTRODUCTION

Macroscopic balance equations derived from the Boltzmann transport equation (BTE) rely on transport coefficients which in part can not be directly determined from experiment [1,2]. A powerful tool to obtain these coefficients is the correlation function analysis of certain microscopic quantities by Monte Carlo (MC) simulations of stationary homogeneous bulk systems [3,4]. The diffusion constant for example can be obtained from the time integral over the velocity autocorrelation function [5]. Since MC simulations are cpu time intensive and the correlation functions are needed for various doping concentrations as well as electric and magnetic field conditions more efficient methods are required.

II. DESCRIPTION OF THE METHOD

Correlation functions are calculated with the joint distribution function $f(\vec{k},t,\vec{k}_0,t_0)$ which can be expressed by the conditional probability $P(\vec{k},t|\vec{k}_0,t_0)$ times the normalized distribution function $f(\vec{k}_0,t_0)$. $P(\vec{k},t|\vec{k}_0,t_0)$ describes the dynamics of the system and $f(\vec{k}_0,t_0)$ the state of the particle ensemble. The correlation function of the microscopic quantities $X(\vec{k})$ and $Y(\vec{k})$ is given by:

$$< X(t)Y(t_0) >= \frac{\Omega^2}{(2\pi)^6} \int d^3k \int d^3k_0 X(\vec{k}) P(\vec{k},t|\vec{k}_0,t_0) f(\vec{k}_0,t_0) Y(\vec{k}_0), \tag{1}$$

where Ω denotes the system volume. $P(\vec{k},t|\vec{k}_0,t_0)$ is the conditional probability (CP) that a particle started at time t_0 with wavevector $\vec{k}_0$ appears at time t with wavevector $\vec{k}$. Since our MC model includes only one particle scattering processes the CP is also the Green's function of the corresponding BTE. We investigate only stationary processes with constant electric and magnetic fields. Thus $P(\vec{k},t|\vec{k}_0,t_0)$ equals $P(\vec{k},t-t_0|\vec{k}_0,0)$. Since the process is Markovian the CP for the

discrete times $(i\delta t, 0)$ with $i \geq 1$ can be calculated as the i-times product of the CP for the time step δt utilizing the Chapman-Kolmogorov equation [6]:

$$P(\vec{k}, i\delta t|\vec{k}_0, 0) = \left[\frac{\Omega}{(2\pi)^3}\right]^{i-1} \int d^3k_{i-1} \cdots \int d^3k_1 P(\vec{k}, \delta t|\vec{k}_{i-1}, 0) \cdots P(\vec{k}_1, \delta t|\vec{k}_0, 0). \tag{2}$$

In our new approach the CP is discretized by a spherical harmonics expansion in the solid angles [7] and an equidistant discretization of the absolute values of $\vec{k}$ and $\vec{k}_0$. The spherical harmonics expansion is especially well suited for this problem because the investigated microscopic quantities involve only spherical harmonics up to the second order. The discrete CP has the form of a matrix and equation (2) reads:

$$\underline{\underline{P}}(i\delta t|0) = \left[\underline{\underline{P}}(\delta t|0)\right]^i. \tag{3}$$

The correlation function is now calculated by multiplying the CP matrix from the left and right with the vectors of $X(\vec{k})$ and $Z(\vec{k}_0) = f(\vec{k}_0, 0)Y(\vec{k}_0)$ as resulting from the discretization:

$$< X(i\delta t)Y(0) >= \underline{X}\left[\underline{\underline{P}}(\delta t|0)\right]^i \underline{Z}. \tag{4}$$

The direct calculation of the i-th power of the CP matrix being very cpu time intensive can be avoided by an iterative calculation of $\left[\underline{\underline{P}}(\delta t|0)\right]^i \underline{Z}$. In the first time step ($i = 1$) the product of the CP matrix and the vector on the right-hand side is performed. The result of this operation is again a vector. For the next time step this vector is multiplied with the CP matrix once more. Thus only matrix-vector operations have to be performed which are much faster than matrix-matrix operations.

The CP can be obtained from the BTE directly with a perturbation series expansion [9,10]. This formulation is equivalent to the MC method but direct numerical evaluation is very tedious and the MC method is normally preferred. But for zero electric field and a scattering rate $S(\epsilon)$ which depends only on energy ϵ the CP has a simple form. Truncating the perturbation series expansion after the second term and including particle number conservation results in the following expression for the CP (arbitrary magnetic field):

$$\begin{aligned} P(\vec{k}, t|\vec{k}_0, 0) = &\exp[-S(\epsilon(\vec{k}))t]\delta\left(\vec{k} - \vec{k}_0 + \frac{e}{\hbar}\int_0^t d\tau \vec{v}(\tau) \times \vec{B}\right) \\ &+ \frac{\Omega}{(2\pi)^3}\int_0^t dt_1 \exp[-S(\epsilon(\vec{k}))(t - t_1)]S\left(\vec{k} + \frac{e}{\hbar}\int_{t_1}^t d\tau \vec{v}(\tau) \times \vec{B}\middle|\vec{k}_0 - \frac{e}{\hbar}\int_0^{t_1} d\tau \vec{v}(\tau) \times \vec{B}\right), \end{aligned} \tag{5}$$

where $S(\vec{k}|\vec{k}_0)$ denotes the transition rate and $\vec{v}$ the particle velocity. Since only one scattering event has been considered in eq. (5), the time t must be chosen sufficiently small compared with the scattering rate. The extension to multiple scattering events for longer times t is straight forward. With eq. (5) the discrete formulation of the CP can be calculated analytically and the setup time is reduced by three orders of magnitude in relation to an evaluation of the CP by the MC method.

In the case of arbitrary electric and magnetic fields the MC method is used, because the discretization of the equation corresponding to eq. (5) for nonzero electric field is very difficult. The discrete CP is evaluated by simulating particles with different initial wavevectors k_0, θ_0, φ_0 (spherical coordinates) for the time δt using a MC method [8]. The initial absolute values of the wavevectors are given by the discretization. The initial angles of the particles θ_0 and φ_0 are

chosen from an equidistant grid between 0 and π and 0 and 2π, respectively†. Since the final absolute values of the particles wavevectors do not match the values given by the discretization, they are mapped onto the grid by linear interpolation. A coefficient of the discrete CP is obtained by summing over all particles with the appropriate k, k_0 multiplied with the proper spherical harmonics of the initial and final state. If the electric and magnetic field are parallel to the polar axsis, the CP has the following symmetry property:

$$P(k,\theta,\varphi,i\delta t|k_0,\theta_0,\varphi_0,0) = P(k,\theta,\varphi-\varphi_0,i\delta t|k_0,\theta_0,0,0), \tag{6}$$

due to the employed Si-model [8]. This effect can be exploited to reduce the variance of the MC method for the setup of the CP by integrating analytically over the angle φ_0 in the spherical harmonics expansion. The setup procedures and the calculation of the correlation functions are well suited for parallelization.

III. RESULTS

The CP matrix has been discretized with about 50 points for the absolute value of $\vec{k}$ and an expansion up to the fourth order involving 25 spherical harmonics. Thus the dimension of the CP matrix is about 1250. 13 microscopic quantities for X and 13 different microscopic quantities for Y have been investigated resulting in 169 auto- and cross-correlation functions. In Table I execution times are listed for the new method and a MC simulation on a 4D 480 SGI computer. The new method is at least eight times faster than the MC simulation. Figure 1 shows stationary expectation values calculated with the new method and MC simulation as a function of the applied field for undoped silicon at room temperature [8] and good agreement is found.

TABLE I. Comparison of execution times for the setup of a CP matrix based on a 4th order expansion, calculation of correlation functions, total time and standard MC simulation for three electric fields.

field	Setup	cor. fun.	total	MC
(kV/cm)	(s)	(s)	(s)	(s)
1	1131	200	1331	48568
10	1179	465	1644	12520
100	858	463	1321	13116

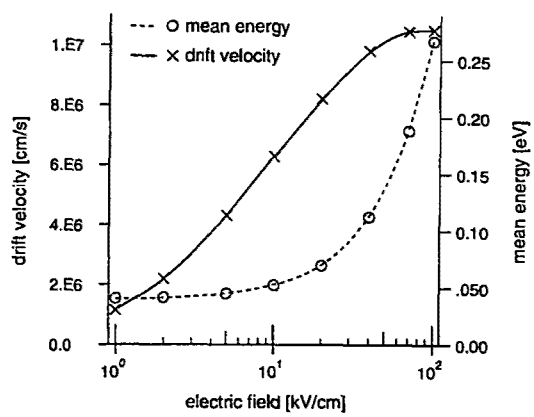

FIG. 1. Stationary expectation values for drift velocity and mean energy with the new method (lines) and MC simulation (symbols).

In Fig. 2 longitudinal and transversal velocity autocorrelation functions are shown and no difference is found between MC simulation and the new method based on an expansion up to the 3rd and 4th order. Results for other correlation functions involving 2nd order spherical harmonics (velocity is 1st order) showed differences between the expansion up to 3rd or 4th order. Therefore the 4th

† The particle weight is modulated in θ_0-direction satisfying the Simpson rule and in φ_0-direction satisfying a trapezoidal rule to ensure sufficient orthogonality of the spherical harmonics in the process of numerical integration with the MC method.

order expansion was used for which the results agreed very well with MC data. In the case of weak correlation the new method is superior to the MC simulation because of the high statistical noise of the MC method.

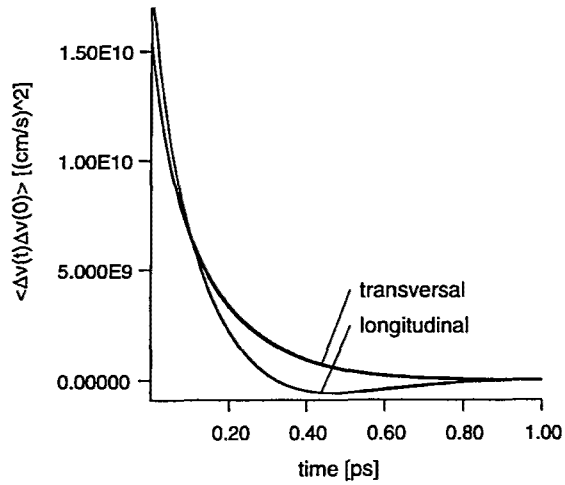

FIG. 2. Autocorrelation functions for longitudinal and transversal velocity calculated with MC and CP matrices based on 3rd and 4th order expansions for $10kV/cm$ $(300K)$.

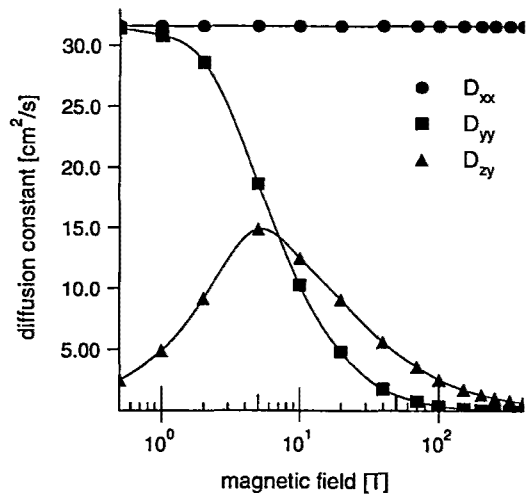

FIG. 3. Elements of diffusion constant tensor (D_{xx}, D_{yy}, D_{zy}) for a magnetic field in x-direction and zero electric field $(300K)$.

In Fig. 3 elements of the diffusion constant tensor for zero electric field are shown as a function of the magnetic field up to $400T$ neglecting quantization effects. The magnetic field lies parallel to the x-axsis which is the polar axsis. The setup time of the CPs was below three seconds using the analytical method mentioned above.

IV. CONCLUSION

A new method for the calculation of correlation functions has been developed which is much faster than the standard MC simulation and less noisy. It agrees very well with MC results for different electric and magnetic fields. The method is well suited for parallelization.

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