Computation of the Electron Distribution Function Employing the Theory of Stochastic Differential Equations

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Abstract

In a previous paper, it has been suggested to employ the theory of stochastic differential equations (SDE) for the modeling of electron transport in semiconductors. It was shown that the differential equations which describe electron transport in semiconductors, and which are used in Monte Carlo simulations, can be interpreted as stochastic differential equations driven by inhomogeneous randomly weighted Poisson processes. Based on this connection, the theory of SDE was employed to demonstrate that the forward Kolmogorov-Feller equation which characterizes the transition probability density function of this random process can be integrated over the initial conditions to obtain the linear Boltzmann transport equation.

In the paper, we will expand on our previous results and present a transport model which leads to the efficient numerical computation of the electron distribution function. The model is based on an approximation of the collision integral in the Boltzmann transport equation by differential operators. As a result of this approximation, the electron distribution is characterized by a second order partial differential equation in momentum space. It turns out that the coefficients of this partial differential equation are the first and second order moments of the scattering transition rate. We will present the derivation of these terms and also present some preliminary results on the computation of the electron distribution function based on this model. Furthermore, by comparing these results with Monte Carlo simulations, we will explore the limits of applicability of this model.

I. Background:

Previously, it has been suggested that the theory of stochastic differential equations can be employed to model current transport in semiconductors, (see Ref. [1]). In this section, we will review some of the previous results and establish a connection between

semi-classical transport theory and the theory of stochastic differential equations. According to semi-classical transport theory, an electron in a semiconductor drifts under the influence of a macroscopic electric field and experiences occasional random jumps in its momentum due to different scattering mechanisms in the crystal, such as, acoustic and optical phonons, ionized impurities, etc. This motion of an electron can be described by the following stochastic differential equation:

$$\frac{d\vec{x}}{dt} = \vec{v}(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k}) \tag{1}$$

$$\hbar\frac{d\vec{k}}{dt} = -q\vec{E} + \vec{F}_r \tag{2}$$

$$\vec{F}_r = \sum_i \hbar\vec{u}_i\delta(t - t_i) \tag{3}$$

Here, $\vec{x}$, $\vec{v}$ and $\vec{k}$ are the electron position, drift velocity and wave vector, respectively, $\vec{E}$ is the electric field, $\varepsilon(\vec{k})$ is the energy-wave vector relationship and $\vec{F}_r$ is the random impulse force on the electron due to scattering. This random force can be characterized by the *scattering rate* $\lambda(\vec{k})$ and the *transition rate* $S(\vec{k}, \vec{k}')$. The probability of scattering in time is given by the following expression:

$$\Pr\{t_i - t_{i-1} > \tau\} = \exp\{-\int_{t_{i-1}}^{t_{i-1}+\tau} \lambda(\vec{k}(t'))dt'\} \tag{4}$$

Given that a scattering event has occurred at some time t_i, the probability density function for the change in the electron wave-vector is expressed as follows:

$$\rho_{\vec{k}_i}(\vec{u}_i) = \frac{S(\vec{k}_i, \vec{k}_i + \vec{u}_i)}{\lambda(\vec{k}_i)} \tag{5}$$

where $\vec{k}(t_i^-) = \vec{k}_i$ and $\vec{k}(t_i^+) = \vec{k}_i + \vec{u}_i$.

Equations (1)-(5) define a Markov process which is discontinuous in wave-vector space (compound Poisson process). In the theory of stochastic differential equations, such a Markov process is generally characterized by a *transition density function*, which satisfies the Kolmogorov-Feller forward equation, (see Refs. [2] and [3] for further details). By formally integrating this equation over the probability density function of the initial state, one obtains the linear Boltzmann transport equation:

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla_{\vec{x}}f - \frac{q\vec{E}(\vec{x},t)}{\hbar}\cdot\nabla_{\vec{k}}f = \int f(\vec{x},\vec{k}',t)S(\vec{k}',\vec{k})d\vec{k}' - \lambda(\vec{k})f \tag{6}$$

where f is the electron distribution function.

This establishes a direct connection between semi-classical transport theory and the theory of stochastic differential equations. It also makes it possible to apply the machinery of stochastic differential equations to semiconductor device modeling.

II. The Transport Model:

In this section, we will present a transport model which is based on the Boltzmann transport equation. According to semi-classical transport theory (2), the total force on the electron is due to the electric field $\vec{E}$ and the random scattering force $\vec{F}_r$. The expected value of this random force can be computed from (3)-(5) and is given by the following expression:

$$\bar{\vec{F}}_r(\vec{k}) = E\left\{\vec{F}_r\right\} = \hbar \int \vec{u} S(\vec{k}, \vec{k} + \vec{u}) d\vec{u} \tag{7}$$

This expression is in fact the first moment of the transition rate S. For acoustic and optical phonon scattering, it can be shown that the expected value of the random force is given by the following expression:

$$\bar{\vec{F}}_r(\vec{k}) = -\hbar \lambda(\vec{k}) \vec{k} \tag{8}$$

which can be interpreted as a drag-force opposite in direction to the electron wave-vector. Substituting this expression into (2), one obtains the following set of stochastic differential equations:

$$\frac{d\vec{x}}{dt} = \vec{v}(\vec{k}) \tag{9}$$

$$\hbar \frac{d\vec{k}}{dt} = \left[-q\vec{E}(\vec{x}, t) - \hbar \lambda(\vec{k}) \vec{k}\right] + \vec{F}_r^0 \tag{10}$$

Here, $\vec{F}_r^0$ denotes the zero mean component of the random (impulse) force.

In order to obtain a transport model suitable for efficient numerical implementation, the integral operator in the Boltzmann transport equation can be approximated by a second order differential operator. This turns out to be equivalent to approximating the zero mean fluctuating force $\vec{F}_r^0$ by the derivative of a zero mean Wiener process (white noise). The variance of the Wiener process is taken to be equal to the momentum dependent variance of the random force:

$$\sigma_{ij}(\vec{k}) = \int u_i u_j S(\vec{k}, \vec{k} + \vec{u}) d\vec{u} \tag{11}$$

This is in fact the second order moment of the transition rate S. The second order moments of the transition rate can be computed by integrating over equal energy surfaces in $\vec{k}$-space (spheroids or ellipsoids). For instance, in the case of a spherical band structure, the second moment in the direction orthogonal to $\vec{k}$ is given by the following expression:

$$\sigma_{k_\perp k_\perp}(\vec{k}) = \frac{1}{3} \sum_m \lambda^{(m)}(\vec{k}) r_m^2(\vec{k}; \beta) \tag{12}$$

and, in the direction parallel to $\vec{k}$, it is given by

$$\sigma_{k_\parallel k_\parallel}(\vec{k}) = \sigma_{k_\perp k_\perp}(\vec{k}) + |\vec{k}|^2 \lambda(\vec{k}) \tag{13}$$

Here, m is the index over different scattering processes, β is the dispersion factor (see Ref. [4]) and r_m is the radius of an equal energy sphere in $\vec{k}$-space after scattering. Similar relations hold in the case of ellipsoidal bands by the use of the Herring-Vogt transformation (see Ref. [5]). Figs. 1 and 2 show the expected value of the random force $\bar{\vec{F}}_r(\vec{k})$ and the variances $\sigma_{k_\perp k_\perp}(\vec{k})$ and $\sigma_{k_\parallel k_\parallel}(\vec{k})$, respectively, as a function of the magnitude of the electron wave vector.

Employing the approximation for the zero mean random force results in a second order partial differential equation for the electron distribution function. In spherical coordinates, this equation has the following form:

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k}) \cdot \nabla_{\vec{x}} f - \nabla_{\vec{k}} \cdot \left(\frac{q\vec{E}(\vec{x},t) - \bar{\vec{F}}_r(\vec{k})}{\hbar}\right) f = \frac{1}{2}\left(\frac{\partial^2}{\partial r \partial r}\sigma_{k_\parallel k_\parallel} f + \frac{1}{r^2}\frac{\partial^2}{\partial \theta \partial \theta}\sigma_{k_\perp k_\perp} f + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi \partial \phi}\sigma_{k_\perp k_\perp} f\right) \tag{14}$$

In the talk, we will present preliminary results on the computation of the electron distribution function employing the above model.

Acknowledgement:

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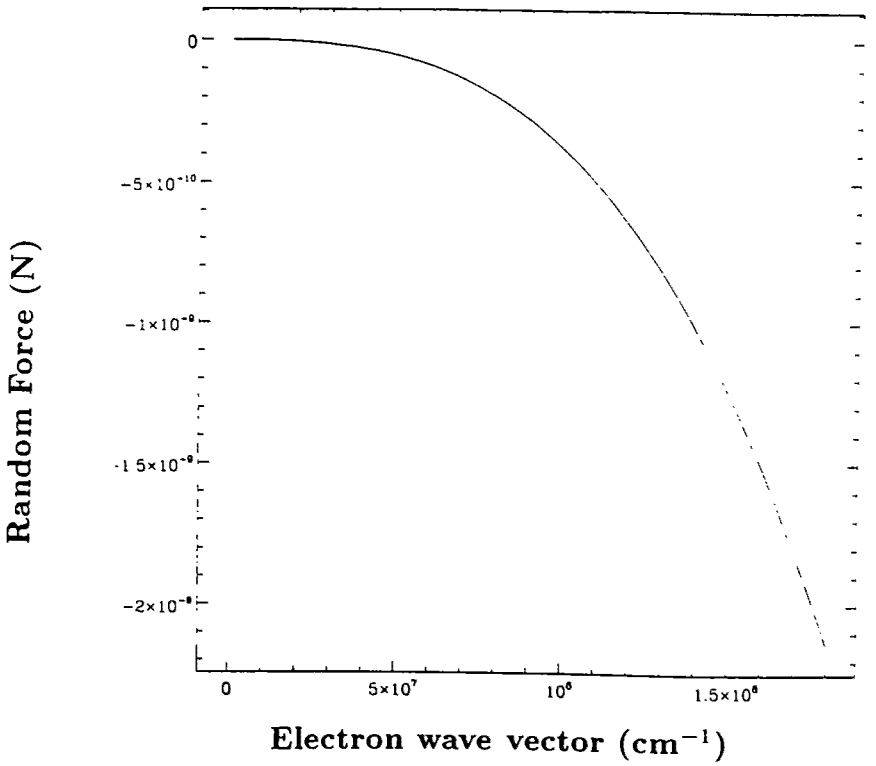

Figure 1. The expected value of the random force vs. the magnitude of the electron wave vector.

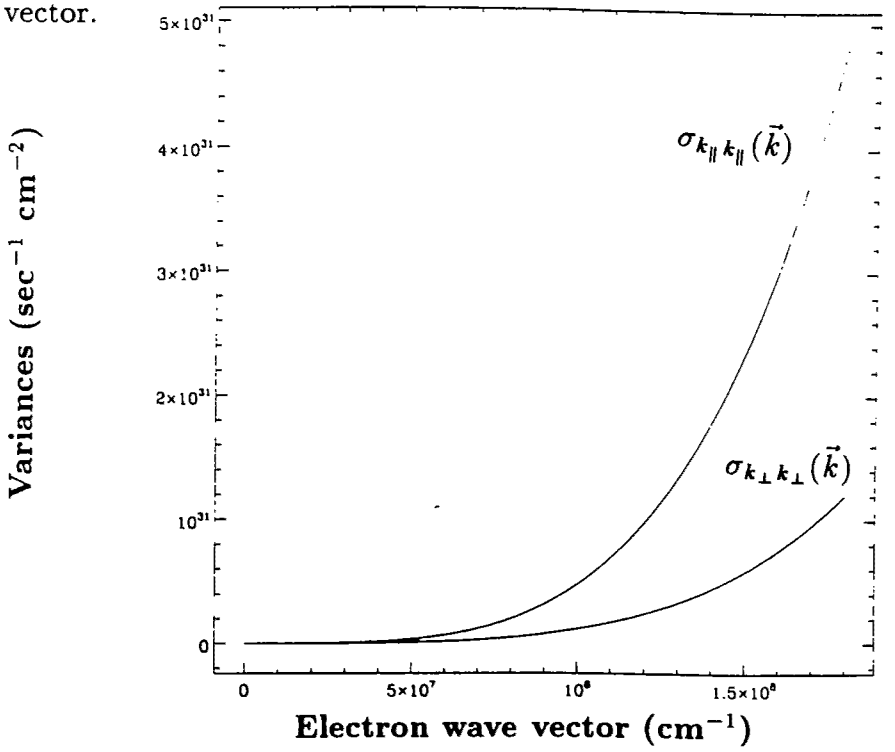

Figure 2. The variances $\sigma_{k_\perp k_\perp}(\vec{k})$ and $\sigma_{k_\parallel k_\parallel}(\vec{k})$, respectively, as a function of the magnitude of the electron wave vector.