APPLICATION OF STOCHASTIC DIFFERENTIAL EQUATION THEORY TO SEMICONDUCTOR TRANSPORT

Can E. Korman
Department of Electrical Engineering and Computer Science
The George Washington University
Washington, DC 20052

Isaak D. Mayergoyz
Electrical Engineering Department and
Institute for Advanced Computer Studies
University of Maryland
College Park, Maryland 20742

Abstract

The paper describes the application of stochastic differential equation (SDE) theory to the modeling of electron transport in semiconductors. The differential equations which describe semiclassical transport of electrons in semiconductors (and which are used in Monte Carlo simulations) can be interpreted as stochastic differential equations driven by inhomogenous randomly weighted Poisson processes. The Poisson process models scattering phenomena in momentum space. The solution of these stochastic differential equations is a Markov process which is usually characterized by a transition probability density function. It is well known in the theory of SDE that this transition probability density satisfies the forward Kolmogorov-Feller equation. The integration of the transition probability function over the initial conditions leads to the electron distribution function. Thus, integrating the Kolmogorov-Feller equation over the initial conditions, we arrive at the linear Boltzman transport equation of semiconductor devices theory.

In the paper, we will explore the described connection between SDE theory and semiclassical transport in semiconductors. In particular, the theory of SDE will be applied to the rigorous derivation of the drift-diffusion model, expressions for the electron mobility and diffusivity, etc. Furthermore, some transport models will be presented which may lead to the efficient computation of the electron distribution function.

1. ELECTRON MOTION DESCRIBED BY 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:

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

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

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

where $\vec{x}$, $\vec{v}$ 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-wavevector relationship in the given energy band and $\vec{F}_r$ is the random impulse force on the electron due to scattering.

The random force is characterized by the *scattering rate* $\lambda(\vec{k})$ and the *transition rate* $S(\vec{k},\vec{k}')$. The probability of scattering is given by

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

Therefore, given the electron wave vector $\vec{k}$, $\lambda(\vec{k})\Delta t$ is the probability that a jump in momentum will occur in a small time interval Δt. Assuming that a scattering event has occurred at some time t_i, the probability density function for the amplitude of the jump is given by,

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

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

2. THE CONNECTION BETWEEN CLASSICAL TRANSPORT THEORY AND THE THEORY OF STOCHASTIC DIFFERENTIAL EQUATIONS

The stochastic differential equations (1) and (2) together with (3)-(5) define a compound Poisson process which is discontinuous in $\vec{k}$-space and is a Markov process . In stochastic differential equation theory, such a process is usually characterized by a *transition density function* g, which satisfies the Kolmogorov-Feller forward equation, (for instance, see Refs. [1] and [2]). As a result, the corresponding equation for the above process is derived to be

$$\frac{\partial g}{\partial t} + \nabla_{\vec{x}} \cdot (\vec{v}g) - \nabla_{\vec{k}} \cdot (\frac{q\vec{E}(\vec{x},t)}{h} g) = \int g(\vec{x}_0, \vec{k}_0, s; \vec{x}, \vec{k}', t) S(\vec{k}', \vec{k}) d\vec{k}' - \lambda(\vec{k})g \tag{6}$$

where $\vec{x}_0$, $\vec{k}_0$ are the initial electron position and wave vector at some time $s < t$. Integrating (6) over the probability density function of the initial state ρ, we obtain the linear Boltzman transport equation:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}} f - \frac{q\vec{E}(\vec{x},t)}{h} \cdot \nabla_{\vec{k}} f = \int f(\vec{x}, \vec{k}', t) S(\vec{k}', \vec{k}) d\vec{k}' - \lambda(\vec{k}) f \tag{7}$$

where f is the electron distribution function defined as

$$f(\vec{x}, \vec{k}, t) = \int g(\vec{x}_0, \vec{k}_0, s; \vec{x}, \vec{k}, t) \rho_{\vec{x}_0, \vec{k}_0, s}(\vec{x}_0, \vec{k}_0) d\vec{x}_0 d\vec{k}_0 \tag{8}$$

Therefore, the linear Boltzman transport equation corresponds to the Kolmogorov-Feller forward equation for the Markov process defined in Eqs. (1)-(5). This result is quite significant since it establishes a direct connection between classical transport theory and the theory of stochastic differential equations. This makes it possible to apply the machinery of stochastic differential equations to semiconductor device modeling and provides

additional insight into the structure of the transport models and the underlying physical processes.

3. DERIVATION OF THE DRIFT-DIFFUSION MODEL BASED ON SDE THEORY

In this section, we will present the rigorous derivation of the drift-diffusion model based on the theory of SDE. According to the stochastic differential equation (2), the momentum of an electron varies 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:

$$\bar{\vec{F}}_r(\vec{k}) = E\left\{\vec{F}_r\right\} = \int \vec{u} S(\vec{k}, \vec{k}+\vec{u}) d\vec{u} \tag{9}$$

Substituting (9) into (2), one obtains the following set of equations:

$$\frac{d\vec{x}}{dt} = \vec{v}(\vec{k}) \tag{10}$$

$$h\frac{d\vec{k}}{dt} = \left[-q\vec{E}(\vec{x},t) + \bar{\vec{F}}_r(\vec{k})\right] + \vec{F}_r^0 \tag{11}$$

where $\vec{F}_r^0$ is the zero mean component of the random force. This representation of the electron motion is quite informative at the physical level. According to this representation, the electron momentum varies due to the electric field $\vec{E}$, a *momentum dependent drag force* $\bar{\vec{F}}_r$ and a *zero mean fluctuating force* $\vec{F}_r^0$.

In order to derive the drift-diffusion equation, four basic assumptions are made on the random process. First, it is assumed that the energy band is spherical and parabolic. This implies that $h\vec{k} = m_e\vec{v}$, where m_e is the effective mass of the electron.

The second assumption is made on the momentum dependent drag force. In (9), it is assumed that the wavevector $\vec{k}$ is small and that the transition rate $S(\vec{k},\vec{k}')$ and the scattering rate $\lambda(\vec{k})$ can be approximated by their values at $\vec{k}=0$. Noting that $S(0,\vec{k}')$ is an even function of $\vec{k}'$, the momentum dependent drag force is approximated to be $\bar{\vec{F}}_r \approx -\lambda(0)m_e\vec{v}$.

The third assumption is to approximate the zero mean random force $\vec{F}_r^0$ by a white noise process. That is, $\vec{F}_r^0 \approx \sigma d\vec{W}_t/dt$, where σ is the variance of the random process and W_t is a standard zero mean Wiener process.

Based on these approximations, the random motion of the electron can now be described by the following stochastic differential equations:

$$\frac{d\vec{x}}{dt} = \vec{v} \tag{12}$$

$$m_e\frac{d\vec{v}}{dt} = -q\vec{E}(\vec{x},t) - \lambda(0)m_e\vec{v} + \sigma\frac{dW_t}{dt} \tag{13}$$

The fourth and final approximation is to neglect the inertia of the electron and assume that $m_e d\vec{v}/dt \approx 0$. As a result, we obtain the following stochastic differential equation:

$$d\vec{x} = -\frac{q}{m_e\lambda(0)}\vec{E}dt + \frac{\sigma}{m_e\lambda(0)}dW_t. \tag{14}$$

This is a differential equation driven by white noise and it describes the evolution of a continuous Markov process. Such a process is usually characterized by a transition probability density function which satisfies the forward Kolmogorov equation [1]. Similar to the analysis in the previous section, the corresponding forward Kolmogorov equation for this process is integrated over the initial distribution function. This results in the following equation:

$$\frac{\partial n}{\partial t} = \nabla \cdot \left(\frac{q}{m_e \lambda(0)} \vec{E} n + \frac{1}{2} (\frac{\sigma}{m_e \lambda(0)})^2 \nabla n \right). \tag{15}$$

Here, we observe that Eq. (15) is, in fact, the drift-diffusion equation. Hence, it is easy to show that the electron mobility and diffusivity are given by the following expressions:

$$\mu_n = \frac{q}{m_e \lambda(0)} \quad , \quad D_n = \frac{1}{2} (\frac{\sigma}{m_e \lambda(0)})^2. \tag{16}$$

Hence, we have obtained the expressions for the low field electron mobility and diffusivity in terms of the transition rate λ. For instance, the electron mobility for silicon can easily be computed by taking $\lambda_{\text{acoustic}}(0) \approx 10^{12}$ sec^{-1}, $\lambda_{\text{optical}}(0) \approx 10^{11}$ sec^{-1} (Ref. [3]), and $m_e = 1.08 m_o$. Since, the total scattering rate is the sum of the individual scattering rates, one obtains $\mu_n = 1478$ cm^2/V-sec which is in agreement with the reported values of low field electron mobility in silicon.

4. A TRANSPORT MODEL BASED ON SDE THEORY

The Boltzman transport equation is an integro-differential equation and does not lend itself to efficient numerical computations. In order to obtain transport equations which are more suitable for efficient numerical implementation, the integral operator in the Boltzman transport equation can be approximated by a second order differential operator. It turns out that this is equivalent to approximating the zero mean fluctuating force $\vec{F}_r^0$ by a zero mean Wiener process whose variance is equal to the momentum dependent variance of the original process. This results in the following partial differential equation for the electron distribution function:

$$\frac{\partial f}{\partial t}(\vec{x}, \vec{k}, t) + \frac{1}{\hbar} \nabla_{\vec{k}} \epsilon(\vec{k}) \cdot \nabla_{\vec{x}} f - \frac{q \vec{E}(\vec{x}, t)}{\hbar} \cdot \nabla_{\vec{k}} f + \frac{1}{\hbar} \nabla_{\vec{k}} \cdot \left[\bar{\bar{F}}_r(\vec{k}) f \right] =$$

$$\frac{1}{2} \sum_{i,j=1}^{3} \frac{\partial^2}{\partial k_i \partial k_j} \left[\sigma_{ij}(\vec{k}) f \right] \tag{17}$$

$$\sigma_{ij}(\vec{k}) = \int u_i u_j S(\vec{k}, \vec{k} + \vec{u}) d\vec{u} \tag{18}$$

From the computational point of view, this partial differential equation is simpler to solve than the Boltzman equation.

5. REFERENCES

[1] I. I. Gihman and A. V. Skorohod, *Stochastic Differential Equations*, (Springer-Verlag, New York, 1972).

[2] D. Kannan, *An Introduction to Stochastic Processes*, (North Holland, New York, 1979).

[3] C. Jacobini and L. Reggiani, Reviews of Modern Phys., 55, 645, (1983).