Semiconductor noise in the framework of semiclassical transport

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The paper describes an approach to semiconductor noise analysis that is entirely within the framework of the semiclassical transport theory. The key aspect that differentiates this approach from other noise models is that this approach directly connects noise characteristics with the physics of scattering in the semiclassical transport model and makes no additional assumptions regarding the nature of noise. Employing the machinery of stochastic differential equation theory, a method is developed to compute the autocovariance function and spectral density of current fluctuations from the solutions of the Boltzmann transport equation (BTE). As a result, current fluctuations due to scattering are directly accounted for without the usual *ad hoc* addition of the ''Langevin source term'' to the transport equation. Simulation results are presented for the noise spectral density and autocovariance functions in silicon due to elastic-acoustic and optical-phonon scattering. The autocovariance and spectral density are computed in bulk silicon for different electric fields and temperatures based on the space-independent solutions of the BTE. In the practical case of Ohmic contacts, an explicit expression for the current noise spectral density is derived in terms of the scattering transition rate, the steady-state distribution function, and the average current density. [S0163-1829(96)02048-6]

I. INTRODUCTION

Noise phenomena in semiconductors have attracted much attention over the past years.[1] With recent technological progress towards low-power and high-density devices, fluctuations in the output signals of semiconductor devices are becoming an important issue both at the circuit and system levels. This paper describes a comprehensive approach to semiconductor noise analysis that is entirely within the framework of semiclassical transport and makes no additional assumptions regarding the nature of noise. This approach can be employed to study the noise characteristics of a wide spectrum of devices where the semiclassical transport theory is applicable.

The mathematical framework of the noise model developed in this paper is the machinery of stochastic differential equations (SDE). In semiclassical transport theory, the differential equations that describe the motion of an electron in a semiconductor can be interpreted as stochastic differential equations, which are driven by inhomogeneous randomly weighted Poisson processes. At the physical level, these processes model the random interband and intraband scattering of electrons in momentum space. The solution to such differential equations is a Markov process, which can be characterized by a transition probability density function. According to the SDE theory, the transition probability density function satisfies the Kolmogorov-Feller equation, which, in the case of semiclassical transport, is identical to the linear (nondegenerate) Boltzmann transport equation with appropriate initial conditions.[2,3] The primary goal of this paper is to present an approach to compute the autocovariance function and spectral density of current fluctuations by using this transition probability density function. The key aspect that differentiates this approach from other microscopic noise models is that this approach is strictly within the framework of semiclassical transport and does not require any *ad hoc* additions of ''Langevin source terms,'' which are generally introduced into transport equations. As a result, this approach directly connects the noise characteristics with the properties of the inhomogeneous randomly weighted Poisson processes, which describe the physics of scattering in the semiclassical transport model. In this sense, our framework is similar to one used in Monte Carlo simulations of noise.[4] However, our approach heavily relies on the interpretation of the semiclassical-transport model as SDE's and the machinery of the Kolmogorov-Feller equation. By using this machinery, it is shown that the key computations of the autocovariance function and the noise spectral density can be reduced to a special initial value problem for the BTE [see formulas (19)–(21)].

It is important to mention that a conceptually similar approach based on the transition probability density function (Green function) was proposed in Refs. 5 and 6 and was extensively used for analytical calculations of current fluctuations under the *relaxation time approximation*. However, there are distinct differences between our work and results reported in Ref. 5. First, we do not use the Green function directly in our calculations but rather proceed to derive formulas (19)–(21) and/or (25) in terms of effective distribution functions, $\mathbf{g}(\mathbf{x},\mathbf{k},\tau)$ and $\mathbf{G}(\mathbf{x},\mathbf{k},\omega)$, which *substantially* simplify numerical calculations. Second, in our approach we do not rely at all on the relaxation time approximation but rather treat the collision integral in all its complexity. This is important in order to accurately take into account the random scattering mechanisms, which are responsible in the first place for the very existence of noise. Finally, we apply our approach not only to the silicon bulk computations but to the very important case of highly doped Ohmic contacts. For this

practically interesting case, we derive integral expressions for the noise spectral density. In addition, it is worthwhile to remark that we justify our approach on the basis of SDE theory, which allows one to clearly relate the semiclassical transport model to the Boltzmann–Green-function formalism.

The paper is organized as follows. In Sec. II, we introduce the basic equations of semiclassical transport theory, which can be construed as SDE's. By employing the machinery of SDE theory, we show that the autocovariance function and spectral density of noise can be computed directly from the solutions of the BTE. In Sec. III, we look at the particular case of noise in bulk silicon where we employ Legendre polynomials to compute the noise spectral density from the solution of the space-independent BTE. We present numerical simulation results for the autocovariance function and spectral density for different electric fields and temperature. These results are shown to be in close agreement with published experimental and Monte Carlo results. In Sec. IV, the practical case of Ohmic contacts adjacent to highly doped regions is considered and an explicit expression for the noise spectral density is derived in terms of the scattering transition rate, the steady-state distribution function, and the average current density. Finally, we reach our conclusions in Sec. V.

II. DERIVATION OF THE NOISE MODEL

According to semiclassical transport theory, an electron in a semiconductor drifts under the influence of electric and magnetic fields and undergoes random jumps in its momentum due to various scattering mechanisms in the crystal caused by acoustic and optical phonons, ionized impurities, interface traps, etc. Neglecting the effects of magnetic fields, the motion of an electron can be described by the following differential equations:

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

$$\hbar\,\frac{d\mathbf{k}}{dt}=-q\mathbf{E}+\mathbf{F}_r, \quad \mathbf{F}_r=\sum_i \hbar\mathbf{u}_i\delta(t-t_i), \tag{2}$$

where $\mathbf{x}$, $\mathbf{v}$, and $\mathbf{k}$ are the electron position, drift velocity, and wave vector (crystal momentum), respectively, $\mathbf{E}$ is the electric field, $\varepsilon(\mathbf{k})$ is the energy–wave-vector relationship in the given energy band, and $\mathbf{F}_r$ is the random impulse force on the electron due to scattering. The random force is characterized by the *transition rate* $W(\mathbf{k},\mathbf{k}')$. By using this rate, we have

$$\mathrm{Prob}\{t_i-t_{i-1}>\tau\}=\exp\left\{-\int_{t_{i-1}}^{t_{i-1}+\tau}\lambda(\mathbf{k}(t'))dt'\right\}, \tag{3}$$

where t_i is the random time at which a scattering event occurs, while $\lambda(\mathbf{k})$ is the *scattering rate* defined as

$$\lambda(\mathbf{k})=\int W(\mathbf{k},\mathbf{k}')d\mathbf{k}'. \tag{4}$$

Therefore, given $\mathbf{k}$, $\lambda(\mathbf{k})\Delta t$ is the probability that a jump in the wave vector $\mathbf{k}$ 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 jump $\mathbf{u}_i$ is given by

$$\chi(\mathbf{u}_i|\mathbf{k}_i)=\frac{W(\mathbf{k}_i,\mathbf{k}_i+\mathbf{u}_i)}{\lambda(\mathbf{k}_i)}, \tag{5}$$

where $\mathbf{k}(t_i^-)=\mathbf{k}_i$ and $\mathbf{k}(t_i^+)=\mathbf{k}_i+\mathbf{u}_i$. The above equations constitute the basis of semi-classical transport theory and they are extensively used in the Monte Carlo simulation of electron transport.[8]

It is clear that the random force $\mathbf{F}_r$ is the derivative of an inhomogeneous randomly weighted Poisson process. For this reason, Eqs. (1) and (2) can be interpreted as stochastic differential equations. Solution of these equations is a Markov process, which is discontinuous in $\mathbf{k}$ space. Such a process is usually characterized by a *transition probability density function or Green function* $\rho(\mathbf{x}',\mathbf{k}',t;\mathbf{x},\mathbf{k},t+\tau)$ and it satisfies the Kolmogorov-Feller equation with respect to the forward coordinates $\mathbf{x}$, $\mathbf{k}$, and τ (for instance, see Refs. 9 and 10). For the stochastic process defined by the SDE's (1) and (2), the Kolmogorov-Feller (forward) equation can be written as follows:

$$\frac{\partial\rho}{\partial\tau}(\mathbf{x}',\mathbf{k}',t;\mathbf{x},\mathbf{k},t+\tau)+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{x}}\rho-\frac{q}{\hbar}\,\mathbf{E}(\mathbf{x},t+\tau)\cdot\nabla_{\mathbf{k}}\rho$$
$$=\int\rho(\mathbf{x}',\mathbf{k}',t;\mathbf{x},\mathbf{k}'',t+\tau)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}''-\lambda(\mathbf{k})\rho, \tag{6}$$

where $(\mathbf{x}',\mathbf{k}')$ are the initial electron position and wave vector at some time t. By integrating the above equation over the initial conditions (backward coordinates), one obtains the well-known linear Boltzmann transport equation.

Generally, noise in semiconductors is characterized by the spectral density of current fluctuations. The spectral density is defined as the Fourier transform of the autocovariance function. The autocovariance function of any random process can be found from the joint probability density function of the random process. With these facts in mind, consider a semiconductor under *steady-state* conditions where a stationary electron distribution function $f(\mathbf{x},\mathbf{k})$ can be introduced. It is clear that this distribution function is the stationary solution of Eq. (6). Let $\mathbf{k}'$ and $\mathbf{k}$ be random electron wave vectors at time instances t and $t+\tau$, respectively. Since the stochastic process is stationary, the joint probability density function of these random vectors is a function of τ only. Consequently, the autocovariance matrix of the electron velocity $\mathbf{v}$ at some point $\mathbf{x}$ can be computed as follows:

$$\hat{C}_{\mathbf{v}}(\tau)=\langle[\mathbf{v}(\mathbf{k})-\langle\mathbf{v}\rangle_{\mathbf{x}}][\mathbf{v}(\mathbf{k}')-\langle\mathbf{v}\rangle_{\mathbf{x}}]^T\rangle$$
$$=\int\int[\mathbf{v}(\mathbf{k})][\mathbf{v}(\mathbf{k}')]^T$$
$$\times[\rho(\mathbf{k}',0,\mathbf{k},\tau)-f(\mathbf{x},\mathbf{k})f(\mathbf{x},\mathbf{k}')]d\mathbf{k}\,d\mathbf{k}', \tag{7}$$

where

$$\langle\mathbf{v}\rangle_{\mathbf{x}}\equiv\int\mathbf{v}(\mathbf{k})f(\mathbf{x},\mathbf{k})d\mathbf{k}. \tag{8}$$

Here, $\rho(\mathbf{k}',0,\mathbf{k},\tau)$ denotes the joint probability density function of $\mathbf{k}'$ and $\mathbf{k}$ and, for notational simplicity, the dependence of this probability density function on the spatial coordinate $\mathbf{x}$ is omitted. It is important to note that when the electron charge density is defined as $n(\mathbf{x})=\int f(\mathbf{x},\mathbf{k})d\mathbf{k}$, $\langle\mathbf{v}\rangle$ given in Eq. (8) should be interpreted as $\langle n\mathbf{v}\rangle$. Consequently, in this context, $\hat{C}_{\mathbf{v}}(\tau)$ defined in Eq. (7) is the autocovariance matrix of the normalized current density $\mathbf{J}/q$. (The instantaneous current is given by $\mathbf{J}=-qn\mathbf{v}$.)

The joint probability density function can be expressed in terms of the transition probability density function and the stationary probability density function as follows:

$$\rho(\mathbf{k}',0,\mathbf{k},\tau)=\rho(\mathbf{k},\tau|\mathbf{k}',0)f(\mathbf{x},\mathbf{k}'). \tag{9}$$

By substituting Eq. (9) into Eq. (7), one obtains the following expression for the autocovariance matrix:

$$\hat{C}_{\mathbf{v}}(\tau)=\int[\mathbf{v}(\mathbf{k})]\Bigg[\int[\mathbf{v}(\mathbf{k}')]^T[\rho(\mathbf{k},\tau|\mathbf{k}',0) - f(\mathbf{x},\mathbf{k})]f(\mathbf{x},\mathbf{k}')d\mathbf{k}'\Bigg]d\mathbf{k}, \tag{10}$$

The transition probability density function is the transient solution of Eq. (6):

$$\frac{\partial\rho}{\partial\tau}(\mathbf{x},\mathbf{k}',0;\mathbf{x},\mathbf{k},\tau)+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{x}}\rho-\frac{q}{\hbar}\mathbf{E}(\mathbf{x})\cdot\boldsymbol{\nabla}_{\mathbf{k}}\rho = \int\rho(\mathbf{x},\mathbf{k}',0;\mathbf{x},\mathbf{k}'',\tau)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}''-\lambda(\mathbf{k})\rho, \tag{11}$$

subject to the following initial condition:

$$\rho(\mathbf{x},\mathbf{k}',0;\mathbf{x},\mathbf{k},\tau)\big|_{\tau=0}=\delta(\mathbf{k}-\mathbf{k}'), \tag{12}$$

where $\delta(\mathbf{k}-\mathbf{k}')$ is the Dirac delta function and the following notation has been adopted:

$$\rho(\mathbf{k},\tau|\mathbf{k}',0)\equiv\rho(\mathbf{x},\mathbf{k}',0;\mathbf{x},\mathbf{k},\tau). \tag{13}$$

As pointed out before, the distribution function f is a stationary solution of Eq. (6):

$$\mathbf{v}(\mathbf{k})\cdot\boldsymbol{\nabla}_{\mathbf{x}}f-\frac{q}{\hbar}\mathbf{E}(\mathbf{x})\cdot\boldsymbol{\nabla}_{\mathbf{k}}f=\int f(\mathbf{k}'')W(\mathbf{k}'',\mathbf{k})d\mathbf{k}''-\lambda(\mathbf{k})f. \tag{14}$$

The formal result presented in Eqs. (10)–(14) is the well-known BTE–Green function approach to compute the noise autocovariance function (see, for instance, Ref. 5). Here, we prove this result by employing the machinery of SDE theory where we interpret the equations describing semiclassical transport as SDE's. It is important to note that the only stochastic information that is needed is the electron scattering rates of semiclassical transport theory. This is natural since the source of noise is the random fluctuations of the electron momentum due to scattering. Since this information is embedded in the corresponding Kolmogorov-Feller (BTE) equation, there is no need to include additional random fluctuations into the system. This is in contrast with the usually held opinion that the BTE reflects the average behavior of the system and that a stochastic field term, referred to as the ''Langevin source term,'' must be added in order to account for the random fluctuations in the current (for instance, see Ref. 11).

From the computational point of view, the BTE–Green function approach has one major drawback. We note from Eq. (10) that in order to compute the autocovariance matrix, the transition probability density function needs to be computed for all initial conditions $\mathbf{k}'$ in momentum space. However, this lengthy computation can be substantially simplified by using the following transformations. By subtracting Eq. (14) from Eq. (11), one finds that the difference of the transient and stationary solutions,

$$\zeta(\mathbf{k},\tau|\mathbf{k}',0)\equiv\rho(\mathbf{k},\tau|\mathbf{k}',0)-f(\mathbf{x},\mathbf{k}), \tag{15}$$

satisfies the equation

$$\frac{\partial\zeta}{\partial\tau}+\mathbf{v}(\mathbf{k})\cdot\boldsymbol{\nabla}_{\mathbf{x}}\zeta-\frac{q}{\hbar}\mathbf{E}(\mathbf{x})\cdot\boldsymbol{\nabla}_{\mathbf{k}}\zeta = \int\zeta(\mathbf{k}'',\tau|\mathbf{k}',0)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}'' - \lambda(\mathbf{k})\zeta, \tag{16}$$

subject to the initial condition:

$$\zeta(\mathbf{k},\tau|\mathbf{k}',0)\big|_{\tau=0}=\delta(\mathbf{k}-\mathbf{k}')-f(\mathbf{x},\mathbf{k}). \tag{17}$$

Next we multiply both Eq. (16) and Eq. (17) by $\mathbf{v}(\mathbf{k}')f(\mathbf{x},\mathbf{k}')$ and integrate over $\mathbf{k}'$. By defining

$$\mathbf{g}(\mathbf{x},\mathbf{k},\tau)\equiv\int d\mathbf{k}'\ \mathbf{v}(\mathbf{k}')f(\mathbf{x},\mathbf{k}')\zeta(\mathbf{k},\tau|\mathbf{k}',0), \tag{18}$$

it is easy to show that this function satisfies the following equation:

$$\frac{\partial\mathbf{g}}{\partial\tau}+\mathbf{v}(\mathbf{k})\cdot\boldsymbol{\nabla}_{\mathbf{x}}\mathbf{g}-\frac{q}{\hbar}\mathbf{E}(\mathbf{x})\cdot\boldsymbol{\nabla}_{\mathbf{k}}\mathbf{g}=\int\mathbf{g}(\mathbf{k}'',\tau)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}'' - \lambda(\mathbf{k})\mathbf{g}, \tag{19}$$

subject to the initial condition:

$$\mathbf{g}(\mathbf{x},\mathbf{k},\tau)\big|_{\tau=0}=[\mathbf{v}(\mathbf{k})-\langle\mathbf{v}\rangle_{\mathbf{x}}]f(\mathbf{x},\mathbf{k}). \tag{20}$$

Here, Eq. (19) should be understood in a component-wise sense. From the expression for the autocovariance matrix [Eq. (10)] it then follows that

$$\hat{C}_{\mathbf{v}}(\tau)=\int[\mathbf{v}(\mathbf{k})][\mathbf{g}(\mathbf{x},\mathbf{k},\tau)]^T d\mathbf{k},\quad \tau\geqslant 0. \tag{21}$$

Thus, it can be seen that the autocovariance matrix can be computed for positive τ by solving the transient Boltzmann transport equation (19) subject to the initial condition (20) and substituting this solution into Eq. (21). Since the autocovariance matrix has even symmetry with respect to τ, the solution of Eq. (19) for $\tau\geqslant 0$ is sufficient.

By definition, the noise spectral density is the time Fourier transform of the autocovariance matrix. Noting the

above symmetry of the autocovariance matrix, the spectral density of the electron velocity is given as follows:

$$\hat{S}_{\mathbf{v}}(\omega)=\int_{-\infty}^{+\infty}\hat{C}_{\mathbf{v}}(\tau)e^{-j\omega\tau}d\tau=2\,\mathrm{Re}\left\{\int_{0}^{+\infty}\hat{C}_{\mathbf{v}}(\tau)e^{-j\omega\tau}d\tau\right\}. \tag{22}$$

By substituting Eq. (21) into Eq. (22), one obtains

$$\hat{S}_{\mathbf{v}}(\omega)=2\,\mathrm{Re}\left\{\int[\mathbf{v}(\mathbf{k})][\mathbf{G}(\mathbf{x},\mathbf{k},\omega)]^{T}d\mathbf{k}\right\}, \tag{23}$$

where

$$\mathbf{G}(\mathbf{x},\mathbf{k},\omega)=\int_{0}^{+\infty}\mathbf{g}(\mathbf{x},\mathbf{k},\tau)e^{-i\omega\tau}d\tau. \tag{24}$$

The last expression suggests that the spectral density can be computed directly in the frequency domain. Indeed, by taking the one-sided Fourier transform of Eq. (19) and by using the initial condition Eq. (20), we obtain the following equation for **G**:

$$j\omega\mathbf{G}-[\mathbf{v}(\mathbf{k})-\langle\mathbf{v}\rangle_{\mathbf{x}}]f(\mathbf{x},\mathbf{k})+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{x}}\mathbf{G}-\frac{q}{\hbar}\,\mathbf{E}(\mathbf{x})\cdot\nabla_{\mathbf{k}}\mathbf{G}$$
$$=\int\mathbf{G}(\mathbf{x},\mathbf{k}'',\omega)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}''-\lambda(\mathbf{k})\mathbf{G}. \tag{25}$$

Hence, the spectral density of the electron velocity fluctuations can be computed directly in the frequency domain by solving Eq. (25) and substituting the solution into Eq. (23).

III. NOISE CHARACTERISTICS IN BULK SILICON

We shall next apply the above machinery to noise computations in bulk silicon. As is typically done in the experimental characterization of noise, we will determine the noise spectral density and autocovariance as functions of electric field, average current, and temperature. In order to compute the noise spectral density, one needs to solve the following space-independent equation:

$$j\omega\mathbf{G}(\mathbf{k},\omega)-[\mathbf{v}(\mathbf{k})-\langle\mathbf{v}\rangle]f(\mathbf{k})-\frac{q}{\hbar}\,\mathbf{E}\cdot\nabla_{\mathbf{k}}\mathbf{G}$$
$$=\int\mathbf{G}(\mathbf{k}'',\omega)W(\mathbf{k}'',\mathbf{k})d\mathbf{k}''-\lambda(\mathbf{k})\mathbf{G}. \tag{26}$$

We will consider bulk silicon with a spherical band structure. An ellipsoidal band structure can easily be incorporated into the following derivations by employing the Herring-Vogt transformation.[12] With a spherical band structure, all six conduction-band valleys are equivalent and one can represent the state of the momentum space with only one valley. For the space-independent problem considered here, the average electron velocity $\langle\mathbf{v}\rangle$ is in the direction of the electric field **E**, which determines the axis of symmetry. In order to facilitate the derivations, it is convenient to introduce the following coordinate system:

$$\mathbf{v}(\mathbf{k})=v_{\parallel}(\mathbf{k})\mathbf{a}_{\parallel}+v_{\perp}(\mathbf{k})\mathbf{a}_{\perp},\quad \mathbf{k}=k_{\parallel}\mathbf{a}_{\parallel}+k_{\perp}\mathbf{a}_{\perp}, \tag{27}$$

where $\mathbf{a}_{\parallel}$ and $\mathbf{a}_{\perp}$ are unit vectors parallel and orthogonal to the average electron velocity $\langle\mathbf{v}\rangle$, respectively. The axial symmetry leads to

$$\mathbf{g}(\mathbf{k},\tau)=g_{\parallel}(\mathbf{k},\tau)\mathbf{a}_{\parallel}+g_{\perp}(\mathbf{k},\tau)\mathbf{a}_{\perp}. \tag{28}$$

Consequently, from Eqs. (21), (27), and (28), one can derive the following expression for the autocovariance matrix:

$$\hat{C}_{\mathbf{v}}(\tau)=\int\begin{pmatrix}v_{\parallel}(\mathbf{k})g_{\parallel}(\mathbf{k},\tau) & v_{\parallel}(\mathbf{k})g_{\perp}(\mathbf{k},\tau)\\ v_{\perp}(\mathbf{k})g_{\parallel}(\mathbf{k},\tau) & v_{\perp}(\mathbf{k})g_{\perp}(\mathbf{k},\tau)\end{pmatrix}d\mathbf{k}. \tag{29}$$

Since the average current flow is in the direction of the average electron velocity, the quantity of primary interest is the autocovariance function of $v_{\parallel}$. It follows from Eq. (29) that the autocovariance function of $v_{\parallel}$ is given by the following expression:

$$C_{I}(\tau)=\int v_{\parallel}(\mathbf{k})g_{\parallel}(\mathbf{k},\tau)d\mathbf{k}. \tag{30}$$

From the definition of the spectral density (23), it also follows that

$$S_{I}(\omega)=2\,\mathrm{Re}\left\{\int v_{\parallel}(\mathbf{k})G_{\parallel}(\mathbf{k},\omega)d\mathbf{k}\right\}, \tag{31}$$

where $G_{\parallel}$ satisfies the following equation:

$$j\omega G_{\parallel}(\mathbf{k},\omega)-[v_{\parallel}(\mathbf{k})-\langle v_{\parallel}\rangle]f(\mathbf{k})-\frac{q}{\hbar}\,\mathbf{E}\cdot\nabla_{\mathbf{k}}G_{\parallel}$$
$$=\int G_{\parallel}(\mathbf{k}',\omega)W(\mathbf{k}',\mathbf{k})d\mathbf{k}'-\lambda(\mathbf{k})G_{\parallel}. \tag{32}$$

At this point, it is useful to employ Legendre polynomials in order to evaluate $S_I(\omega)$. For a spherical band structure, electron energy is a function of the magnitude of the electron wave vector, $\varepsilon(\mathbf{k})=\varepsilon(k)$. Employing the dispersion relationship, $\gamma(\varepsilon)=\hbar^2k^2/2m$, it can be shown that

$$v_{\parallel}(\mathbf{k})=\alpha(k)k_{\parallel}=\alpha(k)kP_{1}(\cos\theta),\quad \alpha(k)=\frac{\hbar}{m\gamma'[\varepsilon(k)]}. \tag{33}$$

The function $G_{\parallel}$ is expressed as follows:

$$G_{\parallel}(\mathbf{k},\omega)=\sum_{n=0}^{\infty}G_{\parallel}^{(n)}(k,\omega)P_{n}(\cos\theta). \tag{34}$$

By substituting Eqs. (33) and (34) into Eq. (31) and by using integration in spherical coordinate (k,θ,ϕ), we obtain

$$S_{I}(\omega)=4\pi\,\mathrm{Re}\left\{\sum_{n=0}^{\infty}\int_{0}^{\infty}dk\;\alpha(k)k^{3}G_{\parallel}^{(n)}(k,\omega)\right.$$
$$\left.\times\int_{0}^{\pi}d\theta\,\sin\theta P_{1}(\cos\theta)P_{n}(\cos\theta)\right\}. \tag{35}$$

Since

$$\int_{0}^{\pi}d\theta\,\sin\theta P_{1}(\cos\theta)P_{n}(\cos\theta)=\tfrac{2}{3}\delta_{1,n}, \tag{36}$$

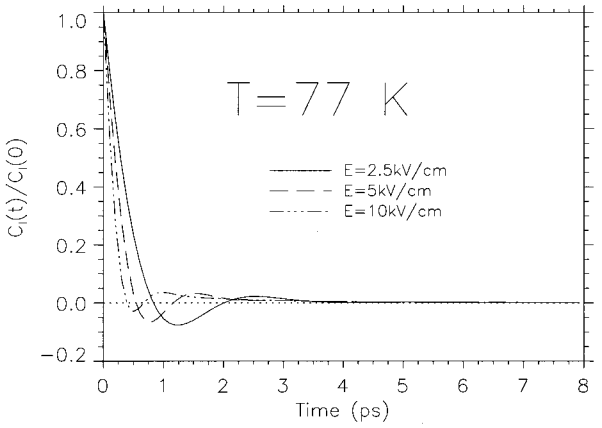

FIG. 1. The normalized autocorrelation function of electron current parallel to the electric field at 77 K. The figure shows reduced velocity correlation times as electrons gain energy from increasing electric fields.

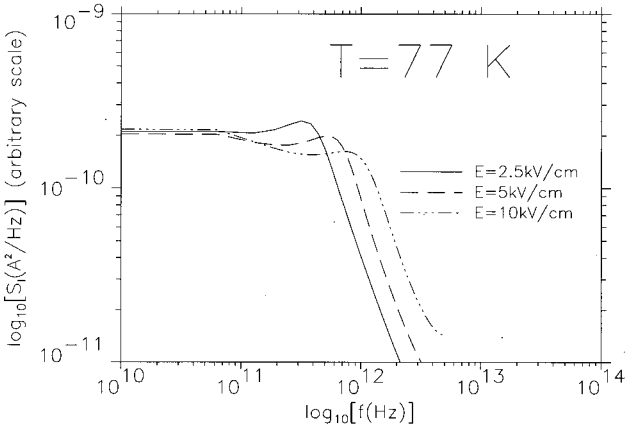

FIG. 3. Spectral density of electron current parallel to the electric field at 77 K. Corresponding to Fig. 1, the spectral density broadens with increasing electric fields.

the spectral density of $v_\parallel$ can be expressed only in terms of the first-order Legendre polynomial expansion of $G_\parallel$ and it is given by the following expression:

$$S_I(\omega)=\frac{8\pi}{3}\,\mathrm{Re}\left\{\int_0^\infty dk\ \alpha(k)k^3G_\parallel^{(1)}(k,\omega)\right\}. \qquad (37)$$

As a result, we have shown that the noise spectral density in bulk silicon can be computed directly from the first-order Legendre polynomial coefficient of the solution of the space independent BTE given in Eq. (32).

The described machinery was employed to compute the noise autocovariance function. The space-independent BTE is solved by employing the Legendre polynomial method.[7] The following figures present numerical simulation results for bulk silicon when noise due to acoustic and optical phonon scattering is considered. An ellipsoidal band structure described in Ref. 8 is considered and the Herring-Vogt transformation is employed in order to simplify the computations. The electric field is assumed to be in the ⟨111⟩ crystallographic direction and enables the computations to be performed in only one conduction-band valley. Figures 1 and 2 show the autocovariance function of the electron current, $C_I(\tau)$, for small values of electric fields (2.5, 5.0, and 10 kV/cm) at the lattice temperatures 77 and 300 K, respectively. Both plots show that correlation times of electron current decrease as the magnitude of the electric field is increased. These figures also show that at these electric fields the correlation time at 77 K is significantly larger than the correlation time at 300 K, indicating the strong influence of temperature on noise characteristics. Figures 3 and 4 show the corresponding spectral densities $S_I(\omega)$ at 77 and 300 K, respectively. It can be seen that the spectral density broadens as a result of increased electric field and temperature. These results are in good agreement with published results on bulk silicon computed by using the Monte Carlo noise simulation technique.[13] Figure 5 shows the autocovariance function for a relatively higher field of 50 kV/cm at temperatures 77, 100, 200, and 300 K. It is interesting to note that the effect of temperature on the correlation time is significantly reduced at high electric fields.

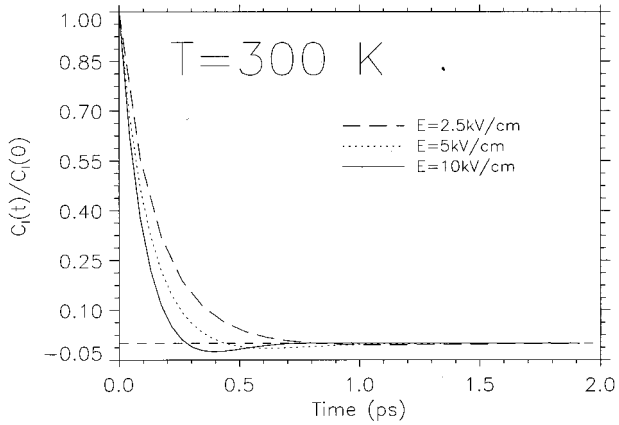

FIG. 2. The normalized autocorrelation function of electron current parallel to the electric field at 300 K. The figure shows reduced velocity correlation times as electrons gain energy from increasing electric fields.

IV. NOISE SPECTRAL DENSITY AT OHMIC CONTACTS

In practice, current noise measurements are made at Ohmic contacts. Consequently, it is of interest to evaluate the noise at Ohmic contacts where, due to high levels of doping, electric fields and $\nabla_{\mathbf{x}}$ can be assumed to be negligible. Under these assumptions, it is easy to see that $G_\parallel$ satisfies the following equation:

$$j\omega G_\parallel(\mathbf{k},\omega)-\int G_\parallel(\mathbf{k}',\omega)W(\mathbf{k}',\mathbf{k})d\mathbf{k}'+\lambda(\mathbf{k})G_\parallel$$
$$=(v_\parallel-\langle v_\parallel\rangle)f(\mathbf{k}). \qquad (38)$$

Furthermore, under these assumptions, it is also clear that a single band distribution function accurately represents the state of the momentum space.

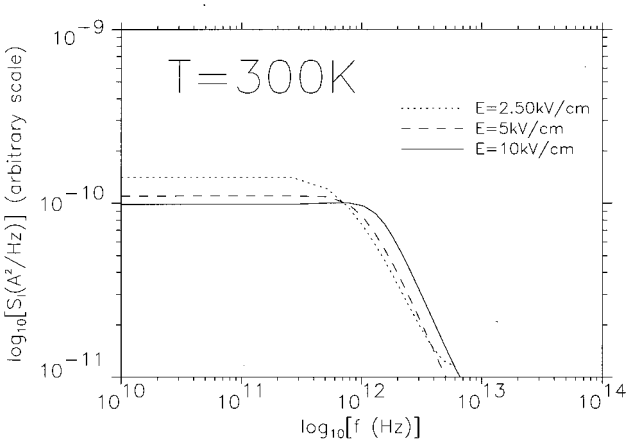

FIG. 4. Spectral density of electron current parallel to the electric field at 300 K. Corresponding to Fig. 2, the spectral density broadens with increasing electric fields.

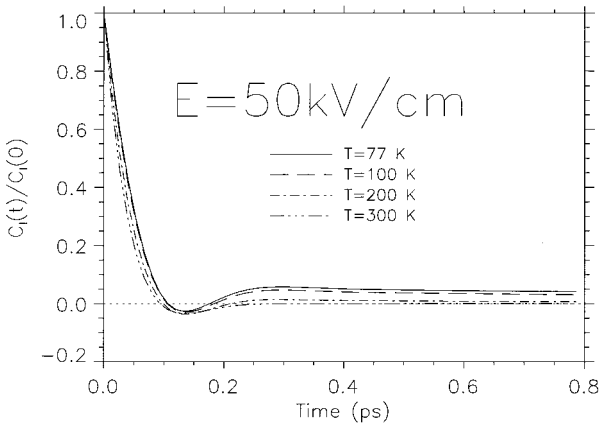

FIG. 5. The normalized autocorrelation function of the parallel component of electron current at an applied electric field of 50 kV/cm for several values of temperature. The figure illustrates that at high electric fields, the effect of temperature on noise autocorrelation function is small.

For the case of isotropic scattering, the above equation allows one to solve for $G_{\parallel}^{(1)}$ explicitly in terms of the total scattering rate and the steady-state distribution function. To this end, we shall represent each term of the above equation in terms of Legendre polynomials. First, we note that for isotropic scattering, the total rate does not depend on the angle of the momentum and consequently,

$$\lambda(\mathbf{k})=\lambda(k). \tag{39}$$

Furthermore, the transition rate only depends on the angle γ between $\mathbf{k}'$ and $\mathbf{k}$, hence, we can employ the following expansion:

$$W(\mathbf{k}',\mathbf{k})=W(k',k,\cos\gamma)=\sum_{l=0}^{\infty} a_l(k',k)P_l(\cos\gamma). \tag{40}$$

The above expression can be transformed by employing the addition theorem for spherical harmonics, which states that

$$P_l(\cos\gamma)=\frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^{*}(\theta',\phi')Y_{lm}(\theta,\phi). \tag{41}$$

As a result, the transition rate can be expressed in terms of spherical harmonics, as follows:

$$W(\mathbf{k}',\mathbf{k})=\sum_{l=0}^{\infty} a_l(k',k)\,\frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^{*}(\theta',\phi')Y_{lm}(\theta,\phi). \tag{42}$$

Furthermore, by substituting

$$P_n(\cos\theta)=\left(\frac{4\pi}{2n+1}\right)^{1/2} Y_{n0}(\theta,\phi) \tag{43}$$

into Eq. (34), $G_{\parallel}$ can be expressed in terms of spherical harmonics as well:

$$G_{\parallel}(\mathbf{k}',\omega)=\sum_{n=0}^{\infty} G_{\parallel}^{(n)}(k',\omega)\left(\frac{4\pi}{2n+1}\right)^{1/2} Y_{n0}(\theta',\phi'). \tag{44}$$

Next, we substitute Eqs. (42) and (44) into the collision integral and obtain

$$\int G_{\parallel}(\mathbf{k}',\omega)W(\mathbf{k}',\mathbf{k})d\mathbf{k}'=\int_0^{\infty} dk'k'^2\sum_{n=0}^{\infty} G_{\parallel}^{(n)}(k',\omega)\left(\frac{4\pi}{2n+1}\right)^{1/2}\sum_{l=0}^{\infty} a_l(k',k)$$
$$\times\frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)\int_0^{2\pi} d\phi'\int_0^{\pi} d\theta'\sin\theta' Y_{lm}^{*}(\theta',\phi')Y_{n0}(\theta',\phi'). \tag{45}$$

Now, in order to simplify the above expression, we employ the orthogonality property of the spherical harmonics and note that the angular integration results in $\delta_{l-n}\delta_{m-0}$. By using this fact and by employing (43), one can show that the scattering integral can be expressed in terms of Legendre polynomials as follows:

$$\int G_{\parallel}(\mathbf{k}',\omega)W(\mathbf{k}',\mathbf{k})d\mathbf{k}'=\sum_{n=0}^{\infty} P_n(\cos\theta)\,\frac{4\pi}{2n+1}\int_0^{\infty} dk'k'^2 a_n(k',k)G_{\parallel}^{(n)}(k',\omega). \tag{46}$$

Next we turn our attention to the right-hand side of Eq. (38) and expand it in terms of Legendre polynomials as well:

$$(v_\parallel - \langle v_\parallel \rangle) f(\mathbf{k}) = [\alpha(k) k \cos\theta - \langle v_\parallel \rangle] \sum_{n=0}^{\infty} f^{(n)}(k) P_n(\cos\theta). \tag{47}$$

Substituting the following recursive relationship for Legendre polynomials into the above equation,

$$\cos\theta \; P_n(\cos\theta) = \frac{n+1}{2n+1} \; P_{n+1}(\cos\theta) + \frac{n}{2n+1} \; P_{n-1}(\cos\theta), \tag{48}$$

one can transform Eq. (47) as follows:

$$(v_\parallel - \langle v_\parallel \rangle) f(\mathbf{k}) = \sum_{n=0}^{\infty} P_n(\cos\theta) \left[\frac{n}{2n-1} \; \alpha(k) k f^{(n-1)}(k) + \frac{n+1}{2n+3} \; \alpha(k) k f^{(n+1)}(k) - \langle v_\parallel \rangle f^{(n)}(k) \right]. \tag{49}$$

Finally, we substitute Eqs. (34), (39), (46), and (49) into Eq. (38), which results in the following integral equations for $G_\parallel^{(n)}$:

$$j\omega G_\parallel^{(n)}(k,\omega) - \frac{n}{2n-1} \; \alpha(k) k f^{(n-1)}(k) - \frac{n+1}{2n+3} \; \alpha(k) k f^{(n+1)}(k) + \langle k_\parallel \rangle f^{(n)}(k) - \frac{4\pi}{2n+1} \int_0^\infty dk' k'^2 a_n(k',k) G_\parallel^{(n)}(k',\omega)$$

$$+ \lambda(k) G_\parallel^{(n)}(k,\omega) = 0. \tag{50}$$

Since the noise spectral density depends only on $G_\parallel^{(1)}$, we consider the first equation:

$$[j\omega + \lambda(k)] G_\parallel^{(1)}(k,\omega) - \frac{4\pi}{3} \int_0^\infty dk' k'^2 a_1(k',k) G_\parallel^{(1)}(k',\omega) = \alpha(k) k [f^{(0)}(k) + \tfrac{2}{5} f^{(2)}(k)] - \langle v_\parallel \rangle f^{(1)}(k). \tag{51}$$

The above equation is derived for a highly doped Ohmic contact under the general condition that the scattering mechanisms are isotropic. In the analysis below, we shall concentrate on the particular case when scattering is due to optical and elastic acoustic phonons, only. A detailed description of these scattering mechanisms can be found in Refs. 4 and 8. For optical phonons, the scattering transition rate has the following form:

$$W^{\mathrm{opt}}(\mathbf{k}',\mathbf{k}) = S^{\mathrm{opt}} \delta(\epsilon(k') - \epsilon(k) \pm \hbar\omega_0), \tag{52}$$

which is independent of the momentum direction, hence, $a_1^{\mathrm{opt}} \equiv 0$. For acoustic phonons, the scattering transition rate has the following form:

$$W^a(\mathbf{k}',\mathbf{k}) = s^a(|\mathbf{k}'-\mathbf{k}|) \, \delta(\epsilon(k') - \epsilon(k) \pm \hbar\omega(|\mathbf{k}'-\mathbf{k}|)), \tag{53}$$

which depends on the momentum direction, hence, $a_1^a \neq 0$. Due to this inelastic collision term, substitution of $a_1^a(k',k)$ into Eq. (51) results in a *difference* equation for $G_\parallel^{(1)}$. In order to avoid the solution of a difference equation, we employ the commonly used elastic, equipartition approximation for acoustic phonons, which results in the following form for the scattering transition rate:[4]

$$W^a(\mathbf{k}',\mathbf{k}) \simeq \tilde{s}^a \delta(\epsilon(k') - \epsilon(k)). \tag{54}$$

For this approximation, the acoustic scattering transition rate is independent of the momentum angle and, consequently, $a_1^a \simeq 0$. As a result, Eq. (51) is easily solved for $G_\parallel^{(1)}(k,\omega)$ as follows:

$$G_\parallel^{(1)}(k,\omega) = \frac{\alpha(k) k [f^{(0)}(k) + \tfrac{2}{5} f^{(2)}(k)] - \langle v_\parallel \rangle f^{(1)}(k)}{j\omega + \lambda(k)}. \tag{55}$$

Now, the noise spectral density is easily obtained by substituting this last expression into Eq. (37):

$$S_I(\omega) = \frac{8\pi}{3} \, \mathrm{Re} \left\{ \int_0^\infty dk \; \alpha(k) k^3 \times \frac{\alpha(k) k [f^{(0)}(k) + \tfrac{2}{5} f^{(2)}(k)] - \langle v_\parallel \rangle f^{(1)}(k)}{j\omega + \lambda(k)} \right\}. \tag{56}$$

Thus, we have derived an explicit expression for the noise spectral density at a highly doped Ohmic contact in terms of the electron distribution function and the total scattering rate. In our derivations, the electric field and $\nabla_{\mathbf{x}}$ terms are assumed to be negligible, and the elastic, equipartition approximation has been used for the acoustic-phonon scattering transition rate.

According to Eq. (56), the noise spectral density depends on the Legendre polynomial coefficients of the electron distribution function f. The choice of the distribution function at Ohmic contacts is a subject of debate for many reasons, mainly because the electrons at Ohmic contacts are considered to be in thermal equilibrium even when there is a net current flow into the contact. In our computations, we will assume that the electron distribution function is given by a shifted Maxwellian:

$$f(\mathbf{k}) = \frac{n\hbar}{\sqrt{2\pi m k_B T}} \exp\left\{ - \frac{\hbar^2}{2 m k_B T} \, |\mathbf{k} - \langle \mathbf{k} \rangle|^2 \right\}, \tag{57}$$

where n is the electron density, k_B is the Boltzmann constant, and T is the lattice temperature. This choice of the distribution function is only employed here for the sake of simplicity of computations and it is not strictly justified.[5] In

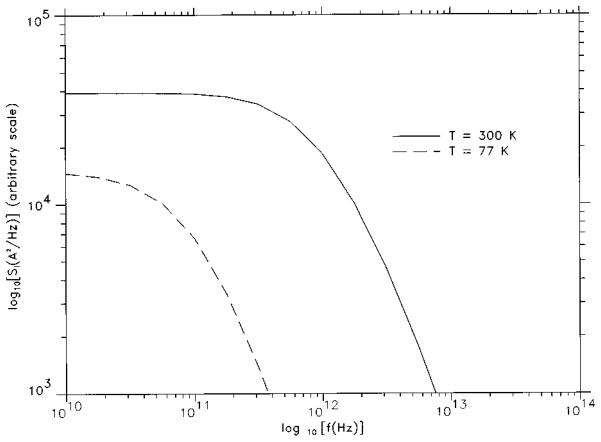

FIG. 6. Spectral density of the parallel component of the electron current at a highly doped Ohmic contact at 77 and 300 K. The figure illustrates the significant effect of temperature on the noise spectral density (or autocorrelation function) when the electric field is assumed to be small.

more sophisticated calculations, the distribution function can be computed from the numerical solution of the stationary BTE. The spherical harmonic expansion technique is quite suitable for this purpose since it leads directly to the determination of $f^{(n)}(\mathbf{k})$.[14]

The above machinery was employed to compute the noise spectral density $S_I(\omega)$ at a highly doped Ohmic contact by substituting the corresponding Legendre polynomial coefficients of Eq. (57) into Eq. (56). Figure 6 shows the noise spectral density at a highly doped Ohmic contact at temperatures 77 and 300 K. As expected, it can be seen that the noise spectral density broadens at higher temperature, similar to previous results of bulk silicon computations.

V. CONCLUSION

An approach was presented to model noise in semiconductors when electron motion is described by the semiclassical transport model. It is shown that the key computations of the autocovariance function and the noise spectral density are reduced to a special initial value problem for the BTE given by Eqs. (19)–(21). The distinct feature of this approach compared to other microscopic noise models is that this approach is strictly within the framework of semiclassical transport and does not require the addition of ''Langevin source terms,'' which are generally introduced into transport equations in order to account for random fluctuations. As a result, this approach directly connects the noise characteristics with the stochastic properties of scattering mechanisms in the semiclassical transport model. Based on this approach, a closed-form expression was derived for the noise spectral density at highly doped Ohmic contacts in terms of the scattering rate and the steady-state electron distribution function. Illustrative numerical simulation results are presented for the autocovariance function and spectral density of current fluctuations due to elastic acoustic and optical phonon scattering in bulk silicon and highly doped Ohmic contacts. Simulated results are found to be similar to those that are reported for noise computations employing the Monte Carlo method.[13]

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