Fokker-Planck approach to nonlocal high-field transport

E. Bringuier
URA 800 du CNRS, Université Pierre et Marie Curie, case 86, 4, place Jussieu, 75 252 Paris Cedex 05, France
(Received 14 April 1997)

The nonequilibrium energy distribution of electrons drifting in a solid subjected to a high electric field is shown to obey a master equation of the Fokker-Planck type allowing for explicit position dependence of the energy distribution, such as occurs in a sharply varying field. Excellent agreement is found between the Fokker-Planck prediction of the energy distribution and a Monte Carlo simulation of transport in the absence of any adjustable parameter. [S0163-1829(97)05434-9]

At low electric fields the drift velocity v_d of an electron in a solid is proportional to the local value of the field F at x, viz. $v_d(x)=\mu F(x)$, with μ possibly a tensor. This comes about because momentum-relaxing collisions occur over a time scale τ_m associated with a spatial scale much smaller than $F/(\partial F/\partial x)$. At low fields the electron energy E is thermal $\approx kT$, and its increase in the field is given up to the lattice at the same rate as momentum, that is, the energy relaxation time $\tau_E \approx \tau_m$, wherefore the energy distribution negligibly departs from that given by equilibrium statistics. At *high* fields entailing average energies well above kT, a distinct state of affairs is met[1] owing to $\tau_E \gg \tau_m$ for high-energy electrons interacting with the lattice principally via the emission of high-frequency phonons of energy $\hbar\omega \ll E$. This is associated with a characteristic energy-variation length $\lambda_E = v_d \tau_E$, much larger than the mean free path over which momentum averaging determines v_d. Therefore, the energy distribution at the location x is not determined by the local value of the field, but also by fields upstream of x, typically between $x-\lambda_E$ and x.

High-field transport in inhomogeneous fields entailing nonlocal effects is crucial to the understanding of submicrometer semiconductor devices. It is usually addressed in Monte Carlo simulations[2] which provide an exact solution to the semiclassical Boltzmann transport equation, but a simpler approach is offered by Ridley's lucky-drift theory.[3] Recently, a critical comparison[4] of both theories in the case of a homogeneous field disclosed two flaws in the latter which led to replace it by a Fokker-Planck approach which subsequently was shown to agree[5] with Monte Carlo predictions in a variety of cases. More precisely, the new approach is equivalent to the Boltzmann transport equation for *drifting* (i.e., not ballistic) electrons wherever the inelastic loss, $\hbar\omega$, is smaller than the energy exchanged with the field between two collisions. The purpose of this paper is to describe nonlocal transport within the Fokker-Planck framework. For simplicity a one-dimensional geometry is considered, where current density and field are oriented along x, and all quantities depend on x only.

The basic quantity $n(E,x,t)$ is the electron energy distribution at x at time t: $n(E,x,t)dEdx$ is defined as the probability of finding the electron in the spatial range $[x, x+dx]$ in the energy interval $[E, E+dE]$. Transitions in E-x space being continuous if $\hbar\omega \ll E$, the probability is conserved locally, and n obeys a continuity equation,

$$\partial n/\partial t + \partial J_E/\partial E + \partial J_x/\partial x = 0, \tag{1}$$

involving a probability current $\mathbf{J}$ in E-x space. Following the general Fokker-Planck scheme,[6] the current is envisioned as the sum of a drift term embodying the average trend, and a diffusion term associated with spreading

$$J_E = W(E,x)n - \frac{\partial(D_{EE}n)}{\partial E} - \frac{\partial(D_{Ex}n)}{\partial x}, \tag{2a}$$

$$J_x = v_d(E,x)n - \frac{\partial(D_{xE}n)}{\partial E} - \frac{\partial(D_{xx}n)}{\partial x}. \tag{2b}$$

W (in eV/s) and v_d (in cm/s) are the components, along the energy and real-space axes, of the local drift velocity of a particle of energy E located at x. The matrix D is a positive semidefinite symmetric one depending on the (E,x) point (time dependences are allowed though not written explicitly). When Eqs. (2a) and (2b) are inserted into Eq. (1), we have a multivariate Fokker-Planck equation, the properties of which are examined at length in van Kampen's treatise.[6] In short, a monoenergetic localized distribution, $n(E,x,0) = \delta(E-E_0)\delta(x-x_0)$, evolves into a Gaussian packet of which the centroid travels in E-x space at speed (W, v_d), and the extension is determined by the diffusion matrix D.

Before proceeding further, let us highlight the physical meaning of the transport coefficients appearing in Eqs. (2a) and (2b). Quantities having straightforward meaning are those referring to real-space motion, namely, v_d and D_{xx} in Eq. (2b). They are just the *spectral* drift velocity and diffusion coefficient in the sense that averaging them over energy yields the conventional drift velocity and diffusion coefficient. The use of spectral quantities is more familiar in gaseous[7] than in solid-state[8] electronics. Specifically, $v_d = \mu(E)F(x)$ and $D_{xx} = \overline{((v_g)_x(v_g)_x\tau_c)}_E$, where $\mu(E)$ is the mobility of a particle of energy E, and D_{xx} is the autocorrelation of the group velocity $\mathbf{v}_g$, with τ_c the correlation time[5] and $\overline{(\ldots)}_E$ the mean value over a constant-energy surface in momentum space. Once the material band structure and electron-phonon dynamics have been specified, $\mu(E)$ and $D_{xx}(E)$ are calculable.[4,9] This has been done in specific nonspherical nonparabolic materials in Ref. 5 where solutions of the x independent (i.e., local) Eq. (1) have been obtained. Generally speaking, at high E scattering times are short and entail small mobilities $\mu(E)$, while group velocities v_g grow

in such a way that the increase in v_g^2 usually outweighs the drop in τ_c, making the high-E spectral part of the motion strongly diffusive. The functions $\mu(E)$ and $D_{xx}(E)$ are pregiven quantities, which are independent of the actual occupation of energy space and thereby of the current state of motion, in contradistinction to the conventional μ and D_{xx} which are ensemble averages of the spectral quantities.

Ensemble average is defined by

$$\langle\ \rangle_E=\frac{\int_0^{+\infty}(\ )n(E,x)dE}{\int_0^{+\infty}n(E,x)dE}, \tag{3}$$

thus involving the distribution n. Integrating Eqs. (1) and (2b) over E leads to

$$\partial\underline{n}/\partial t+\partial\underline{j}_x/\partial x=0, \tag{1'}$$

$$\underline{j}_x=\langle\mu(E)\rangle_E F(x)\underline{n}-\frac{\partial[\langle D_{xx}(E)\rangle_E\underline{n}]}{\partial x}, \tag{2b'}$$

where $\underline{n}=\int_0^{+\infty}n(E,x)dE$ is the usual particle density (in cm^{-1}), and $\underline{j}_x=\int_0^{+\infty}J_x(E,x)dE$ is the usual particle current density (in s^{-1}). Equations (1′) and (2b′) are the familiar particle-conservation and drift-diffusion equations, respectively, *except* that the mobility $\langle\mu(E)\rangle_E$ and diffusion coefficient $\langle D_{xx}(E)\rangle_E$ are high-field quantities depending on the energy distribution $n(E,x,t)$ and thereby on the position and electric field. This stands in stark contrast with the low-field $\langle\mu(E)\rangle_E$ and $\langle D_{xx}(E)\rangle_E$ which are determined by the canonical ensemble averaging $n(E)\sim N(E)\exp(-E/kT)$ [$N(E)$ is the density of conduction-band states].

The second class of transport coefficients appears in Eq. (2a) referring to the motion along the energy axis, and we now proceed to determine them. The component J_E of the probability current along the energy axis reflects the energy gain or loss of the particle. In the semiclassical transport picture, it is made up of two decoupled contributions, one from the field and one from the phonon bath. As shown earlier,[4] energy exchange with the phonon bath gives rise to a drift term (embodying the average exchange) $W_{\mathrm{ph}}(E)n<0$, the diffusion term (embodying the fluctuations about the average) being of order $(\hbar\omega)^2$ and thus negligible in the high-energy limit.[4,5] Energy exchange with the field is just related to the real-space motion J_x, and contributes $qF(x)J_x$ to J_E, where $qF(x)$ is the force exerted on the particle. Then,

$$J_E=W_{\mathrm{ph}}(E)n+qF(x)J_x. \tag{4}$$

Substituting Eq. (2a) for J_E and Eq. (2b) for J_x in Eq. (4), an identity is obtained if and only if

$$W=W_{\mathrm{ph}}(E)+qF(x)^2\mu(E)+D_{xx}(E)\frac{\partial(qF)}{\partial x}, \tag{5a}$$

$$D_{Ex}=qF(x)D_{xx}(E), \tag{5b}$$

$$D_{EE}=qF(x)D_{xE}(E,x)=[qF(x)]^2D_{xx}(E), \tag{5c}$$

the last equality resulting from the symmetry of the diffusion matrix. The novelties introduced by the nonlocal theory are the nondiagonal diffusion coefficients $D_{Ex}=D_{xE}$ and the field gradient in Eq. (5a). The primary transport coefficients, whence all others may be derived through Eqs. (5a)–(5c), are $\mu(E)$ and $D_{xx}(E)$, which are obtainable from the material characteristics.[4,5,9]

We now illustrate the *modus operandi* of the nonlocal Fokker-Planck transport equation in the case of steady-state transport in a uniform F with the condition $n(E,x=0)=\underline{n}_0\delta(E)$ (density $\underline{n}_0$ of cold electrons injected at $x=0$). This is indeed a nonlocal transport problem, considering $n(E,0)$ to be determined by the field $F(x)=0$ at $x<0$, and the step increase in F at $x=0$ to be the field inhomogeneity. From Eqs. (1), (2), and (5) the Fokker-Planck equation is

$$(qF)^2\left[\frac{\partial}{\partial E}+\frac{\partial}{\partial(qFx)}\right]\left[\frac{\mu(E)}{q}n-\frac{\partial(D_{xx}n)}{\partial E}-\frac{\partial(D_{xx}n)}{\partial(qFx)}\right]+\frac{\partial(W_{\mathrm{ph}}n)}{\partial E}=0, \tag{6}$$

which is more conveniently expressed by taking $\xi=qFx-E$ and E as independent variables,

$$\frac{\partial(W_{\mathrm{ph}}n)}{\partial\xi}=\frac{\partial}{\partial E}\left\{[qF^2\mu(E)+W_{\mathrm{ph}}]n-\frac{\partial}{\partial E}(q^2F^2D_{xx}n)\right\}. \tag{7}$$

The boundary conditions are[6] $J_E=0$ at $E=0$ and $+\infty$. Solving for Eq. (7) also requires an ''initial'' condition, namely $n(E,\xi=0)$. At this juncture, it is essential to remember that Eq. (7) can only describe the drift mode, which starts once the electron experiences its first momentum-relaxing collision.[1] Now, immediately after injection the electron travels ballistically, and its distribution in E-x space, as the first scattering event initiates the drift motion, is

$$n(E=qFx,x)=\underline{n}_0(qF\lambda)^{-1}\exp(-x/\lambda), \tag{8}$$

where for definiteness an energy-independent mean free path λ is taken. Ballistic motion will be embedded in the Fokker-Planck framework as the initial condition: since $\xi=0$ at $x=0$, and ξ is conserved along a ballistic path, let

$$n(E,\xi=0)=\underline{n}_0(qF\lambda)^{-1}\exp(-E/qF\lambda) \tag{8'}$$

be the initial condition. (This is in keeping with Ridley's combination of the ballistic and drift transport modes.[1,3])

Specializing now Eq. (7) to the case of nearly-free electrons of effective mass m^*, isotropically exchanging constant-energy phonons at a rate proportional to the density of conduction-band states yields a mean free path λ constant for $E\gg\hbar\omega$, and the functions $\mu(E)=2q\lambda/3m^*v_g(E)$, $D_{xx}(E)=\lambda v_g(E)/3$, and $W_{\mathrm{ph}}(E)=-[2n(\omega)+1]\hbar\omega v_g(E)/\lambda$ are already known[4,5] [$v_g(E)$ denotes

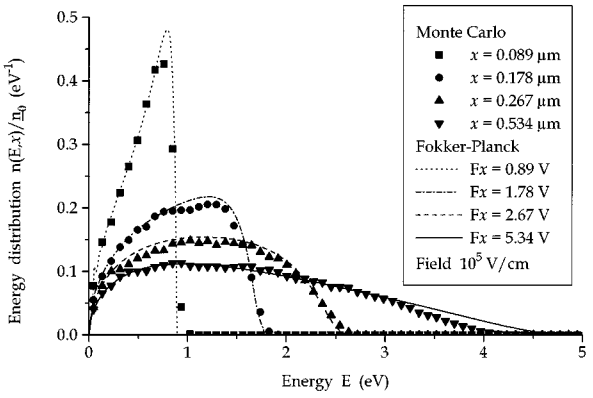

FIG. 1. Monte Carlo (points) and Fokker-Planck (lines) electron energy distributions $n(E,x)$, with distance x covered, or voltage drop Fx, as a parameter. Electric field $F=10^5$ V/cm. (Parameters from Ref. 10: $m^*/m_0=0.22$, $\lambda=282$ Å, $\hbar\omega=29$ meV, $T=300$ K.)

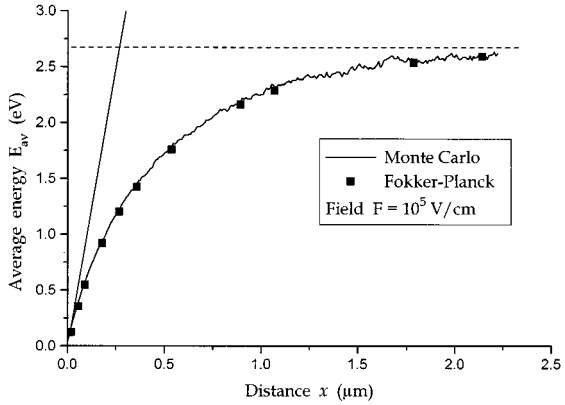

FIG. 2. Fokker-Planck (points) and Monte Carlo (solid line) average electron energies $E_{\rm av}(x)$ against distance x covered, in a uniform electric field $F=10^5$ V/cm, with $E_{\rm av}(0)=0$ as the initial condition. The straight solid line shows the ballistic law $E_{\rm av}(x)=qFx$, and the horizontal dashed line shows the asymptotic $E_{\rm av,\infty}$. Same parameters as in Fig. 1.

$(2E/m^*)^{1/2}$, and $n(\omega)$ is the Bose-Einstein number]. Taking $g(E,\xi)=\sqrt{E}n(E,x)$ as the unknown function, Eq. (7) reads

$$\frac{\partial g}{\partial \xi}=-\frac{\partial}{\partial E}\left[\left(\frac{E_w}{E}-1\right)g-E_w\frac{\partial g}{\partial E}\right], \tag{7'}$$

where $E_w=[2n(\omega)+1](qF\lambda)^2/3\hbar\omega$. The solution $g(E,\xi)$ has been obtained by means of a Crank-Nicholson finite-difference scheme, and the distribution $n(E,x)$ is plotted in Fig. 1 for several values of x. Asymptotically, it is found to become independent of x, viz.

$$n(E,+\infty)=\underline{n_0}\{2\hbar\omega/[2n(\omega)+1]qF\lambda\}^{1/2}\sqrt{E}\,\exp(-E/E_w). \tag{9}$$

As could be expected from Eq. (7) and Ref. 4, Eq. (9) is just the local distribution in a field F and yields an asymptotic average energy $E_{\rm av,\infty}=3E_w/2$. It is found to hold for $x\gg E_{\rm av,\infty}/qF$, which therefore has the meaning of an energy relaxation length λ_E.

Next, a Monte Carlo simulation has been carried out to study the transport of an ensemble of electrons injected in a uniform field F at $x=0$ with zero energy. Typically 25 000 histories have been analyzed using an energy mesh $E_w/30=59$ meV and a position mesh $E_w/60qF=30$ Å, and the energy distribution is shown in Fig. 1. The same parameters (from Ref. 10) are used in obtaining the Monte Carlo and Fokker-Planck data, which are seen to agree very well with each other, with no adjustable parameter. From the data of Fig. 1 the average energy $E_{\rm av}(x)$ at location x is computed and shown in Fig. 2. Again the agreement between the Fokker-Planck and Monte Carlo predictions is excellent, not only in the drift region ($x\gg\lambda$), but also where ballistic electrons bring an important contribution to n. This is attributed to our initial condition (8′) and is analogous to the interpolation of the Sharvin (ballistic) and Drude (diffusive) resistances in a metal wire.[11] Thus, for nonlocal as well as local transport, the Fokker-Planck equation (here, a partial differential equation in two variables, E and x) is equivalent to the Boltzmann partial differentio-integral equation in four variables, p_x, p_y, p_z, and x. This allows a considerably simpler approach to nonlocal transport than present-day Monte Carlo codes. Note that nowhere does our approach rely on a specific band model, although the Monte Carlo simulation supporting the Fokker-Planck prediction has been performed in a parabolic band. The general criterion for the validity of the Fokker-Planck approach is the same in the local and nonlocal cases, namely, the inelasticity $\hbar\omega$ should be small and the electrons are drifting. Therefore the same degree of accuracy that has been observed in the local case[5] is expected in the nonlocal one. A detailed, kinetic-theoretical proof of the equivalence of the Boltzmann and Fokker-Planck transport equations in arbitrary bands and three-dimensional space is planned for future publication.

A final remark is in order. Our nonlocal transport equation is arrived at from a nonequilibrium statistical-mechanical standpoint, with no appeal to kinetic theory. It is interesting to note that special instances of the equation have previously been obtained by means of (lengthy) kinetic-theoretical calculations. We shall give two examples. (i) In the case of an electron submitted to a high field in a weakly ionized gas, and assuming steady-state and uniform J_x, Druyvesteyn[12] has found that $n(E,x)$ obeys an equation which is identical to our Eq. (2a) equated to zero, in which $\mu(E)$ and $D_{xx}(E)$ are those used in Eq. (7′), and $W_{\rm ph}(E)$ stands for the rate of energy loss to the gas atoms. (ii) In the case of a fast neutron slowed down in a medium consisting of heavy atoms, the evolution of $n(E,x,t)$ toward the thermal distribution should be governed by a Fokker-Planck equation where J_E reduces to the loss term and J_x is purely diffusive, since $q=0$. In Ref. 13, the *same* equation is derived from an expansion of the Boltzmann transport equation, in which the small parameter is the energy lost by the neutron in a collision, similar to $\hbar\omega$ in a solid. Therefore our formalism encompasses a variety of physical situations while bypassing heavy calculations.

It is a pleasure to thank Catherine Oppenheim for information on Charpak's wire chambers, Bernadette Thomas for a discussion about partial differential equations, and A. Bourdon for a critical reading of the manuscript.

[1] B. K. Ridley, J. Phys. C **16**, 3373 (1983).
[2] M. V. Fischetti and S. E. Laux, Phys. Rev. B **38**, 9721 (1988); M. V. Fischetti, S. E. Laux, and E. Crabbé, J. Appl. Phys. **78**, 1058 (1995).
[3] B. K. Ridley and F. A. El-Ela, J. Phys., Condens. Matter **1**, 7021 (1989); B. K. Ridley, *ibid.* **2**, 2941 (1990).
[4] E. Bringuier, Phys. Rev. B **52**, 8092 (1995).
[5] E. Bringuier, Phys. Rev. B **54**, 1799 (1996).
[6] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd ed. (Elsevier, Amsterdam, 1992), Chaps. VIII and X.
[7] L. B. Loeb, *Basic Processes of Gaseous Electronics* (University of California Press, Berkeley, 1955), p. 310.
[8] W. Shockley, *Electrons and Holes in Semiconductors* (Van Nostrand, New York, 1950), pp. 293–294. The minus sign in the last formula should be replaced by a plus.
[9] Actually in Ref. 4 an isotropic electron-phonon interaction is considered when writing down the expressions of the energy-dependent drift velocity and diffusion coefficient. Reference 5 considers scattering anisotropy resulting in a correlation time τ_c distinct from τ. The general case will be tackled later.
[10] S. McKenzie and M. G. Burt, J. Phys. C **19**, 1959 (1986).
[11] M. J. M. de Jong, Phys. Rev. B **49**, 7778 (1994).
[12] M. J. Druyvesteyn, Physica (Eindhoven) **10**, 61 (1930); M. J. Druyvesteyn and F. M. Penning, Rev. Mod. Phys. **12**, 87 (1940).
[13] A. Akhiezer and S. Peletminski, *Les méthodes de la physique statistique* (Mir, Moscow, 1980), pp. 49–56 (in French; original Russian edition, 1977).