

## Kinetic theory of high-field transport in semiconductors

E. Bringuier

URA 800 du CNRS, case 86, Université Pierre et Marie Curie, 4, place Jussieu, 75 252 Paris Cedex 05, France

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The paper deals with electron transport in a semiconductor of arbitrary band structure and electron-phonon interaction, subjected to a high, but not necessarily homogeneous, electric field. The Boltzmann transport equation is simplified under the assumption that the occupation of momentum space is almost isotropic, as is the case for a drifting, not ballistic, electron. A closed-form equation for the electron energy distribution ensues: the equation is of the multivariate Fokker-Planck type in four-dimensional energy-position space. The typical relative departure between the Boltzmann and Fokker-Planck transport equations is the ratio of the hard-phonon energy to the average electron energy. Previous electron-transport equations in solids and gases are recovered as instantiations of ours. The hierarchies of scales underlying the derivation of the Fokker-Planck equation are those used in the lucky-drift model. [S0163-1829(98)04204-0]

### I. PURPOSE AND SCOPE

The interest of an analytical description of high-field transport in semiconductors is obvious. It has been remarked that a good understanding of semiclassical transport should be achieved prior to handling quantum effects.<sup>1</sup> Semiclassical transport is contained in Boltzmann's kinetic equation in which a realistic band structure should be used, and the complexity of the problem has led to the use of Monte Carlo solution techniques. A comparison of Monte Carlo simulations in Si in homogeneous electric fields has disclosed<sup>2</sup> "significant, often *vast*, difference even between models which would at first appear to be similar." It was later shown<sup>3</sup> that two models yielding identical predictions in homogeneous fields may exhibit considerable discrepancy in inhomogeneous fields. In view of these findings, it is desirable to devise a theoretical tool as analytical as possible in order to achieve better physical insight and simplicity of computation in transport problems. Statistical mechanics has always afforded a simpler approach than kinetic theory, and this has led us to set up a Fokker-Planck description of transport.<sup>4</sup> While the former considers the momentum-space occupation function  $f(\mathbf{p})$ , the latter is concerned with the energy-space occupation  $f_0(E)$ . The Fokker-Planck equation is a simpler master equation which is used as an approximation to the actual one, i.e., Boltzmann's. In Ref. 4, on the basis of van Kampen's general scheme,<sup>5</sup> we wrote that the approximate equation could in principle be derived from the actual one through an expansion in powers of  $(\hbar\omega/E_{av})^{1/2}$ , and is accurate to order  $(\hbar\omega/E_{av})^{1/2}$ , where  $\hbar\omega$  is the typical phonon energy (optical and zone-edge acoustic phonons, collectively termed hard phonons), and  $E_{av}$  is the average electron energy.

Comparison between Fokker-Planck and Monte Carlo predictions in homogeneous fields demonstrated<sup>6</sup> that simple convergence of the Fokker-Planck distribution towards the exact one always holds as the field  $F \rightarrow +\infty$ , and brought out the condition for uniform convergence over the entire energy range. Recently, we showed<sup>7</sup> that the Fokker-Planck machinery has the inborn capacity to take up transport in inhomogeneous fields as well, where the energy distribution exhibits

explicit position dependence, not accountable for within the dependence of field with position. Again the Boltzmann and Fokker-Planck predictions agreed with each other in the example considered. In the present article, we want to establish the mathematical link between both master equations and its physical meaning. Section II develops the Boltzmann kinetic equation in the case of drifting particles, whereby the Fokker-Planck equation is derived, and Sec. III briefly reviews the links with early and recent works and discloses their common background in physical terms.

### II. KINETIC THEORY OF DRIFTING PARTICLES

#### A. The problem

The particle's motion is semiclassically pictured as a sequence of unscattered flights controlled by the crystal potential and the applied electric force  $q\mathbf{F}$  ( $q$  denotes the charge of the particle), separated by collisions making the crystal momentum  $\mathbf{p}$  change abruptly and at random, at a rate

$$1/\tau(\mathbf{p}) = \int \int \int W_{\mathbf{p},\mathbf{p}'} d^3\mathbf{p}'/h^3 \quad (1)$$

(taking a unit volume of material), where  $W_{\mathbf{p},\mathbf{p}'} d^3\mathbf{p}'/h^3$  is the probability per unit time that an electron with crystal momentum  $\mathbf{p}$  be scattered to the momentum-space volume  $d^3\mathbf{p}'$  about  $\mathbf{p}'$ , and  $h$  is Planck's constant. For definiteness, scattering with lattice vibrations is considered herein, but all nearly elastic scatterings may be lumped together in  $W_{\mathbf{p},\mathbf{p}'}$ , while deeply inelastic mechanisms such as hole-electron pair creation are waived.

The crystal potential determines the spectrum of stationary states  $E(\mathbf{p})$  and the group velocity  $\mathbf{v}_g = \partial E/\partial \mathbf{p}$  (the band index is omitted for simpler notation). If  $\mathbf{r}$  is the position of the particle, the unscattered motion obeys

$$d\mathbf{r}/dt = \mathbf{v}_g(\mathbf{p}), \quad (2a)$$

and the superimposed effect of  $\mathbf{F}$  results in

$$d\mathbf{p}/dt = q\mathbf{F}(\mathbf{r}, t). \quad (2b)$$

An important feature of the spectrum is the density of states per unit energy

$$N(E) \equiv \int \int \int \delta[E - E(\mathbf{p})] d^3\mathbf{p}/h^3. \quad (3)$$

Given the dispersion relation  $E(\mathbf{p})$  and the scattering law, the goal of kinetic theory is to determine the momentum-space occupation function  $f(\mathbf{p}, \mathbf{r}, t)$  at location  $\mathbf{r}$  at time  $t$ . It is the solution of the Boltzmann (or Lorentz<sup>8</sup>) transport equation

$$(\partial f/\partial t) + \mathbf{v}_g(\mathbf{p}) \cdot (\partial f/\partial \mathbf{r}) + q\mathbf{F}(\mathbf{r}, t) \cdot (\partial f/\partial \mathbf{p}) = S\{f\}, \quad (4)$$

where  $S\{f\}$  is the scattering integral

$$S\{f\} \equiv \int \int \int [W_{\mathbf{p}', \mathbf{p}} f(\mathbf{p}', \mathbf{r}, t) - W_{\mathbf{p}, \mathbf{p}'} f(\mathbf{p}, \mathbf{r}, t)] d^3\mathbf{p}'/h^3. \quad (5)$$

The electron energy distribution is determined by the energy-space occupation function  $f_0(E, \mathbf{r}, t)$ , which is the mean value, denoted by  $(\cdots)_E$  of  $f(\mathbf{p}, \mathbf{r}, t)$  over a constant-energy surface  $E(\mathbf{p}) = E$ ,

$$f_0(E, \mathbf{r}, t) \equiv \overline{[f(\mathbf{p}, \mathbf{r}, t)]}_E. \quad (6a)$$

A function of cardinal interest is the deviation  $f_1$  of  $f$  from  $f_0$ ,

$$f_1(\mathbf{p}, \mathbf{r}, t) \equiv f(\mathbf{p}, \mathbf{r}, t) - f_0[E(\mathbf{p}), \mathbf{r}, t], \quad (6b)$$

since the average drift velocity  $\mathbf{v}_d$ , defined as the  $\mathbf{p}$ -space average of  $\mathbf{v}_g$ , is given by

$$\mathbf{v}_d = \frac{\int \int \int \mathbf{v}_g(\mathbf{p}) f_1(\mathbf{p}, \mathbf{r}, t) d^3\mathbf{p}}{\int \int \int f_0(\mathbf{p}, \mathbf{r}, t) d^3\mathbf{p}}, \quad (7)$$

owing to  $E(-\mathbf{p}) = E(\mathbf{p})$ .

### B. The idea of drift

If  $|f_1| \ll f_0$ , the momenta corresponding to a given energy are almost evenly distributed, and the drift velocity  $v_d$  is much less than the instantaneous velocity  $v_g$ . This is what is usually meant by *drift*, the opposite notion being that of a *streaming* particle whose average velocity (directed along the field in an isotropic or cubic material) is of the order of the instantaneous velocity. In Wannier's words,<sup>9</sup> a drifting particle stores large amounts of energy gained in the field in the form of random motion, not visible in the drift motion. The condition for electron transport to exhibit that feature of drift can be understood from Baraff's work<sup>10</sup> where the passage from streaming to drifting electrons is associated with the average energy  $E_{av}$  largely exceeding the collisional loss, namely, a constant optical-phonon energy  $\hbar\omega$ . If  $E_{av}$  is about  $\hbar\omega$ , the electron's energy almost vanishes after the collision, and so too does the velocity. The subsequent acceleration gives rise to a velocity essentially directed along the electric force, that is, the electrons stream down field, and  $v_d$  is of the order of  $v_g$ . In contradistinction, if  $E_{av}$  largely exceeds  $\hbar\omega$ , the velocity after the collision is little changed, *except*

for its direction, the memory of which is lost in the absence of polar scattering, so that the random motion overwhelms the average one. The contrast between the streaming and drifting states may be envisioned differently. Call  $\lambda$  the mean free path. The typical energy *possibly* gained from the field between two scattering events is  $qF\lambda$ , coming about for an electron moving downfield, while the typical energy *actually* gained is  $\hbar\omega$ , since on the average it should balance the loss. If  $qF\lambda \gg \hbar\omega$ , energy balance prevents the electron from proceeding along the electric-field line, and the trajectory is "folded" so that the average direction cosine of the instantaneous trajectory with the field line is<sup>11</sup>  $v_d/v_g \approx \hbar\omega/qF\lambda$ . [Momentum balance and the constancy of effective mass  $m$  entail  $mv_d = qF(\lambda/v_g)$ , whence the typical energy  $E_{av} \approx mv_g^2 \approx (qF\lambda)^2/\hbar\omega$ , and  $\hbar\omega/qF\lambda \approx (\hbar\omega/E_{av})^{1/2}$ , which is the parameter expected to be small.]

In the drifting state, Baraff's theory reproduces Wolff's,<sup>12</sup> which assumes  $|f_1| \ll f_0$  from the outset, but allows for collision anisotropy. Then a collision does not randomize the electron's motion any more, but just lengthens or shortens the mean free path (defined as the mean distance traveled before the direction of motion is randomized), thereby enhancing or reducing  $E_{av}$ . While the anisotropy renormalizes the mean free path,<sup>13</sup> the drift condition keeps the same, viz.,  $E_{av} \gg \hbar\omega$ : the scattering inelasticity should be small. The link between the small inelasticity and  $v_d \ll v_g$  is indeed ubiquitous, and has been noticed in the case of electrons in neutral gases<sup>14</sup> as well as in solids.

We shall henceforth consider drifting particles and develop the Boltzmann transport equation under the condition  $|f_1| \ll f_0$ . In the remainder of this subsection, an equation is derived relating  $f_1$  to  $f_0$ , and Sec. II C gives a closed-form equation on  $f_0$ .

There are many published works dealing with the relationship between the "isotropic" (in the sense of constant-energy average) and "anisotropic" (deviation from the average) parts of  $f$ . Regarding electron transport in gases, they are reviewed in Huxley and Crompton's book,<sup>15</sup> while in semiconductors the relationship has been derived in the spatially uniform case by the present author<sup>4</sup> following Shockley.<sup>16</sup> In the right-hand side of Eq. (5), since  $\hbar\omega \ll E$  the transition probabilities  $W_{\mathbf{p}, \mathbf{p}'}$  connect states lying approximately on the same energy surface  $E(\mathbf{p}) = E$ , so that

$$W_{\mathbf{p}, \mathbf{p}'} = T_{\mathbf{p}, \mathbf{p}'} \delta[E(\mathbf{p}) - E(\mathbf{p}')], \quad (8)$$

$$S\{f\} = -f_1(\mathbf{p})/\tau(\mathbf{p}) + \int \int_E f_1(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3, \quad (9)$$

where  $dS_{\mathbf{p}'}$  is the surface element about  $\mathbf{p}'$ . In the left-hand side of Eq. (4),  $f$  is replaced by  $f_0$ . Proceeding likewise in the spatially nonuniform case yields an integral equation on  $f_1$  involving  $f_0$ :

$$\begin{aligned} & (\partial f_0/\partial t) + \mathbf{v}_g(\mathbf{p}) \cdot (\partial f_0/\partial \mathbf{r}) + q\mathbf{F} \cdot (\partial f_0/\partial \mathbf{p}) \\ & = -f_1(\mathbf{p})/\tau(\mathbf{p}) + \int \int_E f_1(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3. \end{aligned} \quad (10)$$

At steady state the problem is solved (see, e.g., Moll's textbook<sup>17</sup>) if the right-hand side is cast in the relaxation-time form  $-f_1(\mathbf{p})/\tau_c(\mathbf{p})$ . It occurs in the models dealt with in Ref. 6, where  $\tau_c$  is the familiar relaxation time involving the persistence ratio of velocity. The *general* solution can be obtained<sup>18</sup> by introducing the vector mean free path  $\boldsymbol{\lambda}(\mathbf{p})$ , defined by the auxiliary integral equation

$$\boldsymbol{\lambda}(\mathbf{p}) - \tau(\mathbf{p}) \int \int_E \boldsymbol{\lambda}(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3 = \mathbf{v}_g(\mathbf{p}) \tau(\mathbf{p}). \quad (11)$$

Performing the scalar product of Eq. (11) and  $(\partial f_0 / \partial \mathbf{r}) + q\mathbf{F}(\partial f_0 / \partial E)$  shows that

$$f_1(\mathbf{p}, \mathbf{r}, t) = -\boldsymbol{\lambda}(\mathbf{p}) \cdot [(\partial f_0 / \partial \mathbf{r}) + q\mathbf{F}(\partial f_0 / \partial E)] \quad (12)$$

satisfies Eq. (10) if the time dependence is dropped. In case of isotropic scattering [i.e.,  $T_{\mathbf{p}, \mathbf{p}'}$  only depends on  $E(\mathbf{p})$ ],  $\boldsymbol{\lambda}(\mathbf{p})$  is just  $\mathbf{v}_g(\mathbf{p}) \tau(\mathbf{p})$ ; and in case a persistence ratio of velocity can be defined,  $\boldsymbol{\lambda}(\mathbf{p}) = \mathbf{v}_g(\mathbf{p}) \tau_c(\mathbf{p})$ . Otherwise  $\boldsymbol{\lambda}(\mathbf{p})$  is in general not parallel to the velocity, and can be obtained from a variational principle.<sup>18</sup>

The neglect of the time dependence  $(\partial f_0 / \partial t)$  in obtaining  $f_1$  (which in vanishing fields entails the conventional drift-diffusion equation<sup>17</sup>) deserves discussion. Generally speaking,<sup>19</sup> energy, and thence the energy occupation  $f_0$ , vary over the energy-relaxation time  $\tau_E$ , whereas momentum, and thence the momentum occupation, specified by  $f_1$  over a constant- $E$  surface, change over the momentum-relaxation time  $\tau_c$ , which is of the order of the scattering time  $\tau$  unless polar scattering prevails, in which case the drift condition presumed here would be invalid. Now under the very same condition,  $\tau_E / \tau \approx E_{av} / \hbar \omega \gg 1$ , wherefore the "fast" function  $f_1$  follows in time the "slow" function  $f_0$ , the time derivative of which may consistently be disregarded in obtaining  $f_1$ . This is in keeping with our statistical-mechanical approach to high-field transport,<sup>4</sup> where terms of order  $(\hbar \omega / E_{av})^{1/2} \approx v_d / v_g$  are retained while terms of order  $\hbar \omega / E_{av}$  are dropped.

### C. Fokker-Planck equation

Once  $f_1$  is known, the particle current density  $\mathbf{j}$  is obtained as

$$\mathbf{j} = \int \int \int \mathbf{v}_g(\mathbf{p}) f_1(\mathbf{p}, \mathbf{r}, t) d^3 \mathbf{p} / h^3 \quad (13)$$

( $f_0$  is even in  $\mathbf{p}$  while  $\mathbf{v}_g$  is odd), and the spectral current density, denoted by  $\mathbf{J}$ , is obtained by picking out the contribution from the energy shell  $[E, E + dE]$ , that is,

$$\mathbf{j} = \int_0^{+\infty} \mathbf{J} dE, \quad (14a)$$

$$\mathbf{J} = N(E) \overline{[\mathbf{v}_g(\mathbf{p}) f_1(\mathbf{p}, \mathbf{r}, t)]}_E. \quad (14b)$$

Substituting Eq. (12) for  $f_1$  yields, in Cartesian coordinates  $[\mathbf{r} = (x^1, x^2, x^3)]$  and using Einstein's summation convention,

$$J^i = -N(E) \overline{[v_g^i(\mathbf{p}) \lambda^j(\mathbf{p}) [(\partial f_0 / \partial x^j) + qF_j(\partial f_0 / \partial E)]]}_E, \quad (15)$$

In the first term involving  $f_0$  the spatial derivative and energy average may be interchanged, whence

$$J^i = -\frac{\partial}{\partial x^j} [D^{ij}(E) n(E, \mathbf{r}, t)] - qF_j N(E) D^{ij}(E) (\partial f_0 / \partial E), \quad (16)$$

where we have defined

$$D^{ij}(E) \equiv \overline{[v_g^i(\mathbf{p}) \lambda^j(\mathbf{p})]}_E, \quad (17)$$

and

$$n(E, \mathbf{r}, t) \equiv N(E) f_0(E, \mathbf{r}, t) \quad (18)$$

is the spectral carrier density. Introducing a total derivative in the last term of Eq. (16) yields

$$J^i = -\frac{\partial}{\partial x^j} [D^{ij}(E) n(E, \mathbf{r}, t)] - qF_j \frac{\partial}{\partial E} [D^{ij}(E) n(E, \mathbf{r}, t)] + qF_j \mu^{ij}(E) n(E, \mathbf{r}, t), \quad (19)$$

where, by definition,

$$N(E) \mu^{ij}(E) \equiv \frac{\partial}{\partial E} [N(E) D^{ij}(E)]. \quad (20)$$

(The mobility so defined<sup>20</sup> is the ratio of a velocity to an applied force  $qF$ .) The current density describes how the particle flows in real space; in order to describe its behavior in energy space, we introduce the coordinate  $x^0 = E$  and the corresponding component  $J^0$  of the spectral current density,

$$(J^0)_F = q\mathbf{F} \cdot \mathbf{J}, \quad (21)$$

where the subscript  $F$  means that only the energy exchange with the field is accounted for in the motion along the  $x^0$  axis. Since  $x^0$  and  $x^1, x^2, x^3$  have different physical dimensions, the four-dimensional continuum  $(E, \mathbf{r})$  is *not* metric, and ordinary (i.e., contravariant) components should not be identified with covariant ones. From the foregoing (Latin indices  $i, j$  running from 1 to 3),

$$(J^0)_F = -qF_i \frac{\partial}{\partial x^j} [D^{ij}(E) n(E, \mathbf{r}, t)] - qF_i qF_j \frac{\partial}{\partial E} [D^{ij}(E) n(E, \mathbf{r}, t)] + qF_i qF_j \mu^{ij}(E) n(E, \mathbf{r}, t). \quad (22)$$

Rearranging terms so as to introduce total derivatives yields

$$(J^0)_F = -\frac{\partial}{\partial x^j} [qF_i D^{ij}(E) n(E, \mathbf{r}, t)] - \frac{\partial}{\partial E} [qF_i qF_j D^{ij}(E) n(E, \mathbf{r}, t)] + \left[ qF_i qF_j \mu^{ij}(E) + D^{ij}(E) \frac{\partial(qF_i)}{\partial x^j} \right] n(E, \mathbf{r}, t). \quad (23)$$

The contribution  $(J^0)_{ph}$  from the phonon bath does not appear here since the small scattering inelasticity has been dropped out in Eq. (9). If only terms of first order in  $\hbar \omega$

are retained,<sup>4</sup> then  $(J^0)_{\text{ph}}$  is the average rate of energy loss to phonons,  $W_{\text{ph}}(E)n(E, \mathbf{r}, t)$ , where  $W_{\text{ph}}(E) = -[\hbar\omega(\mathbf{p}-\mathbf{p}')/\tau(\mathbf{p}')]_E$  for phonon emission [ $\hbar\omega(\mathbf{p})$  is the phonon dispersion relation]. In the semiclassical picture, phonon scattering is instantaneous and does not shift the particle in real space, thus does not contribute to  $J^i$ . Adding up  $(J^0)_{\text{ph}}$  and  $(J^0)_F$ ,

$$J^0 = \left[ qF_i qF_j \mu^{ij}(E) + D^{ij}(E) \frac{\partial(qF_i)}{\partial x^j} + W_{\text{ph}}(E) \right] n(E, \mathbf{r}, t) - \frac{\partial}{\partial x^0} [qF_i qF_j D^{ij}(E) n(E, \mathbf{r}, t)] - \frac{\partial}{\partial x^j} [qF_i D^{ij}(E) n(E, \mathbf{r}, t)], \quad (24a)$$

$$J^i = qF_j \mu^{ij}(E) n(E, \mathbf{r}, t) - \frac{\partial}{\partial x^0} [qF_j D^{ij}(E) n(E, \mathbf{r}, t)] - \frac{\partial}{\partial x^j} [D^{ij}(E) n(E, \mathbf{r}, t)]. \quad (24b)$$

The latter equations are drift-diffusion equations in  $(E, \mathbf{r})$  space and yield a multivariate Fokker-Planck equation once combined with the continuity equation

$$J^\beta = v_d^\beta(E, \mathbf{r}, t) n(E, \mathbf{r}, t) - \frac{\partial}{\partial x^\alpha} [D^{\beta\alpha}(E, \mathbf{r}, t) n(E, \mathbf{r}, t)], \quad (25a)$$

$$\frac{\partial n}{\partial t} + \frac{\partial J^\beta}{\partial x^\beta} = 0, \quad (25b)$$

where

$$v_d^0(E, \mathbf{r}, t) \equiv qF_i(\mathbf{r}, t) qF_j(\mathbf{r}, t) \mu^{ij}(E) + D^{ij}(E) \frac{\partial(qF_i)}{\partial x^j} + W_{\text{ph}}(E), \quad (26a)$$

$$v_d^i(E, \mathbf{r}, t) \equiv qF_j(\mathbf{r}, t) \mu^{ij}(E), \quad (26b)$$

$$D^{00}(E, \mathbf{r}, t) \equiv qF_i(\mathbf{r}, t) qF_j(\mathbf{r}, t) D^{ij}(E), \quad (26c)$$

$$D^{0i}(E, \mathbf{r}, t) \equiv D^{i0}(E, \mathbf{r}, t) \equiv qF_j(\mathbf{r}, t) D^{ij}(E), \quad (26d)$$

and Greek indices run from 0 to 3. The vector  $(v_d^\beta)$  is a local drift velocity in  $(E, \mathbf{r})$  space, and describes the instantaneous motion of the centroid of a sharply peaked distribution  $n$ , while the tensor  $(D^{\alpha\beta})$  describes the spreading of  $n$  in  $(E, \mathbf{r})$  space. Equations (25a) and (25b) are the three-dimensional version of the multivariate Fokker-Planck equation established earlier<sup>7</sup> from a statistical-mechanical standpoint by-passing kinetic theory. The kinetic-theoretical derivation rests on the assumptions of drift ( $|f_1| \ll f_0$ , or  $v_d \ll v_g$ ) and of small inelasticity ( $\hbar\omega \ll E_{\text{av}}$ ), which are related to each other through  $(\hbar\omega/E_{\text{av}})^{1/2} \approx v_d/v_g$ . The equations so derived are valid up to order  $(\hbar\omega/E_{\text{av}})^{1/2}$ , and the typical error is of order  $\hbar\omega/E_{\text{av}}$ .

Integration of Eq. (25b) over  $E$  gives the familiar, three-dimensional continuity equation. Integration of Eq. (25a)

over  $E$  gives a drift-diffusion expression for the three-dimensional current density  $\mathbf{j}$ , in which the mobility and diffusion coefficient depend on position<sup>7</sup> through  $n(E, \mathbf{r}, t)$ . Applications of such high-field transport equations are deferred to a future paper.

#### D. Boundary conditions

Partial-differential equations require boundary conditions. In the present problem, we need  $n(x^0, x^1, x^2, x^3, t=0)$  and the four-dimensional current density on the boundaries. Real-space boundaries determine the three-dimensional  $\mathbf{J}$  according to their physical features. Energy-space boundaries are such<sup>5</sup> that  $J^0=0$  at  $x^0=0$  and  $+\infty$ .

Ballistic transport (in which electrons stream along the field) is excluded and the Fokker-Planck set of equations should be applied in a region in  $(E, \mathbf{r})$  space where electrons drift. Therefore ballistic effects should be accounted for through a boundary condition, as was demonstrated in one dimension in Ref. 7. We just give an outline of the method in three dimensions. Take, for simplicity, the steady-state case [i.e., less than  $1/\tau_E$  (microwave) frequencies], and denote by  $qV(x^1, x^2, x^3)$  the electric potential energy. Consider that cold electrons ( $E=0$ ) are injected on the equipotential surface  $V=0$ . They first undergo a ballistic flight during which  $x^0 - qV(x^1, x^2, x^3)$  is constant=0, and the Fokker-Planck equations are not applicable. Define a curvilinear coordinate system  $(x'^0, x'^1, x'^2, x'^3)$  such that  $x'^0 = x^0$ ,  $x'^1 = -x^0 + qV(x^1, x^2, x^3)$ , and  $x'^2, x'^3$  locate a point on an equipotential surface (that is, constant  $x'^2$  and  $x'^3$  define an electric-field line). The obvious generalization of Eq. (25b) involves the covariant divergence

$$\frac{DJ'^\beta}{Dx'^\beta} = 0,$$

and the new initial condition involves the surface over which ballistic motion ceases and converts to drift motion, that is,  $x'^1=0$ . Afterwards,  $x'^1$  (the energy released by the electron while drifting towards larger  $V$ 's) takes positive values. The distribution  $n(x'^0, x'^1=0, x'^2, x'^3)$  is determined by ballistic motion starting from zero energy.

### III. LINK WITH OTHER WORKS

#### A. Charged particles in gases

The motion of a free particle of mass  $m$  in a neutral gas is described by  $E = \mathbf{p}^2/2m$ , and  $W_{\text{ph}}(E)$  should be understood as the rate of energy loss in collisions with the neutral gas atoms. If the particle's mass is much smaller than the atom mass  $M$ , scattering is almost elastic, and the average rate of loss is  $-2mE/M$ . Then scattering isotropy entails  $\boldsymbol{\lambda} = \mathbf{v}_g \tau$  and  $D^{ij}(E) = (v_g^i \lambda^j)_E = D(E) \delta^{ij}$ , with  $D(E) \equiv v_g \lambda/3$ . The mobility tensor  $\mu^{ij}(E)$  is given by Eq. (20) and equals  $\mu(E) \delta^{ij}$ , with

$$\mu(E) = \frac{1}{3} \sqrt{\frac{2}{mE}} \frac{d(E\lambda)}{dE}. \quad (27)$$

Then,  $J^0$  of Eq. (24a) reads, in one dimension ( $F$  along  $x^1 = x$ ),

$$J^0 = v_d^0(E, x, t) n(E, x, t) - \frac{\partial}{\partial x^0} [D^{00}(E, x, t) n(E, x, t)] - \frac{\partial}{\partial x^1} [D^{01}(E, x, t) n(E, x, t)], \quad (28a)$$

where

$$v_d^0(E, x, t) = (qF)^2 \mu(E) + D(E) \frac{\partial(qF)}{\partial x} - 2 \frac{m}{M} E, \quad (28b)$$

$$D^{00}(E, x, t) = (qF)^2 D(E), \quad (28c)$$

$$D^{01}(E, x, t) = qFD(E). \quad (28d)$$

Specializing further Eqs. (28a)–(28d) to a homogeneous  $F$ , we obtain Druyvesteyn's result [Eq. (6) of Ref. 14]. More general kinetic equations governing high-field electron transport in gases have been investigated and are reviewed in Huxley and Crompton's book,<sup>15</sup> and they are equivalent to our Fokker-Planck equations. The fact that Boltzmann's kinetic equation combined with the assumption of drift ( $|f_1| \ll f_0$ ) yields an equation of the Fokker-Planck type in energy space [or here, in  $v$  space,  $v = |\mathbf{v}_g| = (2E/m)^{1/2}$ ] seems to have been first pointed out by Davydov<sup>21</sup> and applied to solids.<sup>22</sup> It was later worked out by Wannier<sup>23</sup> who found that no less than eleven integrations were needed. Expression (27) for  $\mu(E)$  appears *inter alia* in articles dealing with charged particle transport in Charpak's wire chambers,<sup>24</sup> and is identical to Shockley's formula in semiconductor physics,<sup>25</sup> written in terms of  $\tau = \lambda/v$ . Energy-independent  $\tau$  yields Drude's formula  $\mu = \tau/m$ , while energy-independent  $\lambda$  leads to Townsend's<sup>26</sup>  $\mu(E) = 2\tau(E)/3m$ .

### B. Electrons in semiconductors

Analytical theories of electron transport in solids bearing relation to the present work are reviewed in Refs. 27, 28, and 4. In recent years, two papers<sup>29,30</sup> have been published in the mathematical literature overlapping ours. Technically speaking, *diffusion scaling* of the Boltzmann equation is performed, i.e., space and time scales are dilated according to<sup>29,30</sup>

$$\mathbf{r}' = \alpha \mathbf{r}, \quad (29a)$$

$$t' = \alpha^2 t, \quad (29b)$$

$$f_\alpha(\mathbf{p}, \mathbf{r}', t') = f(\mathbf{p}, \mathbf{r}, t), \quad (29c)$$

and a Hilbert expansion of the occupation function for  $\alpha \rightarrow 0$  is introduced,

$$f_\alpha = f^{(0)} + \alpha f^{(1)} + \alpha^2 f^{(2)} + \dots \quad (30)$$

The scaling parameter  $\alpha$  is then taken to measure the inelasticity of collisions,

$$\alpha^2 = \hbar \omega / E_{av}, \quad (31)$$

in our notation,<sup>31</sup> and the collision operator  $S\{f\}$  is expanded in powers of  $\alpha^2$ , yielding Eq. (9) as the zeroth-order (elastic)

term. At order  $\alpha^0$ , it is found that  $f^{(0)}$  actually is a function of  $E(\mathbf{p})$ , that is,  $f^{(0)}$  is our  $f_0$ . At order  $\alpha^1$ , the integral equation (11) is obtained and solved by introducing the vector mean free path  $\boldsymbol{\lambda}$ . [In Ref. 30, a possible dependence of  $\boldsymbol{\lambda}$  on  $\mathbf{r}$  due to inhomogeneous ionized-impurity scattering is envisaged; then,  $D^{ij} = D^{ij}(E, \mathbf{r})$  and our  $v_d^0$  should be written  $qF_i qF_j \mu^{ij}(E) + \partial[qF_i D^{ij}(E, \mathbf{r})]/\partial x^j + W_{ph}(E)$  instead of Eq. (26a).] At order  $\alpha^2$ , a solvability condition is obtained which entails an equation on  $f^{(0)}$  that in essence is identical to our Eq. (25b).

The equivalence between the Fokker-Planck approach and the Hilbert expansion of the Boltzmann transport equation just lies in the fact that both are based upon  $\alpha \ll 1$ . In Ref. 4 dealing with uniform transport, it was stated that the Fokker-Planck equation is an approximate master equation which in principle could be derived from the true one (i.e., Boltzmann's) by means of van Kampen's  $\Omega$  expansion,<sup>5</sup> and that the master equation is of diffusion type (thereby allowing use of a nonlinear Fokker-Planck equation). That statement is borne out by the kinetic-theoretical treatment of this article and the more explicitly systematic ones of Ref. 29 [in the case of isotropic scattering,  $\boldsymbol{\lambda}(\mathbf{p}) = \mathbf{v}_g(\mathbf{p}) \tau(\mathbf{p})$ ] and 30 [in the general case,  $\boldsymbol{\lambda}(\mathbf{p})$  not collinear to  $\mathbf{v}_g(\mathbf{p})$ ]. It turns out that  $\Omega^{-1}$  is just  $\alpha$ . [For completeness, we mention a study<sup>32</sup> of a completely different physical system governed by a linear Boltzmann equation (i.e., of the Lorentz type<sup>8</sup>) which can be approximated by a Fokker-Planck equation far from equilibrium.]

The physical meaning of the time scaling  $t' = \alpha^2 t$  has to do with the difference between the relaxation times of energy and momentum<sup>19</sup>  $\tau_E$  and  $\tau$  which are related through  $\tau_E \approx \tau E_{av}/\hbar \omega = \alpha^{-2} \tau$ . Space scaling  $\mathbf{r}' = \alpha \mathbf{r}$  has to do with the difference between the length scales corresponding to time  $\tau$ , over which the motion is ballistic (mean free path  $\lambda = v_g \tau$ ), and to time  $\tau_E$ , over which the particle drifts (energy relaxation length<sup>19</sup>  $\lambda_E = v_d \tau_E$ ). Since  $v_g/v_d$  is of the order of  $(E_{av}/\hbar \omega)^{1/2}$ , then  $\lambda_E \approx \alpha^{-1} \lambda$ . Thereby the device of diffusion scaling rests upon the same ladder of scales  $\hbar \omega/qF\lambda/E_{av}$  as that used in Ridley's lucky-drift model.<sup>19</sup> In short, while the concept of drift means  $v_g \gg v_d$  (Sec. II B), the concept of lucky drift means  $\lambda_E \gg \lambda$ , and Ridley's main finding is that drift entails lucky drift at high  $E_{av}$  where phonon scattering is nearly elastic. The Fokker-Planck approach is an elaboration of the lucky-drift theory in the nonballistic regime:<sup>4</sup> it yields the same typical values of the physical quantities, but is more rigorous in handling the fluctuations about the average in terms of a diffusion coefficient. This comes about because the fluctuation in position between two scattering events is typically  $\pm \lambda$  and entails a large fluctuation in  $E$ , while the average variation in position is  $v_d \tau \ll v_g \tau = \lambda$ , and it is the rationale for the use of a diffusion theory over times  $\lesssim \tau_E$ , or lengths  $\lesssim \lambda_E$ , over which<sup>33</sup>  $E$  and  $\mathbf{p}$  span the range allowed by  $f$ . It is also the reason for the semantic overlap between the notions of drift and diffusion.

### IV. CONCLUSION

In this paper, high-field electron transport in semiconductors has been investigated on the basis of the Boltzmann kinetic equation assuming drift, and the upshot is a multi-

variate Fokker-Planck equation governing the particle density in the energy-position continuum. The latter holds for average energies largely exceeding the phonon energies, except in the presence of ballistic motion which should be subsumed in appropriate boundary conditions. The equation involves local drift velocities and diffusion coefficients endowed with direct physical meaning, and calculable from the material characteristics. The formalism encourages use of a realistic band structure. If the material is covalent, the vector mean free path is obtained straightforwardly. If polar scattering is significant at the typical energies of interest, an integral equation in  $\lambda(\mathbf{p})$  is to be solved, e.g., by means of a variational principle. Great accuracy, however, is not needed, since the tensor components  $D^{ij}$  entering the transport equation are *integrals* over constant- $E$  surfaces. Once the diffusion tensor is known as a function of  $E$ , the statistics of transport are obtained by solving a set of partial-differential equations linear in  $n(E, \mathbf{r}, t)$ . The formalism has been illustrated in a one-dimensional example and found<sup>7</sup> to yield the

exact (Monte Carlo) solution of Boltzmann's transport equation (neglecting terms of order  $\hbar\omega/E_{av}$ ). It can be applied to hot-electron transport problems in short-channel transistor geometries as well. Inclusion of impact ionization events is planned for future work.

Mathematically speaking, the systematic expansion leading from the Boltzmann to the Fokker-Planck equation is in powers of  $\sqrt{\hbar\omega}$ . It involves diffusion scaling of the Boltzmann equation, and the underlying ladder of scales is the same as in Ridley's lucky-drift model. It rests on the strongly diffusive nature of transport at energies high enough that scattering can be considered as nearly elastic.

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