

Statistical mechanics of high-field transport in semiconductors

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The paper is devoted to the statistical-mechanical description of high-field transport in semiconductors within the semiclassical picture, assuming the band structure and electron-phonon interaction to be known. Our goal is to obtain a physical understanding in simple, universal terms without resorting to specific, simplified models for the band structure and/or the electron-phonon interaction. We first examine the lucky-drift model against an exact (analytical and numerical) solution of the Boltzmann transport equation in the simple parabolic case, and two discrepancies are found. The first stems from an incorrect expression for the drift velocity of a hot electron, while the second is associated with the approximate nature of the statistical device yielding the energy distribution. With the aim of retaining the features of simplicity of the lucky-drift description, another approach to the statistics of transport in the high-field regime is developed, based upon a nonlinear Fokker-Planck equation in energy space. While it gives the exact solution in the parabolic case, it has the ability to take up transport in an arbitrary band structure as well, and accounts for the success of the generalized lucky-drift model. The carrier energy distribution is expressed in terms of integrals over constant-energy surfaces in the Brillouin zone; the integrals involve the electron-phonon interaction and have direct physical meaning. The momentum-space distribution is derived approximately from the energy distribution. A simple comprehensive picture of transport statistics emerges that is not linked to a particular material or to specific assumptions regarding the electron-phonon interaction.

I. INTRODUCTION

The fundamental and practical importance of high-field transport in semiconductors is widely known.¹ The quantum mechanics comprises the kinematics (energy-momentum relationship), for which present band-structure models are deemed satisfactory, and the dynamics (electron-phonon interaction), which is incompletely known at high carrier energy. The description of the large-time behavior of a carrier (range of energy and momentum explored, real-space motion . . .) on the basis of those ingredients calls for a statistical-mechanical model, which most frequently rests on the semiclassical Boltzmann transport picture, and numerical solutions are found through Monte Carlo simulations. This technique has reached a high level of sophistication, and yields not only the steady-state solution, but allows for the examination of transients and nonuniform situations.² Yet there is still a need for simple models giving straightforward understanding of general features of transport and prediction of the chemico-physical trends. Not only is it appealing for general solid-state physicists, but it is also our experience that even well-written papers describing Monte Carlo simulations are sometimes basically misunderstood by the device designers calling for them. In 1983, Ridley³ introduced the so-called lucky-drift model of high-field transport in order to find out the main factors controlling the high-energy tail of the carrier distribution, responsible for band-to-band or impurity impact-ionization processes. Shortly after Shichijo and Hess's simulation⁴ including a realistic band structure, he³ could show qualitatively why an electron experiencing many collisions was usually more lucky in attaining high ener-

gies than a ballistic electron, hence the name, lucky drift. He also found that in addition to the mean free path, another characteristic length played a determinant role at high field, namely, the energy relaxation length. Let us say, in short, that Ridley's model is based upon a hierarchy of scales, whether in time, energy, or distance. This first version of the model was developed quantitatively in the case of a parabolic band structure, and good agreement with Baraff's solution of the Boltzmann transport equation was found; but the main features carry over to a nonparabolic monovalley model.³ Later, Burt introduced a variant⁵ of the lucky-drift model and the agreement with Monte Carlo simulations was found to be excellent in the parabolic case,⁶ and moderate in the nonparabolic multivalley case.⁷ More recently, we introduced a third version⁸ of that model in order to use the same expressions for expectation values that are employed in Monte Carlo simulations, so as to sharpen the correspondence between both descriptions. We could make an euristic generalization of the model to arbitrary band structures, and this resulted in a very encouraging, parameter-free comparison with a computer simulation.^{8,9}

In this paper, a critical examination of the lucky-drift model (Sec. II) shows that the apparent agreement⁶ with Monte Carlo results actually comes from the cancellation of two unsuspected flaws. The major one is due to the failure of the Drude formula for the local drift velocity. The second one is rooted in the lucky-drift ansatz yielding the energy distribution. In Sec. III, that ansatz is replaced by a nonlinear Fokker-Planck equation in energy space. Agreement with the prediction of the Boltzmann transport equation is excellent in parabolic bands. However, the energy distribution is obtained analytically for

arbitrary band structure and electron-phonon interaction; the quantities entering the solution are calculated in the Appendixes. Next, Sec. IV applies the Boltzmann equation to obtain the carrier distribution in momentum space, which is shown to depart slightly, and can be derived, from the distribution in energy space. That small departure provides the justification of the Fokker-Planck approach. Section V sketches the conclusions.

II. CRITICAL LOOK AT THE LUCKY-DRIFT MODEL

A. Introduction

The statistics of any transport model consists of at least two parts: (i) calculating the expectation values of the observables, and (ii) obtaining the probability law of energy or momentum. In a previous paper,⁸ we pointed out that some of the expectation values in the original lucky-drift model were not calculated in the standard way of statistical mechanics owing to the use of a helpful fiction, the so-called lucky-drift trajectories. In some, but not all, cases, this fiction led to discrepancies that we chose to eliminate by forsaking the notion of a deterministic real-space trajectory, and by coming back to the statistical-mechanical orthodoxy underlying computer simulations. But at the same time, we retained the idea of lucky-drift trajectories *in energy space*, in order to obtain the probability law $n(E)$, where $n(E)dE$ is the probability for the carrier's energy to be in the interval $[E, E+dE]$, or alternatively the repartition function³ (probability for the energy to exceed E)

$$P(E) = \int_E^{+\infty} n(E') dE'. \quad (1)$$

The lucky-drift expression for $P(E)$ at high E can be obtained easily by noticing^{3,6} that the main contribution is the probability for the carrier to avoid energy relaxation, while drifting from zero energy up to E . Energy relaxation in the drift mode is characterized by an energy relaxation length λ_E , which is the distance traveled by an electron drifting at the velocity $v_d(E)$, during the energy relaxation time $\tau_E(E)$. Considering phonon emission only, the latter is defined by³

$$E/\tau_E(E) = \hbar\omega/\tau(E), \quad (2)$$

where $\tau(E)$ is the collision time, $\hbar\omega$ the phonon energy (assumed constant), and $v_d(E)$ is given by a Drude expression (written here for constant effective mass m^* , i.e., for a parabolic band),

$$v_d(E) = qF\tau(E)/m^*. \quad (3)$$

In the parabolic case $\lambda_E = v_d(E)\tau_E(E)$ is independent of energy,^{3,6} while it depends on E in a nonparabolic band structure.⁸ It usually drops at high E , owing to the increase in the scattering rate.

Since the probability of drifting over dz and thereby gaining $dE' = qF dz$ from the field without relaxing energy to the lattice is $1 - dz/\lambda_E(E') = \exp[-dz/\lambda_E(E')]$,

$$P(E)|_{LD} \simeq \exp \left[- \int_0^E \frac{dE'}{qF\lambda_E(E')} \right], \quad (4a)$$

$$n(E)|_{LD} \simeq [qF\lambda_E(E)]^{-1} \exp \left[- \int_0^E \frac{dE'}{qF\lambda_E(E')} \right]. \quad (4b)$$

The latter equation is just Eq. (44) of Ref. 8 in which the ballistic contribution is dropped. At low E , collisions are infrequent and the electrons travel ballistically rather than by drift. One strength of the lucky-drift model is its ability to combine ballistic and drift motions in calculating^{6,8} $P(E)$. In this paper, we shall be concerned with the high-energy realm and thus disregard the ballistic contribution.

The prediction of Eq. (4b) was compared⁸ to Monte Carlo data for ZnS (a GaAs-like material) from a simulation performed in a realistic band structure, and satisfactory agreement was found without using any adjustable parameter. The available Monte Carlo data comprised the energy distribution about the average energy, for two values of field. In so doing, we followed the spirit of McKenzie and Burt's work,⁶ which was devoted to such a comparison in the simple parabolic case, and obtained a very good agreement for the average energy and the hard-threshold impact-ionization rate over four orders of magnitude.

B. Wolff's theory and the lucky-drift model

It is clear from the outset that the $P(E)$ obtained by the lucky-drift model is approximate. The success of the previous comparisons asks the question of the extent of its accuracy. Obviously the clearest answer should resort to an analytical, instead of numerical, comparison with an exact solution of the Boltzmann transport equation. Such an exact solution exists in the case of a parabolic band structure, with an isotropic electron-lattice interaction characterized by a constant mean free path in which each interaction consists of the emission of a fixed quantum $\hbar\omega$. It is Wolff's theory,¹⁰ which idealizes the non-polar (deformation-potential) interaction with optical phonons. The fact that only emission, and not absorption, is considered, makes it a zero-temperature theory, which can be straightforwardly extended¹¹ to finite temperatures for high-energy carriers ($E \gg \hbar\omega$) thanks¹² to the golden-rule expression of the electron-phonon interaction rate. At finite temperature, one simply has to replace $\hbar\omega$ by $\hbar\omega/[2n(\omega)+1]$, where $n(\omega) = [\exp(\hbar\omega/kT) - 1]^{-1}$ is the Bose-Einstein population of the optical mode. Another simplification of Wolff's solution to the Boltzmann equation is the consideration of a weak anisotropy of the \mathbf{k} -space occupation function $f(\mathbf{k})$, expressed by truncation to the first spherical harmonic,

$$f(\mathbf{k}) = f_0(E) + f_1(E) \cos\theta, \quad (5)$$

where $f_0(E)$ has the meaning of the energy occupation function [that is, $n(E) = N(E)f_0(E)$, $N(E)$ being the density of states], and $|f_1(E)| \ll f_0(E)$. Such an assumption proves to be valid at high field, where the collisions are so frequent that they scatter the electrons in all directions.

Intermediate fields give rise to a larger anisotropy and require higher-order harmonics, and this has been addressed by Baraff.^{13,14} In the lucky-drift picture, it means that electrons reaching high energies do so by drift, not ballistically.

From Boltzmann's equation and Eq. (5), Wolff has derived simple equations for f_0 and f_1 ,

$$d^2f_0/dE^2 + (E^{-1} + E_w^{-1})df_0/dE + f_0/EE_w = 0, \quad (6a)$$

$$f_1 = -qF\lambda df_0/dE, \quad (6b)$$

where $E_w = (qF\lambda)^2/3\hbar\omega$ is a characteristic energy depending on the electric field F and the constant mean free path λ . If we disregard the impact-ionization events considered by Wolff, the only solution of (6a) that remains finite as $E \rightarrow +\infty$ is $f_0(E) \sim \exp(-E/E_w)$, where \sim means henceforth a proportional relationship. Thus,

$$n(E) \sim E^{1/2} \exp(-E/E_w), \quad (7)$$

and the repartition function [Eq. (1)] is

$$P(E) = \Gamma(3/2, E/E_w) / \Gamma(3/2), \quad (8a)$$

where the incomplete Euler function $\Gamma(u, x)$ has an asymptotic expansion,

$$\Gamma(u, x) = \int_x^{+\infty} t^{u-1} e^{-t} dt \simeq x^{u-1} e^{-x} [1 + (u-1)/x + \dots],$$

yielding (for $E \gg E_w$)

$$P(E) \simeq 2(E/E_w)^{1/2} \exp(-E/E_w) / \sqrt{\pi}. \quad (8b)$$

Now the lucky-drift model yields in the high-energy limit,^{6,8}

$$n(E) \sim \exp(-2E/3E_w), \quad (9a)$$

$$P(E) \simeq \exp(-2E/3E_w). \quad (9b)$$

The discrepancy between Wolff's theory and the lucky-drift model is twofold: (i) there is a misfit in the dominant exponential term, and (ii) the subdominant, preexponential factor is different. In contrast, if we calculate the average energies, they agree to be $E_{av} = 3E_w/2$.

The question which immediately arises is the following: Since the Monte Carlo simulation gives an exact solution to the Boltzmann transport equation, it should yield Wolff's result, and therefore disagree with the lucky-drift prediction, contrary to McKenzie and Burt's findings.⁶ They compared the average energies given by the lucky-drift and Monte Carlo models, and found excellent agreement, as expected. They compared the high-energy tails given by both models by calculating the hard-threshold impact-ionization rate α_n at $E = 1.5, 2.0,$ and 3.0 eV, taking a set of GaAs parameters. The ionization rate as a function of E ,

$$\alpha_n = qF \frac{P(E)}{\int_0^E P(E') dE'}, \quad (10)$$

is proportional to $P(E)$ for $E_{av} \ll E$, in which case the denominator is E_{av} . For $E_{av} \gtrsim E$ (where E_{av} is calculated as $3E_w/2$, i.e., discarding impact-ionizing events), a large

fraction of carriers reaches the threshold, $P(E') \approx 1$ for $0 \leq E' \leq E$, and $\alpha_n \approx qF/E$ becomes hardly sensitive to the $P(E)$ function. Therefore, only in the $E_{av} \ll E$ case do we truly probe the high-energy tail of the distribution. This requires that, at a given E, F should not be too high, though high enough for the lucky-drift concept to be applicable. Consequently, the relevant range of field should obey

$$2\hbar\omega \ll qF\lambda \ll (2E\hbar\omega)^{1/2}, \quad (11a)$$

so that $E_{av} \ll E$ corresponds to

$$(E/2\hbar\omega)^{1/2} \ll E/qF\lambda. \quad (11b)$$

In Ref. 6, $(E/2\hbar\omega)^{1/2}$, calculated at room temperature, ranges between 7 and 10, while $E/qF\lambda$ actually never exceeds 20, so that (11b) is not satisfied and Wolff's asymptotic form is never reached, and the discrepancy between Eqs. (8b) and (9b) cannot be disclosed. The same is true of Ridley's comparison³ with Baraff's curves, which are the numerical solution of Boltzmann's equation.

C. Monte Carlo simulation

For the sake of completeness, we have performed a Monte Carlo simulation corresponding to Wolff's theory. At finite temperature, emission and absorption processes have been treated exactly, namely,

$$[1/\tau(E)]_{em} = [n(\omega) + 1]v_g(E - \hbar\omega)/\lambda_0, \quad (12a)$$

$$[1/\tau(E)]_{abs} = n(\omega)v_g(E + \hbar\omega)/\lambda_0, \quad (12b)$$

where $v_g(E) = (2E/m^*)^{1/2}$, m^* is the effective mass, and $\lambda_0 = [2n(\omega) + 1]\lambda$ is the zero-temperature mean free path. We have taken two sets of parameters, those of Ref. 6 ($\lambda_0 = 550$ Å, $m^*/m_0 = 0.22$, $\hbar\omega = 29$ meV) and those of Refs. 8 and 9 ($\lambda_0 = 45$ Å, $m^*/m_0 = 0.30$, $\hbar\omega = 42$ meV) at $T = 300$ K. No impact-ionizing events were introduced in order to study the effect of the electron-phonon interaction alone up to very high energies. The high-energy tail has been probed by counting the number of collision-free flights ending above nE_{av} ($1 \leq n \leq 7$), which yields¹⁵ an estimator of $P(nE_{av})$. More than 10^9 scattering events, real or fake, were simulated in order to get a reproducible $P(7E_{av})$. This is confronted to the Wolff and lucky-drift predictions in Table I, part of which are displayed in Fig. 1. One can see that Wolff's and the Monte Carlo solutions to the Boltzmann transport equation agree extremely well with each other, as they should, while the lucky-drift prediction steadily deviates as E becomes higher. This holds at high fields, while at lower fields the agreement between Wolff's and the Monte Carlo solutions is not as good, as expected owing to the simplifications in the former. In the low/intermediate ($0-2E_{av}$) energy range, the lucky-drift and Monte Carlo figures agree with each other, in consistency with the findings of Ref. 6: this means that (i) the average energies obtained by both approaches are the same, and (ii) the errors in the exponential term and the prefactor cancel each other around E_{av} . In the case of a realistic band

structure, our comparison⁸ between Monte Carlo data and the generalized lucky-drift model was made over a small energy range around E_{av} . Therefore, we attribute the good agreement obtained⁸ to such cancellation of errors in the exponential and nonexponential factors in the intermediate-energy range, and to the very close⁸ values of E_{av} obtained from both approaches. The results of this paper strongly suggest that for $E \gg E_{av}$, the Monte Carlo and lucky-drift predictions would disagree, but the available Monte Carlo data⁸ are restricted to the intermediate energy range.

(In passing we could see that Wolff's solution is closer to the Monte Carlo results than is the analytical theory of Baraff,¹⁴ based on the maximum anisotropy approximation. That theory is designed to represent analytically the whole energy distribution over a large field range, comprising the low-energy part, which contains ballistic electrons responsible for anisotropy at moderate fields, and thereby cannot be very accurate as regards the high-energy tail.)

D. The lucky-drift velocity revisited

Since the lucky-drift approach is deliberately approximate, and was successful in interpolating the ballistic and drifting behaviors of a hot electron,^{3,6} it should not be blamed for the absence of the $E^{1/2}$ factor in $P(E)$ [Eqs. (8b) and (9b)], but in view of the results of Sec. II C the dominant, exponential dependence should be corrected. The argument of the exponential is $-E/qF\lambda_E$, where in $\lambda_E = v_d(E)\tau_E(E)$ the energy-dependent drift velocity is given by a Drude expression Eq. (3). The idea behind Eq. (3) is the central idea of lucky drift, that is, the electron relaxes crystal momentum and attains a state of drift while its energy is almost unaffected by the collisions as

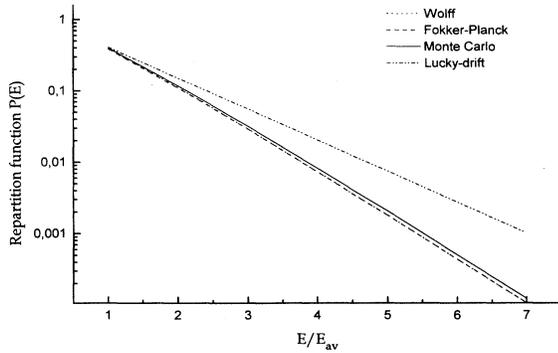


FIG. 1. Semilogarithmic plot of the repartition function $P(E)$ (probability for the carrier's energy to exceed E) as a function of energy E over the $[E_{av}, 7E_{av}]$ range. The band structure is parabolic, and the electron-phonon interaction is isotropic with a constant mean free path. Parameter values $\lambda_0 = 550 \text{ \AA}$, $m^*/m_0 = 0.22$, $\hbar\omega = 29 \text{ meV}$, $T = 300 \text{ K}$, field $F = 0.1 \text{ MV/cm}$ (from Table I). The results calculated from four theories [Wolff's (Ref. 10, dotted line), Monte Carlo (Sec. II C), lucky-drift (Ref. 6), and Fokker-Planck Eq. (27) (dashed line)] are shown. The Wolff and Fokker-Planck figures are almost indistinguishable.

TABLE I. Comparison of $P(nE_{av})$ ($1 \leq n \leq 7$, $E_{av} = (qF\lambda_0)^2 / \{2\hbar\omega[2\pi(\omega) + 1]\}$) obtained from different theories of high-field transport in a parabolic band structure [Wolff's (Ref. 10), Fokker-Planck Eq. (27), Monte Carlo (Sec. II C), and lucky-drift (Ref. 6)]. Two sets of parameters have been considered, from Ref. 6 ($\lambda_0 = 550 \text{ \AA}$, $m^*/m_0 = 0.22$, $\hbar\omega = 29 \text{ meV}$, "low-energy GaAs") and Refs. 8 and 9 ($\lambda_0 = 45 \text{ \AA}$, $m^*/m_0 = 0.30$, $\hbar\omega = 42 \text{ meV}$, "high-energy ZnS"), at $T = 300 \text{ K}$. Two values of field F have been used in each case. Wolff's figures [Eq. (6a)] are universal. The first set (GaAs at 0.1 MV/cm) has been plotted as Fig. 1.

Model	Parameters	$10 \times P(E_{av})$	$10 \times P(2E_{av})$	$10^2 \times P(3E_{av})$	$10^3 \times P(4E_{av})$	$10^3 \times P(5E_{av})$	$10^4 \times P(6E_{av})$	$10^4 \times P(7E_{av})$
Wolff		3.92	1.12	2.93	7.38	1.82	4.40	1.06
Fokker-Planck		3.88	1.10	2.96	7.33	1.81	4.40	1.06
Monte Carlo	"GaAs" $F = 0.1 \text{ MV/cm}$	4.00	1.18	3.18	8.29	2.08	5.07	1.23
Lucky drift		4.11	1.51	5.57	20.5	7.53	27.7	10.2
Fokker-Planck		3.90	1.11	2.92	7.36	1.81	4.40	1.05
Monte Carlo	"GaAs" $F = 0.15 \text{ MV/cm}$	3.97	1.15	3.08	7.99	1.93	4.41	1.03
Lucky drift		3.96	1.46	5.36	19.7	7.25	26.7	9.81
Fokker-Planck		3.88	1.11	2.95	7.52	1.88	4.61	1.12
Monte Carlo	"ZnS" $F = 1 \text{ MV/cm}$	4.09	1.24	3.47	9.34	2.45	6.23	1.52
Lucky drift		4.51	1.66	6.12	22.5	8.28	30.5	11.2
Fokker-Planck		3.91	1.11	2.93	7.42	1.83	4.45	1.07
Monte Carlo	"ZnS" $F = 2 \text{ MV/cm}$	3.97	1.15	3.09	7.96	1.99	5.00	1.16
Lucky drift		4.06	1.49	5.49	20.2	7.43	27.3	10.1

$E \gg \hbar\omega$. This assumes that the variation in E and thence in τ is negligible over the scattering time, in other words that the change in τ would give a small, first-order correction to the Drude expression, which applies for a constant collision time.

However natural such an assumption looks, it is incorrect. As a matter of fact, the variation of the collision time as the electron is being accelerated by the field between two collisions brings a *zero-order correction to the drift velocity*.¹⁶ In the case of parabolic dispersion relation and isotropic scattering, Shockley¹⁶ arrives at

$$v_d(E) = qF\tau(E) \left[1 - \left(\frac{2}{3}\right) \frac{d \ln(1/\tau)}{d \ln E} \right] / m^* . \quad (13)$$

This was needed to explain why the energy-dependent Drude mobility fails to give the conventional mobility upon integration over energy in the thermalized transport regime, a discrepancy we also pointed out in the high-field transport regime.⁸ For deformation-potential scattering $1/\tau \sim E^{1/2}$, whence $v_d(E) = 2qF\tau(E)/3m^*$, and λ_E is reduced by a factor $\frac{2}{3}$. Then the lucky-drift $n(E)$ has the same exponential term as Wolff's [Eq. (8b)]; the only difference is in the slowly varying prefactor, which in turn causes the average energies to disagree. The prefactor is reminiscent of a density of states, and this points to the approximate nature of the ansatz^{3,5,8} used to calculate $P(E)$ ("lucky-drift trajectories" in energy space).

Based on Shockley's reasoning,¹⁶ Appendix A brings a closer insight into the failure of Drude's formula, and gives a general expression for the local drift velocity, even in anisotropic band structures and almost regardless (see Sec. IV B) of the form of the electron-phonon interaction. The upshot of all this is that v_d can be meaningfully defined as a function of energy, and this is used in the next section.

III. A FOKKER-PLANCK APPROACH

A. Aim

In the previous section, we pointed out two flaws in the lucky-drift model. The major one stemmed from an incorrect expression for the energy-dependent drift velocity yielding in turn a wrong energy relaxation length; it was cured by substituting Shockley's to Drude's formula. The second flaw has to do with the statistics, and its consequences in an arbitrary band structure are difficult to guess. This section is aimed at designing a statistical-mechanical model for high-field transport, assuming the carrier kinematics (band structure) and dynamics (lattice scattering) to be known, that retains some essential features of the lucky-drift description. The first feature is the real-space description of the electron's motion in terms of a local drift velocity—in fact, such a description is valid for nonballistic motion, which is always true at high enough energy at steady state.⁴ The use of a slowly varying velocity (on times $\tau \ll t \ll \tau_E$) allows straightforward visualization of the motion, which is fast and possibly ballistic at low energy where collisions are infrequent, and slow at high energy where the scattering rate is very

large. The second feature is the use of energy E as the basic variable, instead of \mathbf{k} in computer simulations: this is made possible by the fact that for hot electrons, momentum is relaxed very rapidly compared to energy, so that momentum is randomized on scales over which energy hardly changes. The consideration of E instead of \mathbf{k} or $\mathbf{p} = \hbar\mathbf{k}$ spares to the physicist or device engineer a detailed consideration of the structure of phase space: the main transport properties can be understood on the basis of a one-variable function, the density of states $N(E)$.

That such a program can be envisioned, is strongly suggested by the generalized lucky-drift model introduced previously,⁸ in which the energy relaxation length involving $v_d(E)$ and $\tau_E(E)$ gives a realistic probability law $n(E)$ if suitable energy dependences are used. The relationship between E space and \mathbf{p} space is tackled in Sec. IV and used in the appendixes for deriving the general expressions for all the relevant quantities. In the remainder of this section, we shall take for granted that a local drift velocity can be defined as a function of energy alone in spite of band-structure and electron-phonon anisotropies, and the reader is advised that any doubts he may have should be postponed until Sec. IV. The next two subsections introduce the Fokker-Planck approach for finding $n(E)$ in a generic material: in subsection D, we set out the physical meaning of our solution, and in subsection E make the link with Wolff's theory and the generalized lucky-drift model.

B. Equation of evolution in energy space

The problem is to find how the probability distribution $n(E, t)$ evolves in time owing to energy exchange with the field and the phonon bath. Since the integral of the probability density is conserved in time, and since the energy changes can be assumed almost continuous for hot carriers ($\hbar\omega \ll E$), it is possible to write down an equation of continuity,

$$\partial n / \partial t + \partial J_E / \partial E = 0 , \quad (14)$$

in which J_E (in s^{-1}) is a density of probability current in E space. Equation (14) is analogous to the conservation of probability (in real space) in Schrödinger's wave mechanics. This idea has been introduced for dealing with hot-electron problems independently by Kurosawa¹⁷ and Levinson.¹⁸ The next step is to write the probability current as the sum of a drift term and a diffusion term,

$$J_E = W(E)n(E) - \partial[D(E)n(E, t)] / \partial E . \quad (15)$$

When (15) is input into (14), we have a Fokker-Planck equation,¹⁹ W has the meaning of a drift velocity in energy space, and D is called the diffusion coefficient. If D is a function of E , we are dealing with a nonlinear Fokker-Planck equation.¹⁹ Strictly speaking, the drift and diffusion currents cannot be defined unambiguously in the case of a variable diffusion coefficient.²⁰ For instance, Kurosawa¹⁷ uses another, equivalent definition. The reasons why we cast J_E in the form (15) is that an initially peaked distribution $n(E, 0) = \delta(E - E_0)$ will become,

after some time, shifted and broadened in such a way^{17,19} that the average shift, or drift in energy space, obeys

$$d\langle E - E_0 \rangle / dt = W(E_0), \quad (16a)$$

so that $W(E_0)$ is the average rate of energy gain (or loss) of the particle, while the broadening caused by the randomness associated with the energy exchange is

$$d\langle (E - E_0)^2 \rangle / dt = 2D(E_0). \quad (16b)$$

More specifically,^{17,19} the Dirac distribution $\delta(E - E_0)$ is changed into a Gaussian packet centered at $E_0 + W(E_0)t$, with a variance $2D(E_0)t$. This holds at times t short enough that $W(E)$ and $D(E)$ retain their values at E_0 . Hence, $W(E_0)$ (in eV/s) represents the speed at which the center of the packet moves in energy space, starting from E_0 , while the diffusion term embodies the variance caused by the energy exchange experienced by the electron both from the field and the phonon bath. General conditions to be obeyed by diffusion coefficients^{17,19} are $D(E) > 0$, except at $E = 0$, where $D(0)$ vanishes.

The time evolution of the probability density has two origins, namely, the energy exchange with the field and lattice vibrations. The rates of change of $n(E, t)$, due to the field and the lattice are additive in the semiclassical transport picture, viz. $\partial n / \partial t = (\partial n / \partial t)_F + (\partial n / \partial t)_{ph}$, with the subscript "F" standing for the field and "ph" for the phonons. In modern language, this means that the intracollisional field effect is ignored.²¹ Thus, the current J_E is the sum of two terms, each being a superposition of drift and diffusion,¹⁷

$$J_E = J_F + J_{ph}, \quad (17)$$

$$W(E) = W_F(E) + W_{ph}(E), \quad D(E) = D_F(E) + D_{ph}(E).$$

We are thus led to deal with four coefficients (actually,

functions of E) displayed in Table II, and we proceed to examine each in turn.

The field-related drift velocity in energy space, $W_F(E)$ (in eV/s) is related to the drift velocity in real space $v_d(E)$ already discussed in Sec. II D,

$$W_F(E) = qFv_d(E). \quad (18)$$

It is usually positive, though a negative value is *a priori* conceivable in an energy range where electrons traveling upfield (giving rise to Bloch oscillations) are possible. Equation (13) gives $v_d(E)$ for isotropic band structure and electron-phonon interaction; Appendix A gives the general expression for $v_d(E)$ and $W_F(E) = q\mathbf{F} \cdot \mathbf{v}_d(E)$. Realistic calculations of $W_F(E)$ and $D_F(E)$ in specific materials are planned for future publications.

Kurosawa derives (18) in another way. The evolution of E_{av} due to field is

$$\begin{aligned} (dE_{av}/dt)_F &= \int_0^{+\infty} E [\partial n(E, t) / \partial t]_F dE \\ &= \int_0^{+\infty} E (-\partial J_F / \partial E) dE \\ &= \int_0^{+\infty} J_F dE = \int_0^{+\infty} n(E, t) W_F(E) dE. \end{aligned} \quad (19)$$

Since n is an arbitrary probability density, $W_F(E)$ should be identified with the rate of energy gain from the field, viz., $qFv_d(E)$. From (19) one can see that the diffusion term averages to zero and does not affect the average energy, but only the shape of the distribution.

The phonon-related drift velocity in energy space $W_{ph}(E)$ is oriented downwards. In the simple case of emission of phonons of fixed frequency ω at a time rate $1/\tau(E)$,

$$W_{ph}(E) = -\hbar\omega/\tau(E), \quad (20)$$

in general, see Appendix B.

TABLE II. The physical quantities used and obtained in the Fokker-Planck approach. The W 's are energy rates, or drift velocities, giving the average motion in energy space, and the D 's are half energy variances per unit time representing the tendency to spread in energy space. The f 's are occupation functions (probability for a state to be occupied); $f(\mathbf{p})$ can be written down explicitly for cubic material [Eq. (42) appearing in this table], in general it is given by Eq. (40). ϵ denotes $(3/2)(\hbar\omega/qF\lambda_0)^2$ and E'_w means $(1 + \epsilon)(qF\lambda_0)^2 / \{3\hbar\omega[2n(\omega) + 1]\}$.

Physical quantity	Notation and structure	General expression	Parabolic form
Average energy gain from field (eV/s)	$W_F(E) = q\mathbf{F} \cdot \mathbf{v}_d(E)$	(A8)	$2(qF)^2\lambda/3m^*v_g(E)$
Average energy loss to phonons (eV/s)	$W_{ph}(E) = -\hbar\omega/\tau(E)$	(B7)	$-\hbar\omega v_g(E)/\lambda_0$
Field-related diffusion coefficient (eV ² /s)	$D_F(E) = \overline{\{[q\mathbf{F} \cdot \mathbf{v}_g(\mathbf{p})]^2\tau(\mathbf{p})\}}_E$	(A11) or (21)	$(qF)^2\lambda v_g(E)/3$
Phonon-related diffusion coefficient (eV ² /s)	$D_{ph}(E) = (\hbar\omega)^2/2\tau(E)$	(B8)	$(\hbar\omega)^2 v_g(E)/2\lambda$
Energy occupation function	$f_0(E) = \exp \left\{ \int^E [W_{ph}(E')/D_F(E')] dE' \right\}$	(28b)	$E^{-\epsilon/1+\epsilon} \exp(-E/E'_w)$
Momentum-space occupation function	$f(\mathbf{p}) = f_0(E(\mathbf{p})) \left[1 - \frac{W_{ph}(E(\mathbf{p}))}{(q\mathbf{F} \cdot \mathbf{v}_g \cos\theta)_{E(\mathbf{p})}} \cos\theta \right]$	(40)	$f_0(E)[1 + (3\hbar\omega/qF\lambda_0) \cos\theta]$

C. Diffusion coefficients in energy space

There are two ways to derive the diffusion coefficients. The one employed in previous works consists in using general statistical-mechanical arguments regarding the occupation of phase space. The other one we shall employ here consists in directly calculating the variance, after time t , of a distribution of carriers initially peaked at energy E_0 : by equating the variance to $2D(E_0)t$, $D(E_0)$ is obtained. We first review and criticize the earlier method before introducing ours.

To determine D_F , consider that the particle only exchanges energy with the field, not with the phonon bath. Since the particle is coupled to a reservoir of momentum and energy, at steady state it is equally likely to be in any phase-space volume d^3p , so that $n(E) \sim N(E)$. If this $n(E)$ is input into (15), $J_E = 0$ and $D_F(0) = 0$ entail upon integration,

$$D_F(E) = \frac{1}{N(E)} \int_0^E W_F(E') N(E') dE'. \quad (21)$$

Equation (21) can be derived from elementary arguments *à la Shockley*, see Appendix A, where $D_F(E)$ is expressed as an integral over the constant-energy surface $E(\mathbf{p}) = E$. This gives a closer physical insight into the field-related diffusion in energy space than the general statistical-mechanical argument. Let us set off the gist of the result. If the energy at zero time is E , and if t is taken to be the typical collision time τ , then the typical energy after t is $E \pm qF\lambda$, where $\lambda = v_g \tau$ is the typical mean free path at energy E ; $E + qF\lambda$ (respectively, $E - qF\lambda$) is for an electron traveling downfield (respectively, upfield). Now if we remember that the *average* energy change is $qFv_d\tau$, with $v_d \ll v_g$, then the variance in energy $(qF\lambda)^2 - (qFv_d\tau)^2 \simeq (qF\lambda)^2$. Hence the carrier motion in energy space, due to field, is strongly diffusive. By equating $(qF\lambda)^2$ to $2D_F\tau$, we get $D_F \approx \frac{1}{2}(qFv_g)^2\tau$. Exact equations valid for arbitrary band structure and electron-phonon interaction can be found in Appendix A, which also contains a mathematical proof of Eq. (21).

Let us now turn to the phonon-related diffusion coefficient D_{ph} . Kurosawa obtains it by requiring that when the carrier exchanges energy with the lattice only (that is, $F = 0$), then $n(E)$ will be the canonical distribution $N(E) \exp(-E/kT)$. If this $n(E)$ is input into (15), $J_E = 0$ and $D_{ph}(0) = 0$ entail upon integration,

$$D_{ph}(E) = \frac{\exp(E/kT)}{N(E)} \int_0^E W_{ph}(E') N(E') \times \exp(-E'/kT) dE'. \quad (22)$$

Levinson¹⁸ arrives at the same conclusion, and notices that an energy-space version of the fluctuation-dissipation theorem ensues. The reasoning is entirely right, but is *not* suited to our purpose. Indeed one can see that Kurosawa's or Levinson's $W_{ph}(E)$ [from Eqs. (3.7) and (3.8) of Ref. 17] corresponds to the energy relaxation rate associated with acoustic phonons at equipartition,

$$W_{ph}(E) = \alpha E^{1/2} (2kT - E). \quad (23)$$

This means that the lattice can thermalize the electron through the exchange of low-energy, zone-center acoustic phonons. In our case, the dominant interaction proceeds by optical and zone-edge acoustic phonons, that for simplicity we model as quanta of fixed energy $\hbar\omega$. It turns out that a particle cannot reach a canonical distribution by exchanging quanta of fixed energy with a reservoir. Therefore, we need determine $D_{ph}(E)$ directly from the very features of the electron-phonon interaction. Consider the simple case of optical-phonon emission at a rate $1/\tau(E)$. In the absence of F , the change of the population $n(E, t)dE$ during dt is caused by loss ($E \rightarrow E - \hbar\omega$) and gain ($E + \hbar\omega \rightarrow E$):

$$(\partial n / \partial t)_{ph} = n(E + \hbar\omega, t) / \tau(E + \hbar\omega) - n(E, t) / \tau(E). \quad (24a)$$

Upon second-order expansion with respect to $\hbar\omega \ll E$, Eq. (24a) may be written

$$(\partial n / \partial t)_{ph} = \hbar\omega [\partial(n/\tau) / \partial E] + \frac{1}{2} (\hbar\omega)^2 [\partial^2(n/\tau) / \partial E^2], \quad (24b)$$

which can be cast in the form $-\partial J_{ph} / \partial E$, with

$$W_{ph}(E) = -\hbar\omega / \tau(E), \quad D_{ph}(E) = \frac{1}{2} (\hbar\omega)^2 / \tau(E). \quad (25)$$

Drift velocities and diffusion coefficients are gathered in Table II.

D. General features of the energy distribution

The steady-state distribution of electrons submitted both to the field and the coupling to phonons corresponds to a vanishing probability current, $J_E = 0$. This amounts to stating that the loss to phonons is balanced by the gain from the field:

$$-W_{ph}(E) + \frac{1}{n} \frac{d(D_{ph}n)}{dE} = W_F(E) - \frac{1}{n} \frac{d(D_F n)}{dE}. \quad (26)$$

If in (26) diffusion terms are dropped, we recover the conventional energy-balance equation yielding the typical energy of the distribution^{8,9} $-W_{ph}(E) = W_F(E)$, or $E / \lambda_E(E) = qF$ in the spatial lucky-drift notation. Therefore, the Fokker-Planck description leads to the same typical energy as the lucky-drift model, but differs from the latter in dealing with the fluctuations about the average. According to the foregoing subsection $D_{ph} / D_F \approx (\hbar\omega / qF\lambda)^2 \ll 1$, so that at high field the fluctuations are essentially due to the energy exchange with the field, not to the exchange of quanta with the lattice, contrary to the vanishing-field case where the variance of the canonical distribution arises from the thermalized lattice.

The solution of (26) is

$$n(E) = \exp \left[\int^E \frac{W_{\text{ph}}(E') + W_F(E') - dD_F(E')/dE' - dD_{\text{ph}}(E')/dE'}{D_F(E') + D_{\text{ph}}(E')} dE' \right]. \quad (27)$$

Neglecting $D_{\text{ph}} \ll D_F$ in the denominator, and noting that in the numerator $W_F(E') - dD_F(E')/dE'$ according to (21) is $D_F(E') d \ln [N(E')]/dE'$, we arrive at

$$n(E) = N(E) \exp \left[\int^E \frac{W_{\text{ph}}(E')}{D_F(E')} dE' \right], \quad (28a)$$

if we also neglect $-dD_{\text{ph}}(E')/dE'$. From (25) taking this term into account would change $W_{\text{ph}}(E') = -\hbar\omega/\tau$ appearing in (28a) into

$$-(\hbar\omega/\tau) \left[1 + \frac{1}{2} \hbar\omega d \ln(1/\tau)/dE \right].$$

The last term is low if the collision rate varies slightly over $\hbar\omega$, which is usually true except in the vicinity of an intervalley separation energy in a direct-gap material, where $N(E)$ and as a result $1/\tau(E)$ exhibit sharp variations. There $D_{\text{ph}}(E)$ is high over a narrow energy range so that the contribution to the *integral* in (27) is insignificant anyway. The point of greater concern regarding intervalley transitions is that the collision rate varies so sharply over $\hbar\omega$ that writing down the local equation (14) for the conservation of probability is approximate: this is also apparent in the expansion (24b) leading to W_{ph} and D_{ph} . The Fokker-Planck approach will soften intervalley transitions: we take the optimistic view that uncertainty broadening would anyway do the same, since in practical cases \hbar/τ exceeds $\hbar\omega$.

Equation (28a) is a particularly simple expression for the energy distribution. The prefactor $N(E)$ is reminiscent of the field's propensity to populate phase space uniformly, and thereby favors energy ranges where the density of states is high, whereas the exponential term does not favor high-energy states owing to the energy loss to phonons $W_{\text{ph}}(E) < 0$. Note that a strong W_{ph} can be overcome by a large D_F embodying the field's ability to broaden the distribution. From (28a), the nonequilibrium occupation function is

$$f_0(E) = \exp \left\{ \int^E [W_{\text{ph}}(E')/D_F(E')] dE' \right\}. \quad (28b)$$

It is generally not expressible in terms of an electron temperature unless the integrand is constant with respect to E' as occurs in parabolic bands.

E. Link with Wolff's theory and the lucky-drift model

In this subsection, Eq. (28a) is first confronted to Wolff's distribution in the case of a constant mean-free-path, isotropic interaction with phonons of fixed frequency, and then to the $n(E)$ given by the generalized lucky-drift model of Ref. 8.

Consider an electron interacting isotropically with a flat optical-phonon branch in a parabolic band structure; for simplicity, we take zero temperature. The field- and

phonon-related drift velocities in energy space are [see Eqs. (13) and (25)]:

$$W_F(E) = 2(qF)^2 \tau(E) / 3m^*, \quad W_{\text{ph}}(E) = -\hbar\omega/\tau(E),$$

where $1/\tau(E) = v_g(E)/\lambda$, and $\lambda = \lambda_0$. The diffusion coefficients are [see Eqs. (21) and (25)]

$$D_F(E) = (2E/m^*)^{1/2} (qF)^2 \lambda / 3,$$

$$D_{\text{ph}}(E) = (2E/m^*)^{1/2} (\hbar\omega)^2 / 2\lambda.$$

We check that $D_{\text{ph}}/D_F \ll 1$ at high enough fields, as noticed earlier. Application of (28a) straightforwardly yields.

$$n(E) \sim E^{1/2} \exp(-E/E_w),$$

which is precisely Wolff's distribution (7). In Tables I and II, we have computed the exact result of (27), without neglecting $D_{\text{ph}}(E)$, and at finite temperature. It is seen in Table I and Fig. 1 that the agreement of the Fokker-Planck prediction with Wolff's or the Monte Carlo figures is excellent.

We now turn to the link between the Fokker-Planck approach and the generalized lucky-drift model.⁸ In the foregoing subsection, it was noticed that the "typical" carrier energy, corresponding to energy balancing between gain from the field and loss to phonons, was approximately the same in both frameworks. We want here to compare the full distributions in a universal way, without considering a specific material for which the exact D_F and W_{ph} should be obtained from the detailed band structure and electron-phonon interaction according to the formulas of the appendices.

If in Eq. (28a) we take $W_{\text{ph}}(E) = -\hbar\omega/\tau(E)$, we are left to seek an approximate universal expression for $D_F(E)$. To this end, we consider Eq. (21), and notice that the drift velocity $v_d(E)$ is roughly proportional to the collision time $\tau(E)$, which in turn is roughly proportional to $1/N(E)$ according to the golden rule, or even Dyson's equation, provided that (i) energy be conserved in a collision event, and that (ii) all \mathbf{k}' within the final energy shell be reached with more or less the same probability. The latter feature is true of the nonpolar (deformation potential) interaction, but is not verified by the polar interaction, which strongly favors final \mathbf{k}' close to the initial \mathbf{k} , that is, a small part of the energetically accessible phase space. [If quantum effects are so strong as to broaden the final energy, an isotropic interaction should yield $1/\tau(E)$ broadly $\sim N(E)$, the proportionality being poor at intervalley separation energies in direct-gap semiconductors, where $N(E)$ exhibits sharp variations.] It follows that the integrand in Eq. (21) is approximately constant with respect to E' , so that we may equate it to its value at the upper energy E , and obtain upon integration

$$D_F \approx qFv_d(E)E. \quad (29)$$

Then the Fokker-Planck prediction (28a) becomes, if we recognize that $E'\tau(E')/\hbar\omega = \tau_E(E')$ [Eq. (2)] and $v_d(E')\tau_E(E') = \lambda_E(E')$,

$$n(E) \approx N(E) \exp \left[- \int^E \frac{dE'}{qF\lambda_E(E')} \right]. \quad (30)$$

This is close to the lucky-drift expression Eq. (4b). The difference between the Fokker-Planck [Eq. (30)] and lucky-drift [Eq. (4b)] predictions lies in the preexponential factor, which in the latter roughly varies with E as $[N(E)]^2/E$. Compared to the former, there is an extra factor of $N(E)/E$. In the parabolic case, such a factor $\sim E^{-1/2}$ was pointed out in Sec. II when lucky drift was confronted to Wolff's theory, and is not very serious as far as the asymptotic behavior is concerned and the correct $v_d(E)$ is used, but it is now clear that for sharply varying $N(E)$ it matters. Another superiority of the Fokker-Planck approach is that it provides us with definite expressions for its basic quantities, while those entering the generalized lucky-drift model were guessed in an heuristic manner in our previous work⁸ [not to mention the erroneous $v_d(E)$ disclosed in Sec. II]. As a final point, we note that D_{ph}/D_F in the lucky-drift language is $\hbar\omega / (2qF\lambda_E) \approx \hbar\omega/E_{av}$, a very small quantity.

IV. MOMENTUM SPACE DISTRIBUTION

We have hitherto fastened our attention on the distribution in energy space, embodied in $n(E)$. There are, however, a number of observables that are not only energy, but also momentum, dependent. The simplest one is v_g , whose mean value is the average drift velocity. Realistic impact-excitation or impact-ionization rates are also strongly momentum dependent ("anisotropic"). It is, therefore, very desirable to complete the knowledge of $n(E)$ or the occupation function $f_0(E)$ with that of $f(\mathbf{p})$. The second motivation for obtaining $f(\mathbf{p})$ is to justify the Fokker-Planck approach together with the expressions for W_F and D_F (Appendix A), and for W_{ph} and D_{ph} (Appendix B).

A. Calculation of momentum-space distribution

The usual way of obtaining $f(\mathbf{p})$ is to write the Boltzmann transport equation, as is done, for instance, in Wolff's theory.¹⁰ We shall use the equivalent elementary approach of Shockley,²² who considers the traffic in momentum space in a pictorial way which readily suggests the relevant approximations. The main idea behind Shockley's treatment of low-field conductivity is that electron-lattice scattering with acoustic phonons is almost elastic, so that the electron-phonon interaction connects electron states located on a constant-energy surface in the Brillouin zone. As has been remarked many times,¹⁸ the case of hot electrons emitting or absorbing high-frequency phonons is very similar. We shall, therefore, consider as a working approximation that the electron-phonon interaction effects transitions over a constant-energy surface, or within a constant-energy shell of fixed thickness $dE \approx \hbar\omega$. This quasielastic approxima-

tion amounts to writing the transition probability as

$$W_{\mathbf{p},\mathbf{p}'} = T_{\mathbf{p},\mathbf{p}'} \delta[E(\mathbf{p}) - E(\mathbf{p}')], \quad (31)$$

and the principle of detailed balancing $W_{\mathbf{p},\mathbf{p}'} = W_{\mathbf{p}',\mathbf{p}}$ entails $T_{\mathbf{p},\mathbf{p}'} = T_{\mathbf{p}',\mathbf{p}}$. Let $f(\mathbf{p})$ be the occupation function of momentum space (per unit volume of the crystal), that is, $f(\mathbf{p})d^3p/h^3$ is the probability for the carrier's momentum to lie in the momentum volume d^3p . From $f(\mathbf{p})$, the probability density in energy space $n(E)$ is obtained as

$$n(E) = \int \int \int f(\mathbf{p}) \delta[E(\mathbf{p}) - E] d^3p / h^3. \quad (32)$$

The density of states (per unit volume of the crystal) is given by

$$N(E) = \int \int \int \delta[E(\mathbf{p}) - E] d^3p / h^3 = \int \int_E dS_p / |v_g| h^3, \quad (33)$$

where $\int \int_E$ means the integral over the surface $E(\mathbf{p}) = E$, and dS_p is the corresponding surface element. The occupation function in energy space appearing in Eqs. (5) and (28b) is $f_0(E) = n(E)/N(E)$; it is the energy-shell average of $f(\mathbf{p})$.

In the absence of a field, all states belonging to a constant-energy surface are evenly occupied, and it is liable to say that $f(\mathbf{p})$ is a microcanonical distribution, that is, $f(\mathbf{p}) = f_0(E)$. This is obvious from the examination of the collision term in Boltzmann's transport equation and the detailed balancing principle. In this state of affairs, the average v_g over the constant-energy surface vanishes. If the field is present, there will appear a deviation from uniformity, commonly called "anisotropy," giving rise to a nonvanishing average of v_g directed along \mathbf{F} in cubic materials. Since the average drift velocity is an order of magnitude smaller than the group velocity, the deviation from uniformity should, in general, be small. This is conspicuously clear in Wolff's solution for a spherical parabolic band structure Eq. (6b): at a high field, the anisotropic part of the occupation function is small, and is expressed as the first spherical harmonic Y_1^0 . (At an intermediate field, the anisotropy is stronger, the occupation function is more forward oriented, and this is related to the occurrence of ballistic electrons.^{13,14}) Thus, we shall consider that at constant E , the occupation function slightly departs from $f_0(E)$, and we proceed to determine the deviation $f_1(\mathbf{p})$:

$$f(\mathbf{p}) = f_0(E(\mathbf{p})) + f_1(\mathbf{p}). \quad (34)$$

If integrals over \mathbf{p} space are to be calculated, $f(\mathbf{p}) = f_0(E(\mathbf{p}))$ may be used as a first approximation, as is done in the Appendixes, unless the outcome is zero, as occurs with an odd function of \mathbf{p} . Then it is necessary to resort to the nonuniform part f_1 .

In Wolff's theory, f_1 can be obtained from f_0 [Eq. (6b)]. In order to obtain the general relation, we consider a small momentum volume d^3p containing $\delta n = f(\mathbf{p})d^3p/h^3$ electrons of a given spin. The rate of change of δn is threefold. First, the field bring to \mathbf{p} , at time t , particles which were at $\mathbf{p} - \mathbf{q}\mathbf{F} dt$ at time $t - dt$, whence

$$\left[\frac{d(\delta n)}{dt} \right]_F = -q\mathbf{F} \cdot (\partial(\delta n)/\partial \mathbf{p}) = -q\mathbf{F} \cdot (\partial f/\partial \mathbf{p}) d^3 p / h^3. \quad (35)$$

Second, out scattering ($\mathbf{p} \rightarrow \mathbf{p}'$) depopulates momentum volume $d^3 p$ at a rate

$$\begin{aligned} \left[\frac{d(\delta n)}{dt} \right]_{\text{out}} &= - \int \int \int \delta n W_{\mathbf{p}, \mathbf{p}'} d^3 p' / h^3 \\ &= -\delta n / \tau(\mathbf{p}), \end{aligned} \quad (36)$$

where the scattering time $\tau(\mathbf{p})$ is defined as

$$\begin{aligned} 1/\tau(\mathbf{p}) &= \int \int \int W_{\mathbf{p}, \mathbf{p}'} d^3 p' / h^3 \\ &= \int \int_{E(\mathbf{p})} T_{\mathbf{p}, \mathbf{p}'} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3. \end{aligned} \quad (37)$$

Third, in scattering ($\mathbf{p}' \rightarrow \mathbf{p}$) from states lying (approximately) in the same energy shell gives

$$\left[\frac{d(\delta n)}{dt} \right]_{\text{in}} = \left[\int \int_E f(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3 \right] d^3 p / h^3. \quad (38a)$$

By breaking up $f(\mathbf{p}')$ into a uniform and a nonuniform part [Eq. (34)] and accounting for detailed balance, the in-scattering term reads

$$\begin{aligned} \left[\frac{d(\delta n)}{dt} \right]_{\text{in}} &= \left[f_0(E) / \tau(\mathbf{p}) \right. \\ &\quad \left. + \int \int_E f_1(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3 \right] d^3 p / h^3. \end{aligned} \quad (38b)$$

Equating the total rate of change of δn to zero at steady state yields,

$$\begin{aligned} q\mathbf{F} \cdot (\partial f / \partial \mathbf{p}) &= -f_1(\mathbf{p}) / \tau(\mathbf{p}) \\ &\quad + \int \int_E f_1(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3, \end{aligned} \quad (39)$$

which could be obtained [within the quasielastic approximation Eq. (31)] from Boltzmann's transport equation. Equation (39) is an integro-differential equation which can be converted into an integral equation for f_1 if the left-hand side is approximated²² to $q\mathbf{F} \cdot (\partial f_0 / \partial \mathbf{p}) = q\mathbf{F} \cdot \mathbf{v}_g (df_0/dE)$. Then,

$$\begin{aligned} f_1(\mathbf{p}) &= q\mathbf{F} \cdot \mathbf{v}_g(\mathbf{p}) \tau(\mathbf{p}) (-df_0/dE) \\ &\quad + \tau(\mathbf{p}) \int \int_E f_1(\mathbf{p}') T_{\mathbf{p}', \mathbf{p}} dS_{\mathbf{p}'} / |\mathbf{v}'_g| h^3 \end{aligned} \quad (40)$$

is the desired generalization of Wolff's relationship Eq. (6b). To check that $f_1(\mathbf{p})$ is small compared to f_0 , we notice that the integral term in (40) (related to scattering anisotropy¹⁰) is of the order f_1 unless it vanishes, so that the order of magnitude of f_1 is always given by the first term in the right-hand side of (40). Now from Eq. (28b), $df_0/dE = f_0(E) W_{\text{ph}}(E) / D_F(E)$, whence

$$f_1(\mathbf{p}) \approx q\mathbf{F} \cdot \mathbf{v}_g(\mathbf{p}) \tau(\mathbf{p}) \frac{\hbar\omega / \tau(E)}{((q\mathbf{F} \cdot \mathbf{v}_g)^2 \tau)_E}, \quad (41)$$

where $(\)_E$ means the energy-shell average, $1/\tau(E) = (1/\tau(\mathbf{p}))_E$, and $D_F(E)$ was obtained from (A11). Generally speaking $f_1/f_0 \approx \hbar\omega / qF\lambda(E)$ is much less than unity, with $\lambda(E)$ the mean free path at the energy of interest.

In general, f_1 is not a combination of the spherical harmonics $Y_1^{0, \pm 1}$ only. In view of Wolff's work,¹⁰ it is reasonable, however, to assume that at high energy and field, first-order spherical harmonics prevail in f_1 , and derive the coefficients of $Y_1^{0, \pm 1}$. Pushing the expansion to higher orders is dubious, since Eq. (40) is already approximate. Taking a cubic material where only Y_1^0 is present and $f_1(\mathbf{p}) = f_1(E) \cos\theta$, we multiply Eq. (40) by $q\mathbf{F} \cdot \mathbf{v}_g(\mathbf{p}) dS_{\mathbf{p}} / |\mathbf{v}_g|$ and integrate over the energy shell:

$$\begin{aligned} f_1(E) &= \frac{D_F(E)}{(q\mathbf{F} \cdot \mathbf{v}_g \cos\theta)_E} \left[-\frac{df_0}{dE} \right] \\ &= \frac{-W_{\text{ph}}(E)}{(q\mathbf{F} \cdot \mathbf{v}_g \cos\theta)_E} f_0(E), \end{aligned} \quad (42)$$

where use has been made of (A11) and (28b). The advantage of expressing $f_1(E)$ in this way is the relation it bears to the power brought by the field, namely,

$$\begin{aligned} \int \int \int q\mathbf{F} \cdot \mathbf{v}_g f(\mathbf{p}) dS_{\mathbf{p}} dE / |\mathbf{v}_g| h^3 \\ &= \int_0^{+\infty} dE N(E) (q\mathbf{F} \cdot \mathbf{v}_g f)_E \\ &= \int_0^{+\infty} dE N(E) D_F(E) (-df_0/dE) \\ &= \int_0^{+\infty} dE n(E) [-W_{\text{ph}}(E)]. \end{aligned} \quad (43)$$

In the preceding chain of equations, the energy-dependent integrands are identical. We, thus, see that the shell average $(q\mathbf{F} \cdot \mathbf{v}_g f)_E$, multiplied by the number of states $N(E)dE$, yields the power received by the phonon system. The last equation is arrived at by using the approximate $f_0(E)$ of Eq. (28b) in which D_{ph} is neglected, and this approximation is good. A rigorous result for that power is

$$\begin{aligned} \int_0^{+\infty} J_F(E) dE, \\ \text{i.e.,} \\ \int_0^{+\infty} qFv_d(E) [n(E)dE] - d[D_F(E)n(E)]. \end{aligned} \quad (44)$$

The first term is the power production due to the average rate (drift term in J_F), while the second is related to the variance (diffusion term in J_F). Since $J_F = -J_{\text{ph}}$, the same can be said in terms of phonon-related probability current, but the phonon-related diffusion current is negligible. Upon integration over all energies, the second term of (44) does not contribute and the former expression of power is recovered:

$$\int_0^{+\infty} qFv_d(E) N(E) f_0(E) dE,$$

thereby proving that the momentum-space average of

$v_g(\mathbf{p})$ is the same as the energy-space average of $v_d(E)$ if $f_1(\mathbf{p})$ is taken to be a first-order harmonic with a coefficient given by Eq. (42).

B. Validity of the Fokker-Planck description

Generally speaking, the Fokker-Planck equation is a special type of master equation which is often used as an approximation to the actual one.¹⁹ In semiclassical transport, the latter is deemed to be Boltzmann's, which refers to momentum space. Now in the case of isotropic band structure and electron-phonon interaction, Levinson¹⁸ actually derived the Fokker-Planck equation from Boltzmann's under the assumptions that $\hbar\omega \ll E$ and the anisotropic part of the distribution $f_1(\mathbf{p})$ is small compared to the isotropic part $f_0(E)$. The generalized procedure is to consider the constant-energy surface $E(\mathbf{p})=E$ and assume its occupation to be almost microcanonical, that is, $|f_1(\mathbf{p})| \ll f_0(E)$, and obtain the first two moments (mean and variance) of energy change, yielding $W(E)$ and $D(E)$. This is done in the Appendixes. *Taking the Fokker-Planck $f_0(E)$, the almost microcanonical occupation of states at constant E is proved in Sec. IV A for $\hbar\omega/qF\lambda(E) \ll 1$, thereby establishing the Fokker-Planck description of high-field transport in a self-consistent manner.* One may alternatively notice that $|f_1(\mathbf{p})| \ll f_0(E)$ is equivalent to having $v_d(E) \ll v_g(E)$. Now lucky-drift and the effective-mass approximation, which is never very wrong as far as velocities are concerned, give $v_d(E_{av}) \approx (\hbar\omega/m^*)^{1/2}$ and $v_g(E_{av}) \approx (2E_{av}/m^*)^{1/2}$, so that the condition for the Fokker-Planck approach to apply is simply $\hbar\omega \ll E_{av}$, namely, that the carriers are hot. The typical accuracy is $(\hbar\omega/E_{av})^{1/2}$.

The condition $qFv_d(E) \ll qFv_g(E)$ also states that an initially peaked distribution $n(E,0) = \delta(E - E_0)$ spreads in energy space much more than it shifts. [Actually, $W(E) = qFv_d(E) - \hbar\omega/\tau(E)$ has the same order of magnitude as $W_F(E)$, and $D(E) \approx D_F(E)$.] It means that the master equation underlying the nonlinear Fokker-Planck equation is of the diffusion type,²³ and the latter can be derived from the former by taking the energy quantum $\hbar\omega$ as an expansion parameter, since $v_d/v_g \approx (\hbar\omega/E_{av})^{1/2} \ll 1$. We shall leave this point as a parentheses (admittedly cryptic), and refer the reader to van Kampen's treatise²³ for a rigorous justification.

The prominent role played by constant-energy surfaces in the high-field transport problem stems from the electron-phonon interaction connecting states of (almost) equal energy as $\hbar\omega \ll E_{av}$. While the field tends to populate the whole phase space evenly, it is the quasielastic electron-phonon interaction that makes the constant-energy surfaces play their role. There is a condition, however, which is that at constant energy, the electron-phonon coupling should not be strongly preferential toward certain states within the shell $E(\mathbf{p})=E$. It is this condition that makes the occupation of an energy surface almost microcanonical. As is known, the condition is not obeyed by the polar coupling, which at high energy forbids large $\mathbf{k}' - \mathbf{k}$. Before closing this section, we, therefore, comment on polar scattering.

The condition $|f_1(\mathbf{p})| \ll f_0(E)$ is not valid for forward peaked $f(\mathbf{p})$, as occurs in purely polar materials at high field (and also in nonpolar materials at intermediate fields^{13,14}). For them the first obstacle is that it is not possible to split apart the determination of $n(E) = N(E)f_0(E)$ and of $f_1(\mathbf{p})$: the determination of the coefficients, especially $W_F(E)$, will chiefly involve knowledge of the "anisotropic" part of the distribution, $f_1(\mathbf{p})$, which in this work is consistently neglected. The second obstacle is that if $f(\mathbf{p})$ peaks forward (in cubic material), $W_F = qFv_d$ tends towards qFv_g , entailing the breakdown of the nonlinear Fokker-Planck description,²³ which rests on $v_d \ll v_g$. For purely polar materials, a totally different treatment is called for,³ and they will not be considered here. In medium-to-large-gap polar materials, such as GaAs, ZnS, or SiO₂, the nonpolar interaction eventually prevails at high enough energy owing to the large density of states, and the fact that as far as is known deformation-potential scattering is essentially isotropic. This will make $f(\mathbf{p})$ mainly energy, rather than momentum, dependent at high enough^{13,14} field. [In this respect, it is worthy of remark that Wolff's theory allows for scattering anisotropy, but this does not affect $|f_1|/f_0$ whatsoever, see Eqs. (10) and (13) of Ref. 10 where $\text{const}=0$ in the absence of impact ionization.] At first sight, near isotropy in $f(\mathbf{p})$ holds at high energy, where nonpolar scattering prevails, but according to remarks above, diffusion in energy space by the field is so strong as to smear out the anisotropy in the low energy $f(\mathbf{p})$ as well. Practically speaking, if an GaAs the field is high enough that E_{av} reaches or overtakes the intervalley separation 0.35 eV, we expect the occupation function $f(\mathbf{p})$ to reduce to its isotropic part $f_0(E)$ at all energies, except for a small $f_1(\mathbf{p})$ as discussed in Sec. IV A.

V. CONCLUSIONS

This paper has developed an alternative framework for dealing with the statistics of high-field transport in semiconductors within the semiclassical picture. While the conventional approach rests on the Boltzmann transport equation in momentum space, we propose a Fokker-Planck equation in energy space, the coefficients of which have a direct physical meaning (Table II). The electron's motion in energy space is the superposition of an average motion of velocity $W_F(E) + W_{ph}(E)$, and of Brownian motion tending to enhance the variance of the energy distribution, described by the diffusion coefficient $D(E) \approx D_F(E)$. At steady state, Eq. (28b) yields the energy occupation function $f_0(E)$ as a functional of $W_{ph}(E)$ and $D_F(E)$, which are expressed as integrals over constant-energy surfaces in the Brillouin zone involving the band structure and the electron-phonon interaction. This allows us to guess by inspection, or at worse at the expense of quadratures, the relevance to transport problems of some features of the electron-phonon interaction, which experimentally¹² and theoretically²⁴ is incompletely known at high energy.

The momentum-space occupation $f(\mathbf{p})$ can also be obtained in so far as it differs slightly from $f_0(E(\mathbf{p}))$: the

difference $f_1(\mathbf{p})$ is given by Eq. (40). This is the generalization of Wolff's theory in which the anisotropic part f_1 of $f(\mathbf{p})$ is small. And $|f_1| \ll f_0$, which is tantamount to $v_d \ll v_g$, is the condition for the Fokker-Planck approach to be valid—and expresses Ridley's state of lucky drift.³ It excludes narrow-gap polar materials in which $f(\mathbf{p})$ is strongly forward oriented at high field.

Monte Carlo simulations can, in principle, provide $f(\mathbf{p})$ with higher accuracy in so far as the semiclassical framework is valid, and a quantitative comparison between the Fokker-Planck and Monte Carlo predictions in specific materials, taking the same, realistic band-structure and electron-phonon parameters, is planned as a further work. *The expected typical accuracy is $(\hbar\omega/E_{av})^{1/2}$.* The Fokker-Planck vs Monte Carlo comparison displayed in Fig. 1 is already very encouraging. But the main asset of the Fokker-Planck description is its being largely analytical and endowed with immediate physical meaning.

We have been concerned with steady-state transport in this paper, because it is the minimal goal of any transport theory. But the Fokker-Planck equation can handle non-stationary problems as well. Another issue of interest usually addressed in the Monte Carlo framework consists in nonlocal effects, and it is not unrealistic to expect that simple features of nonlocal transport could be understood within the present framework, or a variant thereof, just as Ridley²⁵ demonstrated the versatility of the original lucky-drift theory by building an analytical nonlocal theory of ionization waves on that basis.

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APPENDIX A

In this appendix, we calculate the average and the variance of the energy gain of an electron between two collisions. According to Eqs. (16a) and (16b) the former leads to $W_F(E)$ and thereby to the instantaneous real-space drift velocity in the revisited sense of Sec. II D, and the latter to the diffusion coefficient $D_F(E)$ defined and derived in another way in Sec. III C. The dispersion relation $E(\mathbf{p})$ is assumed to be known (band structure). We also assume that the scattering rate $1/\tau$ is known as a function of \mathbf{p} [electron-phonon interaction, Eq. (37)].

We follow Shockley's line of reasoning.¹⁶ Consider an electron of momentum \mathbf{p}_0 and energy $E_0 = E(\mathbf{p}_0)$ at time $t=0$. By ∂_F , we denote the differential operator $q\mathbf{F} \cdot \partial/\partial\mathbf{p}$ (derivative along $q\mathbf{F}$, in s^{-1}). (Vector \mathbf{F} denotes minus the electric field, and $q > 0$ the elementary charge, $q\mathbf{F}$ is the force exerted on the electron.) The energy change after t before any collision occurs is

$$E(t) - E_0 = (\partial_F E)_0 t + \frac{1}{2} (\partial_F^2 E)_0 t^2 + \dots, \quad (\text{A1})$$

where the subscript 0 means that the quantity is calculated at \mathbf{p}_0 . Then the probability for the electron starting from \mathbf{p}_0 not to experience a collision between 0 and t is

$$c(t) = \exp \left\{ - \int_0^t dt' / \tau[\mathbf{p}(t')] \right\}, \quad (\text{A2})$$

where account is taken of the change in τ as \mathbf{p} changes in time according to $d\mathbf{p}/dt = q\mathbf{F}$. Upon first-order expansion¹⁶ of $\tau(\mathbf{p}_0 + q\mathbf{F}t')$,

$$c(t) = \exp(-t/\tau_0) [1 + \frac{1}{2}(t/\tau_0)^2 (\partial_F \tau)_0] + O(F^2), \quad (\text{A3})$$

where τ_0 means $\tau(\mathbf{p}_0)$. In (A3), the exponential gives the nonscattering probability if τ were constant while the electron is being accelerated by the field, and the second factor is the lowest-order correction due to the change in τ . From (A3), we obtain the averages (denoted by $\langle \rangle$) over a collision-free flight,

$$\langle t \rangle = \tau_0 [1 + (\partial_F \tau)_0], \quad \langle t^2 \rangle = 2\tau_0^2 [1 + 3(\partial_F \tau)_0]. \quad (\text{A4})$$

The former is the average collision time, it is shorter than τ_0 if in the course of the flight $\tau(\mathbf{p})$ decreases owing to \mathbf{p} reaching a phase-space region, where the scattering rate is higher.

From (A1) and (A4), the average energy gained over a flight is, to order F^2 ,

$$\langle E(t) - E_0 \rangle = \{ (\partial_F E)_0 + [\partial_F (\tau \partial_F E)]_0 \} \tau_0, \quad (\text{A5})$$

which can be rewritten as

$$\langle E(t) - E_0 \rangle = q\mathbf{F} \cdot \{ \mathbf{v}_g(\mathbf{p}_0) + [\partial_F (\mathbf{v}_g \tau)]_0 \} \tau_0. \quad (\text{A6})$$

This is equivalent to Shockley's equation¹⁶ giving the average vector displacement over a flight. To the vector mean free path $\mathbf{v}_g(\mathbf{p}_0)\tau_0$, a term is added which describes how that free path varies owing to $q\mathbf{F}$. Thus,¹⁶

$$(dE/dt)_F = q\mathbf{F} \cdot \{ \mathbf{v}_g(\mathbf{p}_0) + [\partial_F (\mathbf{v}_g \tau)]_0 \} \quad (\text{A7})$$

is the rate of energy gain from the field for an individual electron starting from $\mathbf{p} = \mathbf{p}_0$. We now average that rate over the energy shell $E(\mathbf{p}) = E_0$ taking a uniform (i.e., microcanonical, see Sec. IV) occupation of that shell. The number of states corresponding to a surface element dS_p in \mathbf{p} space is proportional to $dS_p/|\mathbf{v}_g|$, so that the microcanonical ensemble average of (A7) gives $W_F(E_0) = \overline{(dE/dt)_F}_{E_0}$:

$$W_F(E_0) = q\mathbf{F} \cdot \mathbf{v}_d(E_0), \quad (\text{A8a})$$

$$\mathbf{v}_d(E_0) = \frac{\int \int_{E_0} \partial_F [\mathbf{v}_g \tau(\mathbf{p})] dS_p / |\mathbf{v}_g|}{\int \int_{E_0} dS_p / |\mathbf{v}_g|}. \quad (\text{A8b})$$

$\overline{(\)}_{E_0}$ denotes the ensemble average over the constant-energy surface $E(\mathbf{p}) = E_0$, and $\int \int_{E_0}$ denotes the surface integral over $E(\mathbf{p}) = E_0$. This also holds for a surface consisting of several sheets. Averaging (A7) wipes out the group-velocity term owing to $E(-\mathbf{p}) = E(\mathbf{p})$, and there remains the vector drift velocity $\mathbf{v}_d(E_0)$ at the energy E_0 . In materials other than cubic, \mathbf{v}_d is not necessarily directed along \mathbf{F} . In Sec. III, $qFv_d(E)$ should be under-

stood as $q\mathbf{F}\cdot\mathbf{v}_d(E)$. In the isotropic case, (A8b) leads to Eq. (13).

We turn to the calculation of the diffusion coefficient $D_F(E)$ used in Sec. III. Consider the *variance* in the energy $E(t)-E_0$ acquired from the field between two collisions, instead of its average. From (A1), we have

$$\langle [E(t)-E_0]^2 \rangle = [(\partial_F E)_0]^2 \langle t^2 \rangle + O(F^3), \quad (\text{A9})$$

whence from (A4)

$$\langle [E(t)-E_0]^2 \rangle = 2\tau_0^2 [(\partial_F E)_0]^2 + O(F^3). \quad (\text{A10})$$

Since the average of the energy gain of the electron ensemble at E_0 is of order F^2 , its square is negligible compared to (A10), which therefore yields the desired variance upon ensemble average over the energy shell. If it is equated to $2D_F(E_0)\tau_0$ (to lowest order in F), we get the diffusion coefficient in energy space,

$$D_F(E_0) = \frac{\int \int_{E_0} \tau(\mathbf{p})(\partial_F E)^2 dS_{\mathbf{p}}/|\mathbf{v}_g|}{\int \int_{E_0} dS_{\mathbf{p}}/|\mathbf{v}_g|}. \quad (\text{A11})$$

The average displacement of the carrier packet in energy space, starting from $E=E_0$, is proportional to the drift velocity, while the ‘‘Brownian’’ (undirected) spread is related to the group velocity, which typically is an order of magnitude larger than \mathbf{v}_d . This is why $\{\langle [E(t)-E_0] \rangle\}^2$ is negligible compared to $\langle [E(t)-E_0]^2 \rangle$. (This is also the rationale for a nonlinear Fokker-Planck description of the fluctuations, as explained in Sec. IV B and Ref. 23.)

Equations (A8) and (A11) yield $W_F(E) = qFv_d(E)$ and $D_F(E)$ from elementary arguments. We proceed to demonstrate that $D_F(E)$ and $W_F(E)$ are linked through Eq. (21) obtained on general statistical-mechanical grounds. We have to check that

$$\int \int_E \tau(\mathbf{p})(\partial_F E)^2 dS_{\mathbf{p}}/|\mathbf{v}_g| = \int_0^E dE' \int \int_{E'} \partial_F(\tau \partial_F E) dS_{\mathbf{p}}/|\mathbf{v}_g|. \quad (\text{A12})$$

The right-hand side can be converted into the volume integral of $\partial_F(\tau \partial_F E)$ over the domain $E(\mathbf{p}) < E$. Next, if we interpret $\partial_F g$ as $\text{div}(q\mathbf{F}g)$ (with g , any scalar function), the Ostrogradsky theorem yields

$$\int \int \int_{E(\mathbf{p}) < E} \partial_F(\tau \partial_F E) d^3\mathbf{p} = \int \int_E (\tau \partial_F E) q\mathbf{F}\cdot d\mathbf{S}_{\mathbf{p}}. \quad (\text{A13})$$

Lastly, we write the vector surface element $d\mathbf{S}_{\mathbf{p}}$ as $(\partial E/\partial \mathbf{p})dS_{\mathbf{p}}/|\mathbf{v}_g|$. Q.E.D. It must be noted¹⁶ that the $\tau(\mathbf{p})$ to be used in this appendix is the relaxation time of the energy-space mean free path, which may differ from the collision time.

APPENDIX B

This appendix derives the phonon-related drift velocity $W_{\text{ph}}(E)$ and diffusion coefficient $D_{\text{ph}}(E)$ in energy space, the electron-phonon interaction $W_{\mathbf{p},\mathbf{p}'}$ being known. First, we address the question of phonon emission and absorption (absent in Sec. III) from a flat phonon branch. Second, keeping only phonon emission for simplicity, we obtain $W_{\text{ph}}(E)$ and $D_{\text{ph}}(E)$ in the general case.

Emission and absorption of phonons of fixed energy. In Sec. III C, only emission of phonons of fixed energy was considered. If absorption is taken into account, two more terms have to be added to (24a), and the second-order expansion yields

$$W_{\text{ph}}(E) = -\hbar\omega/\tau_{\text{em}}(E) + \hbar\omega/\tau_{\text{abs}}(E), \quad (\text{B1})$$

$$D_{\text{ph}}(E) = \frac{1}{2}(\hbar\omega)^2 [1/\tau_{\text{em}}(E) + 1/\tau_{\text{abs}}(E)],$$

where $1/\tau_i(E)$ ($i = \text{em,abs}$) should, in general, be understood as a constant-energy average of $1/\tau_i(\mathbf{p})$ as explained below. If $1/\tau(\mathbf{p})$ is the sum of the emission and absorption rates, and if the ratio of these rates is assumed^{11,12} to be $[n(\omega)+1]/n(\omega)$, then

$$W_{\text{ph}}(E) = \frac{-\hbar\omega/[2n(\omega)+1]}{\tau(E)}, \quad D_{\text{ph}}(E) = \frac{(\hbar\omega)^2}{2\tau(E)}. \quad (\text{B2})$$

Optical and acoustic phonons. Considering only phonon emission for simplicity, the energy relaxation rate for a carrier of momentum \mathbf{p} is given by

$$W_{\text{ph}}(\mathbf{p}) = - \int \int \int W_{\mathbf{p},\mathbf{p}'} \hbar\omega_{\mathbf{p}'-\mathbf{p}} d^3\mathbf{p}'/h^3, \quad (\text{B3})$$

where $W_{\mathbf{p},\mathbf{p}'}$ is the transition probability per unit time from state \mathbf{p} to state \mathbf{p}' , and $\hbar\omega_{\mathbf{p}'-\mathbf{p}}$ is the energy of the corresponding phonon. If several phonons connect \mathbf{p} and \mathbf{p}' , a sum over branches has to be performed. [If $\hbar\omega_{\mathbf{p}'-\mathbf{p}}$ is independent of \mathbf{p} and \mathbf{p}' , $W_{\text{ph}}(\mathbf{p})$ reduces to $\hbar\omega/\tau(\mathbf{p})$ according to Eq. (37)]. In view of the quasielasticity of the interaction ($W_{\mathbf{p},\mathbf{p}'} = T_{\mathbf{p},\mathbf{p}'}\delta[E(\mathbf{p})-E(\mathbf{p}')]$, Eq. (31)), we convert $W_{\text{ph}}(\mathbf{p})$ into a surface integral:

$$W_{\text{ph}}(\mathbf{p}) = - \int \int_{E(\mathbf{p})} T_{\mathbf{p},\mathbf{p}'} \hbar\omega_{\mathbf{p}'-\mathbf{p}} dS_{\mathbf{p}'}/|\mathbf{v}'_g| h^3, \quad (\text{B4})$$

which can be written as

$$W_{\text{ph}}(\mathbf{p}) = - \overline{(\hbar\omega_{\text{op}})}_{\mathbf{p}}/\tau_{\text{op}}(\mathbf{p}) - \overline{(\hbar\omega_{\text{ac}})}_{\mathbf{p}}/\tau_{\text{ac}}(\mathbf{p}), \quad (\text{B5})$$

where $\overline{(\)}_{\mathbf{p}}$ means, an average of $\hbar\omega_{\mathbf{p}'-\mathbf{p}}$ with a weighting factor $T_{\mathbf{p},\mathbf{p}'}/|\mathbf{v}'_g| h^3$ over the energy shell $E(\mathbf{p}')=E(\mathbf{p})$, and

$$1/\tau(\mathbf{p}) = \int \int_{E(\mathbf{p})} T_{\mathbf{p},\mathbf{p}'} dS_{\mathbf{p}'}/|\mathbf{v}'_g| h^3 = 1/\tau_{\text{op}}(\mathbf{p}) + 1/\tau_{\text{ac}}(\mathbf{p}). \quad (\text{B6})$$

In (B5), the acoustic term is usually neglected owing to the small acoustic-phonon energy. But it should not be overlooked that the *total* scattering rate (B6), including the acoustic-phonon scattering rate, is the one that appears in drift velocities. While acoustic-phonon scattering hardly contributes to W_{ph} and D_{ph} , it may affect W_F (and D_F) in reducing the drift velocities and thereby the energy exchanged with the field. An occurrence of this phenomenon can be found in Fischetti's theory²⁶ for SiO_2 .

Finally, from (B4), we obtain $W_{\text{ph}}(E)$ as the micro-canonical average of $W_{\text{ph}}(\mathbf{p})$ over the energy surface $E(\mathbf{p})=E$:

$$W_{\text{ph}}(E) = \frac{-\int \int_E (dS_{\mathbf{p}}/|\mathbf{v}_g|) \int \int_E (dS_{\mathbf{p}'}/|\mathbf{v}'_g| h^3) \hbar \omega_{\mathbf{p}'-\mathbf{p}} T_{\mathbf{p},\mathbf{p}'}}{\int \int_E dS_{\mathbf{p}}/|\mathbf{v}_g|} \quad (\text{B7})$$

Similarly, one obtains the phonon-related diffusion coefficient,

$$D_{\text{ph}}(E) = \frac{\int \int_E (dS_{\mathbf{p}}/|\mathbf{v}_g|) \int \int_E (dS_{\mathbf{p}'}/|\mathbf{v}'_g| h^3)^{\frac{1}{2}} (\hbar \omega_{\mathbf{p}'-\mathbf{p}})^2 T_{\mathbf{p},\mathbf{p}'}}{\int \int_E dS_{\mathbf{p}}/|\mathbf{v}_g|}, \quad (\text{B8})$$

which is usually negligible (see Sec. III D) within the validity range of the Fokker-Planck approach ($\hbar \omega/E_{\text{av}} \ll 1$).

If both phonon emission and absorption take place, (B7) and (B8) should be supplemented with the absorption term, see (B1).

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- ¹Proceedings of the 8th International Conference on Hot Carriers in Semiconductors (HCIS-8), Oxford, UK, 1993, edited by J. F. Ryan and A. C. Maciel [Semicond. Sci. Technol. **9**, 411 (1994)].
- ²M. V. Fischetti and S. E. Laux, Phys. Rev. B **38**, 9721 (1988).
- ³B. K. Ridley, J. Phys. C **16**, 3373 (1983).
- ⁴H. Shichijo and K. Hess, Phys. Rev. B **23**, 4197 (1981).
- ⁵M. G. Burt, J. Phys. C **18**, L477 (1985).
- ⁶S. McKenzie and M. G. Burt, J. Phys. C **19**, 1959 (1986).
- ⁷S. McKenzie and M. G. Burt, Semicond. Sci. Technol. **2**, 275 (1987).
- ⁸E. Bringuier, Phys. Rev. B **49**, 7974 (1994).
- ⁹E. Bringuier, J. Appl. Phys. **75**, 4291 (1994).
- ¹⁰P. A. Wolff, Phys. Rev. **95**, 1415 (1954).
- ¹¹C. R. Crowell and S. M. Sze, Appl. Phys. Lett. **9**, 242 (1966).
- ¹²E. A. Eklund, F.R. McFeely, and E. Cartier, Phys. Rev. Lett. **69**, 1407 (1992).
- ¹³G. A. Baraff, Phys. Rev. **128**, 2507 (1962).
- ¹⁴G. A. Baraff, Phys. Rev. **133**, A26 (1964).
- ¹⁵P. J. Price, in *Lasers, Junctions, Transport*, edited by R. K. Willardson and Albert C. Beer, Semiconductors and Semimetals Vol. 14 (Academic, New York, 1979), p. 249.
- ¹⁶W. Shockley, *Electrons and Holes in Semiconductors* (Van Nostrand, New York, 1950), pp. 293–294. Note that there is a misprint in the sign appearing in the last formula [rewritten as Eq. (13) in the present paper], which should be replaced by a plus.
- ¹⁷T. Kurosawa, J. Phys. Soc. Jpn. **20**, 937 (1965).
- ¹⁸I. B. Levinson, Fiz. Tverd. Tela (Leningrad) **6**, 2113 (1964) [Sov. Phys. Solid State **6**, 1665 (1965)].
- ¹⁹N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (Elsevier, Amsterdam, 1981), Chap. VIII.
- ²⁰N. G. van Kampen, J. Phys. Chem. Solids **49**, 673 (1988).
- ²¹J. Bardeen and W. Shockley, Phys. Rev. **80**, 69 (1950).
- ²²W. Shockley, in *Electrons and Holes in Semiconductors* (Ref. 16), p. 272.
- ²³N. G. van Kampen, in *Stochastic Processes in Physics and Chemistry* (Ref. 19), Chap. IX.
- ²⁴M. V. Fischetti and J. M. Higman, *Monte Carlo Device Simulation: Full Band and Beyond* (Kluwer, Norwell, MA, 1991), pp. 123–160.
- ²⁵B. K. Ridley, J. Phys. Condens. Matter **2**, 2941 (1990).
- ²⁶M. V. Fischetti, Phys. Rev. Lett. **53**, 1755 (1984); M. V. Fischetti, D. J. DiMaria, S. D. Brorson, T. N. Theis, and J. R. Kirtley, Phys. Rev. B **31**, 8124 (1985).