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Energy-diffusion equation for an electron gas interacting with polar optical phonons

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We present a novel method to solve explicitly the Boltzmann equation for highly energetic electrons interacting with polar optical phonons and scattering mainly in the forward direction. In this approach, the collision integral of the Boltzmann equation is reduced to a differential operator which is much easier to manipulate than the integral form and does not require a relaxation-time approximation. The relaxation of the distribution function with time as well as the spatial evolution of highly energetic electrons are calculated and closed-form expressions for the distribution function are given. In both cases the behavior of the electron distribution is characterized by two fundamental parameters: a drift factor which represents the net rate of phonon emission, and a broadening factor which is proportional to the latter and also to time and distance.

I. INTRODUCTION

The theory of high-field transport in semiconductors is closely related to the solution of the Boltzmann equation for high carrier energies.[1] Owing to its complexity (integro-differential equation), the Boltzmann equation cannot be solved explicitly. In the past two general methods of approximation have been proposed. The first relies on the concept of electron temperature and assumes a Maxwellian form of the isotropic part of the electron distribution function.[2,3] Unfortunately, this analytical method applies only to the case of very high electron densities. The other methods use numerical techniques (iterative and Monte Carlo) to solve the Boltzmann equation.[4,5] These methods are more exact but are rather time consuming and costly and therefore not easily applicable to semiconductor device models.

Recently, transient transport phenomena at high energies have been the subject of considerable interest in connection with "ballistic transport" in very short devices.[6] The idea is that for small device dimensions (of the order of the mean free path) the charge carriers suffer only a few collisions and gain extremely high speeds. In the calculations semiempirical (Newton) equations such as the following are often used[7]:

$$\frac{d}{dt} m v_d = qE - \frac{m v_d}{\tau_m} , \tag{1a}$$

$$\frac{d}{dt} \epsilon = q v_d E - \frac{\epsilon - \epsilon_0}{\tau_\epsilon} , \tag{1b}$$

where ϵ and ϵ_0 are the average and the zero-field energy, respectively, v_d is the drift velocity, E the electric field, m the effective mass, and τ_m and τ_ϵ are the empirical momentum and energy relaxation times.

This method has been subject to controversy since the boundary conditions have been oversimplified and spatial inhomogeneities and the statistical nature of the charge transport have been neglected.[8-10] Moreover, the criteria that define the mean free path are often based on the low-field and steady-state values of the physical parameters, whereas the calculations are applied to high-field and transient phenomena. The numerical methods, Monte Carlo, etc., also have their limitations. In addition to their high cost, they cannot easily be applied to complicated device structures.

In this paper we present a new derivation of the Boltzmann equation for fast electrons scattered by polar optical phonons (POP). This approach can be used to obtain closed-form integrations of the Boltzmann equation even for sophisticated device structures, provided the electrons are injected at high energies and the electric fields away from the injecting barrier can be treated as perturbation. Injection of electrons over barriers was proposed recently[11] to achieve extremely high electron velocities over large distances. It is important in many heterojunction structures[12] and planar doped barrier devices.[13] Our solution of the Boltzmann equation is similar in character to the treatment of Dumke.[14] He pointed out that the strong anisotropy of the POP relaxation process makes the derivation of a diffusion equation for highly energetic electrons possible. His analysis was based on the flux conservation in energy space. Our approach yields similar expressions but is directly derived from the Boltzmann equation for scattering by POP at high energies. We use the Fermi golden rule for the calculation of the rates of phonon emission and absorption and restrict our analysis to moderate electric fields and therefore neglect the intracollisional field effect. For GaAs the fields can reach 5×10^3 V/cm without modifying appreciably the electron-phonon transition probability.[15]

The general features of the theory are discussed in the next section. Section III treats some applications of a general nature, and details of the derivations are left to the Appendix. Discussions of specific devices are left to planned future publications.[13,16]

II. THEORY

Our treatment is applicable to moderately polar semiconductors such as GaAs, InP, etc. We assume in this analysis that the conduction band is spherical and that the dispersion relation between the carrier energy and its wave vector is parabolic. However, we restrict the highest possible velocity to values smaller than $\sim10^8$ cm/s as dictated by band-structure considerations. Satellite valleys are not taken into account. The electron gas is assumed to be nondegenerate under these high-energy conditions. With these limitations the collision integral for the POP scattering can be written as follows:

$$\hat{C}_{\mathrm{POP}}f=\int[W_e(\vec{k}'\to\vec{k})+W_a(\vec{k}'\to\vec{k})]f(\vec{k}')D(\vec{k}')d\vec{k}'-f(\vec{k})\int[W_e(\vec{k}\to\vec{k}')+W_a(\vec{k}\to\vec{k}')]D(\vec{k}')d\vec{k}' \;. \tag{2}$$

Here $D(\vec{k})$ is the density of states at wave vector $\vec{k}$, equal to $V/(2\pi)^3$ where V is the semiconductor volume. The function $W_{a,e}(\vec{k}'\to\vec{k})$ is the transition probability from $\vec{k}'$ to $\vec{k}$ for an electron interacting with one POP. The labels a and e denote absorption and emission processes, respectively. In the framework for the Fröhlich Hamiltonian one obtains[17]

$$W_{a,e}(\vec{k}'\to\vec{k})=\frac{8\pi^2}{V}\left[\frac{\hbar}{2m\omega}\right]^{1/2}\frac{\alpha\hbar\omega^2}{|\vec{k}'-\vec{k}|^2}(N_q+\tfrac{1}{2}\pm\tfrac{1}{2})\delta(\epsilon'-\epsilon\pm\hbar\omega)\;, \tag{3}$$

where ω is the POP frequency, for which any dispersion is neglected, and α is Frölich's electron-phonon coupling constant. N_q is the equilibrium phonon distribution given by

$$N_q=\left[\exp\left[\frac{\hbar\omega}{k_BT}\right]-1\right]^{-1}, \tag{4}$$

where k_B is the Boltzmann constant and T is the lattice temperature. By substituting (3) into (2) and distinguishing both the absorption and emission term, the collisional integral takes the form

$$\hat{C}_{\mathrm{POP}}f=\frac{\alpha}{\pi(1-\gamma)}\frac{(\hbar\omega)^{3/2}}{(2m)^{1/2}}\left[\int\frac{d\vec{k}'f(\vec{k}')}{|\vec{k}'-\vec{k}|^2}[\delta(\epsilon'-\epsilon-\hbar\omega)+\gamma\delta(\epsilon'-\epsilon+\hbar\omega)]\right.$$
$$\left.-f(\vec{k})\int\frac{d\vec{k}'}{|\vec{k}-\vec{k}'|^2}[\delta(\epsilon'-\epsilon+\hbar\omega)+\gamma\delta(\epsilon'-\epsilon-\hbar\omega)]\right], \tag{5}$$

where $\gamma=\exp(-\hbar\omega/k_BT)$. With the use of the properties of the δ function for a parabolic band the factor depending on the wave-vector difference can be written as

$$\frac{1}{|\vec{k}'-\vec{k}|^2}\delta(\epsilon'-\epsilon\pm\hbar\omega)=\frac{\hbar^2}{4m}\frac{1}{[\epsilon(\epsilon\pm\hbar\omega)]^{1/2}}\frac{\delta(\epsilon'-\epsilon\pm\hbar\omega)}{[1-1/(2\epsilon/\hbar\omega\pm1)^2]^{-1/2}-\cos\Theta}\;. \tag{6}$$

Here Θ is the angle between $\vec{k}'$ and $\vec{k}$. For high energies the scattering probability is strongly anisotropic. For $\epsilon\geq2\hbar\omega$ small-angle scattering ($\cos\Theta\simeq1$) is almost 20 times more probable than large-angle scattering ($\cos\Theta\lesssim0$) in the case of emission. For absorption the ratio is more than 2.5 larger (Fig. 1). Therefore, for

$\epsilon \geq 2\hbar\omega$ we assume forward scattering to be dominant and write

$$\frac{\delta(\epsilon'-\epsilon\mp\hbar\omega)}{|\vec{k}'-\vec{k}|^2}\simeq R_{\pm}(\epsilon)\delta(\cos\Theta-1)\delta(\epsilon'-\epsilon\mp\hbar\omega)\,, \tag{7}$$

where

$$R_{\pm}(\epsilon)=\frac{2\hbar^2}{m}\frac{1}{[\epsilon(\epsilon\pm\hbar\omega)]^{1/2}}\operatorname{arcsinh}\begin{cases}(\epsilon/\hbar\omega)^{1/2}\\ [(\epsilon/\hbar\omega)-1]^{1/2}\,.\end{cases} \tag{8}$$

Neglecting the azimuthal dependence of the distribution function (azimuthal symmetry), the collision integral takes the form

$$\hat{C}_{\mathrm{POP}}f=\frac{2\alpha\omega}{(1-\gamma)}\left[\frac{\operatorname{arcsinh}\sqrt{\epsilon/\hbar\omega}}{\sqrt{\epsilon/\hbar\omega}}f(\epsilon+\hbar\omega,\cos\theta)+\frac{\operatorname{arccosh}\sqrt{\epsilon/\hbar\omega}}{\sqrt{\epsilon/\hbar\omega}}f(\epsilon-\hbar\omega,\cos\theta)\right.$$
$$\left.-\frac{1}{\sqrt{\epsilon/\hbar\omega}}(\operatorname{arccosh}\sqrt{\epsilon/\hbar\omega}+\gamma\operatorname{arcsinh}\sqrt{\epsilon/\hbar\omega})f(\epsilon,\cos\theta)\right]\,, \tag{9}$$

where θ is the polar angle of the vector $\vec{k}$. For high energy the coefficients of the distribution function in the right-hand side (rhs) are almost equal, and we may assume

$$\frac{\operatorname{arcsinh}\sqrt{\epsilon/\hbar\omega}}{\sqrt{\epsilon/\hbar\omega}}\simeq\frac{\operatorname{arccosh}\sqrt{\epsilon/\hbar\omega}}{\sqrt{\epsilon/\hbar\omega}}\equiv S(\epsilon)\,, \tag{10}$$

and we can expand f, which gives

$$\hat{C}_{\mathrm{POP}}f\simeq\frac{2\alpha\hbar^2\omega^3}{(1-\gamma)}S(\epsilon)\left[\frac{1-\gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}f(\epsilon,\cos\theta)+\frac{1+\gamma}{2}\frac{\partial^2}{\partial\epsilon^2}f(\epsilon,\cos\theta)\right]\,. \tag{11}$$

Expression (11) is much easier to handle than the corresponding integral expression. It gives a useful differential form to the collisional operator $\hat{C}_{\mathrm{POP}}$. The collisional operator includes two terms: The first is the drift term in energy space, which is independent of temperature. It represents the net rate of phonon emission. The second term (second derivative) is the diffusion term, which is a function of temperature through the factor $(1+\gamma)/(1-\gamma)$. The above procedure is valid under the condition that the function f varies very slowly in an energy interval of width $\hbar\omega$. Generally this condition can only be verified self-consistently. However, we can anticipate that the procedure is certainly valid for large electron energy.

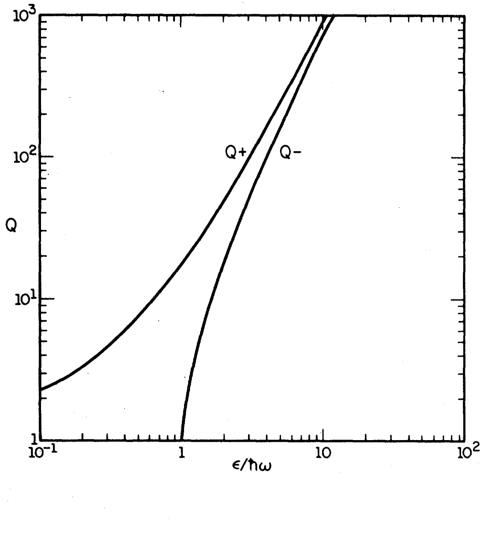

FIG. 1. Anisotropy Q factor for the transition probability in POP scattering as a function of the electron energy. The Q factor is the ratio between the transition probability for small angle ($\cos\Theta=1$) to the transition probability for large angle ($\cos\Theta=0$). The Q factor is calculated with Eq. (6) and the + and − signs are for the absorption and the emission, respectively.

III. APPLICATIONS

In this section we derive special solutions of Eq. (11). In equilibrium we have the following:

$$\frac{2\Gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}f+\frac{\partial^2}{\partial\epsilon^2}f=0\,, \tag{12}$$

where

$$\Gamma=\frac{1-\gamma}{1+\gamma} . \tag{13}$$

The solution of this equation is

$$f(\epsilon)=K\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right] , \tag{14}$$

which is Maxwellian in form. K is a constant of integration. Moreover, for $\gamma\to 1$ we obtain $2\Gamma/\hbar\omega\simeq 1/k_BT$. Figure 2 gives the temperature variation of the factor $1/2\Gamma$. We see that the equilibrium solution is not Maxwellian at low temperature but approaches a Maxwell distribution for high temperature in accordance with our approximations. For GaAs and room temperature the deviations from the Maxwellian solution are smaller than 15%.

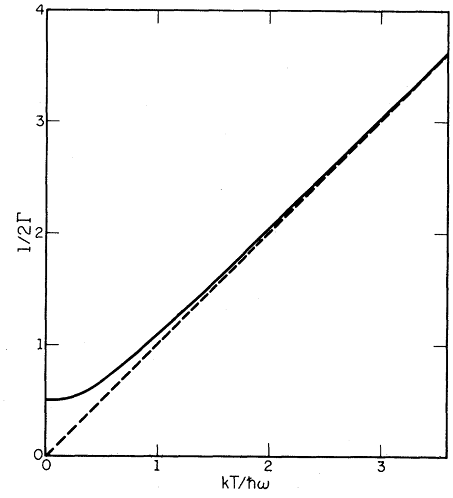

FIG. 2. Variation of the inverse of the Γ factor in function of the temperature normalized to the phonon energy.

A. Time-dependent solution

One of the main interests in reducing device dimensions is to achieve a very fast temporal response to external perturbations. Here we apply our formalism to simple relaxation processes. The field-free energy relaxation of charge carriers is an example of temporal evolution of the distribution function. Specifically, we consider the case of high-energy injection and neglect the external electric field. The electron concentration is assumed to be spatially homogeneous. This particular situation sheds light on the high-energy relaxation process when POP scattering is important, and it is also important for the photoconductivity at high fields.[18] With these assumptions and Eq. (11) we arrive at

$$\frac{\partial}{\partial t}f(\epsilon,t)=\frac{\alpha}{\Gamma}\hbar^2\omega^3S(\epsilon)\left[\frac{2\Gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}f(\epsilon,t)+\frac{\partial^2}{\partial\epsilon^2}f(\epsilon,t)\right] . \tag{15}$$

Using a δ-like energy distribution at $t=0$, and the equilibrium distribution of Eq. (14) at $t=\infty$, we have

$$f(\epsilon,t)=\sum_{\nu}U_\nu(t)Q_\nu(\epsilon) \tag{16}$$

by separating variables. $U_\nu(b)$ and $Q_\nu(t)$ are, respectively, solutions of

$$\frac{\partial}{\partial t}U_\nu(t)+\omega\nu U_\nu(t)=0 \tag{17a}$$

and

$$\frac{\partial^2}{\partial\epsilon^2}Q_\nu(\epsilon)+\frac{2\Gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}Q_\nu(\epsilon)+\frac{\nu}{(\hbar\omega)^2\beta}Q_\nu(\epsilon)=0 , \tag{17b}$$

with

$$\beta=\frac{\alpha S(\epsilon_0)}{\Gamma} .$$

For simplicity, we have assumed that the slowly varying function $S(\epsilon)$ is constant and equal to its value $S(\epsilon_0)$ at the injection energy ϵ_0. The general solution is

$$f(\epsilon,t)=\exp\left[-\frac{\Gamma\epsilon}{\hbar\omega}\right]\left\{\sum_{\nu<\beta\Gamma^2}\left[A'_\nu\exp\left[\frac{\sigma\epsilon}{\hbar\omega}\right]+B'_\nu\exp\left[-\frac{\sigma\epsilon}{\hbar\omega}\right]\right]\exp(-\nu\omega t)\right.$$
$$\left.+\sum_{\nu>\beta\Gamma^2}\left[A_\nu\exp\left[i\frac{\mu\epsilon}{\hbar\omega}\right]+B_\nu\exp\left[-i\frac{\mu\epsilon}{\hbar\omega}\right]\right]\exp(-\nu\omega t)\right\} , \tag{18}$$

with

$$\sigma=(\Gamma^2-\nu/\beta)^{1/2}\,, \tag{19a}$$

$$\mu=(\nu/\beta-\Gamma^2)^{1/2}\,. \tag{19b}$$

From the boundary conditions one obtains

$$A'_\nu=0\,, \tag{20}$$

and the initial condition yields

$$2\left[\frac{\hbar^2}{2m}\right]^{3/2}\frac{\delta(\epsilon-\epsilon_0)}{\sqrt{\epsilon_0}}=\exp\left[-\frac{\Gamma\epsilon}{\hbar\omega}\right]\left\{\sum_{\sigma=0}^{\Gamma}B_\sigma\exp\left[-\left[\frac{\sigma\epsilon}{\hbar\omega}\right]\right]+\sum_{\mu=0}^{\infty}\left[A_\mu\exp\left[\frac{i\mu\epsilon}{\hbar\omega}\right]+B_\mu\exp\left[-\frac{i\mu\epsilon}{\hbar\omega}\right]\right]\right\}. \tag{21}$$

If we choose $A_\mu=B_\mu=\frac{1}{2}C(\mu)$, a Fourier analysis gives

$$C(\mu)=\frac{4}{\pi}\left[\frac{\hbar^2}{2m}\right]^{3/2}\left[\frac{\exp(\Gamma\epsilon_0/\hbar\omega)}{\sqrt{\epsilon_0}}\cos\left[\frac{\mu\epsilon_0}{\hbar\omega}\right]-\frac{1}{2}\left[\frac{2m}{\hbar^2}\right]^{3/2}\sum_{\sigma=0}^{\Gamma}B_\sigma\frac{\sigma}{\sigma^2+\mu^2}\right]. \tag{22}$$

The coefficients B_σ are determined by requiring that the energy distribution function remain normalized for any time. However, this procedure is long and tedious; therefore, we use the trial solution

$$B_\sigma=K(t)\delta_{\sigma,\Gamma}\,, \tag{23}$$

where $K(t)$ is a function of time which must satisfy

$$K(0)=0 \tag{24a}$$

and

$$K(\infty)=\frac{4}{\sqrt{\pi}}\left[\frac{\hbar\Gamma}{m\omega}\right]^{3/2}, \tag{24b}$$

since for $t=\infty$ the normalized equilibrium function is

$$f_0(\epsilon)=\frac{4}{\sqrt{\pi}}\left[\frac{\hbar\Gamma}{m\omega}\right]^{3/2}\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right]. \tag{25}$$

The expression

$$K(t)=\frac{4}{\sqrt{\pi}}\left[\frac{\hbar\Gamma}{m\omega}\right]^{3/2}\left[1-\exp\left[-\frac{\Gamma^2}{2}\beta\omega t\right]\right] \tag{26}$$

gives an error of less than 5%. Therefore, Eq. (18) becomes

$$f(\epsilon,t)=K(t)\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right]+\exp\left[-\left[\frac{\Gamma\epsilon}{\hbar\omega}+\Gamma^2\beta\omega t\right]\right]\int_0^\infty d\mu\, C(\mu)\cos\left[\frac{\mu\epsilon}{\hbar\omega}\right]e^{-\mu^2\beta\omega t}\,, \tag{27}$$

where we have replaced the summation by an integral. Finally, after tedious algebra (see Appendix A) a closed-form expression for the distribution function can be obtained:

$$f(\epsilon,t)=\frac{2\Gamma}{\sqrt{\pi}}K(t)\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right]\int_0^{\sqrt{\beta\omega t}}dz\exp\left[-\left[\Gamma z-\frac{\epsilon}{2\hbar\omega z}\right]^2\right]$$
$$+\frac{1}{2\sqrt{\pi}}\left[\frac{\hbar^2}{m\beta[\epsilon_0(\hbar\omega)^2]^{1/3}\omega t}\right]^{3/2}\exp\left[-\frac{(\epsilon-\epsilon_0+2\Gamma\beta\hbar\omega^2 t)^2}{4\hbar^2\omega^3\beta t}\right]. \tag{28}$$

The energy distribution function consists of two parts. The first term of the rhs is the equilibrium distribution function which is zero at $t=0$. The second term of the rhs is the diffusion (plus drift) term in energy space. The "drift velocity" in energy space is given by the factor $2\Gamma\beta\hbar\omega^2$ and represents the net rate of POP emission as expected. Thus in our approach it is independent of the temperature ($\Gamma\beta=$const). The broadening factor of the distribution function is proportional to time and is given by $4\hbar^2\omega^3\beta t$. It is also proportional to the rate of phonon emission and thus, to the drift factor. It is an increasing function of the temperature ($\beta \propto 1/\Gamma$). Typically, the process can be described as follows: Initially, the distribution function is strongly peaked at $\epsilon=\epsilon_0$, then, under the influence of the POP scattering, mainly emission, it drifts toward low energy and is broadened (Fig. 3).

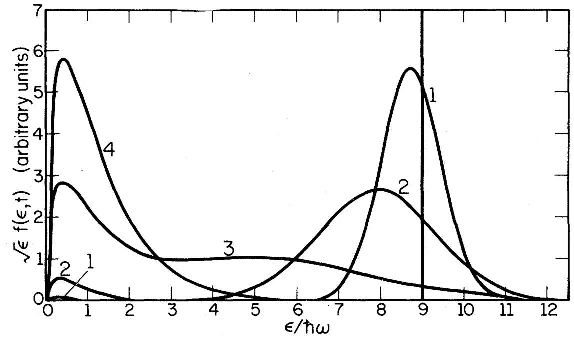

FIG. 3. Temporal evolution of the energy distribution function at $T=300$ K. The starting energy ϵ_0 is $9\hbar\omega$. The δ function is represented by the vertical line. (1) $\beta\omega t=0.25$, (2) $\beta\omega t=1$, (3) $\beta\omega t=4$, (4) $\beta\omega t=\infty$. For GaAs the $\beta\omega$ factor is 7.31×10^{12} s^{-1}.

B. Space-dependent solution—one-dimensional case

Another problem of importance is the charge transport in the presence of a spatially inhomogeneous carrier concentration in the x direction. In this case we start from the equation

$$\sqrt{2\epsilon/m}\,\frac{\partial}{\partial x}f(\epsilon,x)+eE\sqrt{2\epsilon/m}\,\frac{\partial}{\partial \epsilon}f(\epsilon,x)$$

$$=\frac{\alpha}{\Gamma}\hbar^2\omega^3 S(\epsilon)\left[\frac{2\Gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}f(\epsilon,x)+\frac{\partial^2}{\partial\epsilon^2}f(\epsilon,x)\right]. \tag{29}$$

In order to simplify the calculation we assumed $\theta=0$, i.e., all the electrons are injected in the x direction with a velocity parallel to the electric field. As mentioned in Sec. II the scattering does not change the injection direction for high energy. Before solving Eq. (29) a general consideration must be made concerning the field term. If we neglect the spatial diffusion of the distribution function, Eq. (29) has no stationary solution for $eE>0$. Indeed the field term is proportional to $\sqrt{\epsilon}$ and increases with energy whereas the first derivative of the rhs is approximately constant. This means that for a certain value of energy the second derivative of the distribution function changes its sign. A more detailed analysis shows that the distribution decreases with energy and suddenly increases to a nonzero value for high energy.[19] This is the well-known "runaway effect," i.e., an unbounded increase in electron thermal and drift velocity in the presence of POP scattering only.[20] In this work we will deal with relatively small electric fields and will not consider this effect which occurs at very high energy where other scattering mechanisms [intervalley scattering (GaAs) or impact ionization (InAs)] play a more significant role.

As in the preceding section we consider an idealized monoenergetic distribution function represented by a δ function at $x=0$. Moreover, we set $S(\epsilon)=S(\epsilon_0)=C^t$, a constant, where ϵ_0 is the initial electron energy. Equation (29) is too complicated to be solved exactly; therefore we must proceed with successive approximations. In the spatial diffusion term $\partial f/\partial x$ we approximate $\sqrt{\epsilon}$ by a constant value $\sqrt{\epsilon_0}$ and treat the deviations as a perturbation. The electric field is also treated as a perturbation. This reduces Eq. (29) to a more manageable form,

$$\frac{\partial^2}{\partial\epsilon^2}f(\epsilon,x)+\frac{2\Gamma}{\hbar\omega}\frac{\partial}{\partial\epsilon}f(\epsilon,x)-\frac{\sqrt{2\epsilon_0/m}}{\beta\omega}\frac{\partial}{\partial x}f(\epsilon,x)$$

$$=F(\epsilon,x)\,, \tag{30}$$

where

$$F(\epsilon,x)=\frac{1}{(\hbar\omega)^2}\left[\frac{eE}{\beta\omega}\sqrt{2\epsilon/m}\,\frac{\partial}{\partial\epsilon}f(\epsilon,x)+(\sqrt{2\epsilon/m}-\sqrt{2\epsilon_0/m}\,)\frac{1}{\beta\omega}\frac{\partial}{\partial x}f(\epsilon,x)\right] \tag{31}$$

is a correction term. With the use of the same procedure as in the preceding section the general solution of the homogeneous equation is written as

$$f_0(\epsilon,x)=\frac{2}{\sqrt{\pi}}\exp\left[-\frac{\Gamma\epsilon}{\hbar\omega}\right]\int_0^{\Gamma}d\sigma\,B(\sigma)\exp\left[-\frac{\sigma\epsilon}{\hbar\omega}\right]\int_0^{\sqrt{\beta^*\omega x}}dz\,\exp\left[-\left[\sigma z-\frac{\epsilon}{2\hbar\omega^2}\right]^2\right]$$
$$+\frac{2}{\sqrt{\pi}}\left[\frac{\hbar^2}{m\beta^*[\epsilon_0(\hbar\omega)^2]^{1/3}\omega x}\right]^{3/2}\exp\left[-\frac{(\epsilon-\epsilon_0+2\Gamma\beta^*\hbar\omega^2x)^2}{4\beta^*\hbar^2\omega^3x}\right], \tag{32}$$

with $\beta^*=\sqrt{m/2\epsilon_0}\beta$. The $B(\sigma)$ coefficients are determined from the normalization of the distribution function. Notice that the normalization factor of the transient term is different from (28). This results from the fact that the "initial" ($x=0$) distribution is strongly anisotropic (Appendix C). Again, the distribution function consists of two parts: the terms of the equilibrium function, which are vanishing at $x=0$, and the drifted-diffused distribution function represented by the last term of the rhs. The broadening factor is now given by $4\beta^*\hbar^2\omega^3x$ and is inversely proportional to the injection velocity $\sqrt{2\epsilon_0/m}$, whereas the "drift velocity" in energy space is now $2\Gamma\beta^*\hbar\omega^2$, as expected from kinetic consideration.

According to our procedure the distribution function $f_0(\epsilon,x)$ is only the zero-order approximation. We need to use the first-order approximation $f_1(\epsilon,x)$ to properly include the dependence on the electric field and the diffusion term of Eq. (30). The corrected distribution function contains both the zero- and first-order terms,

$$f(\epsilon,x)=f_0(\epsilon,x)+f_1(\epsilon,x)\,, \tag{33}$$

where

$$f_1(\epsilon,x)=\int_0^x dx'\int_0^\infty d\epsilon'\,G(\epsilon-\epsilon';x-x')F(f_0(\epsilon',x'))\exp\left[-\frac{\Gamma}{\hbar\omega}(\epsilon-\epsilon')\right], \tag{34}$$

with

$$F(f_0(\epsilon,x))=\frac{1}{(\hbar\omega)^2}\left[\frac{eE}{\beta^*\omega}\sqrt{\epsilon/\epsilon_0}\frac{\partial}{\partial\epsilon}f_0(\epsilon,x)+(\sqrt{\epsilon/\epsilon_0}-1)\frac{1}{\beta^*\omega}\frac{\partial}{\partial x}f_0(\epsilon,x)\right]. \tag{35}$$

Here the electric field E is eventually dependent on the x position. The Green's function $G(\epsilon-\epsilon';x-x')$ is given by the following (see Appendix B):

$$\begin{aligned}G(\epsilon-\epsilon';x-x')&=0\quad\text{if } x'>x\\&=-\hbar\omega\left[\frac{\beta^*\omega}{4\pi(x-x')}\right]^{-1/2}\\&\quad\times\exp\left\{-\left[\left[\frac{\epsilon-\epsilon'}{2\hbar\omega}\right]^2\frac{1}{\beta^*\omega(x-x')}+\Gamma^2\beta^*\omega(x-x')\right]\right\}\quad\text{if } x'<x\,.\end{aligned} \tag{36}$$

Here several remarks must be made concerning our derivation: The entire procedure is based on a one-dimensional calculation because we assumed $\cos\theta=1$. This approximation is reasonable for high energy where the scattering is in the forward direction but it is a very bad approximation for low energy $\epsilon\leq\hbar\omega$ where the POP scattering is quasi-isotropic. However, Fig. 1 indicates that the onset of anisotropy occurs already for $\epsilon\gtrsim\hbar\omega$. This means that only the distribution function near the equilibrium is affected by the isotropic scattering. Under this condition we can use Eq. (23) of the preceding section to scale the equilibrium distribution function and provide a good normalization factor for this three-dimensional function. Then the transient term of the distribution function (32) is totally anisotropic while the equilibrium term is isotropic. Moreover, instead of taking the exact solution of our differential operator, nonvalid at low energy, we assume for the asymptotic (equilibrium) distribution function the exact equilibrium distribution function, which is Maxwellian at the lattice temperature. The first term of Eq. (32) can be written

$$f_{\mathrm{as}}(\epsilon,x)=\frac{1}{\sqrt{\pi}}\frac{\hbar\omega}{k_BT}K(x)\exp\left[-\frac{\epsilon}{k_BT}\right]\times\int_0^{\sqrt{\beta^*\omega x}}dz\exp\left[-\left[\frac{\hbar\omega}{2k_BT}z-\frac{\epsilon}{2\hbar\omega z}\right]^2\right], \quad (37)$$

where $f_{\mathrm{as}}(\epsilon,x)$ is asymptotic, $K(x)$ is given by

$$K(x)=\left[\frac{\hbar^2}{2\pi m k_BT}\right]^{3/2}[1-\exp(-\chi\Gamma^2\beta^*\omega x)], \quad (38)$$

and $x=0.42$ gives the optimum normalization constant. Then we obtain a solution that is good for high energy and short distance as well as for low energy and long distance. Within this framework the equilibrium distribution is not modified by the first-order perturbation. The corrections introduced by the field term and the residual diffusion term affect only the transient part of the distribution function. Figure 4 presents the results for GaAs at zero field. The space evolution of the distribution function is very similar to the time evolution except for a slight shift toward the low energy which comes from the perturbation term. We have also plotted the true equilibrium distribution function.

IV. CONCLUSION

The purpose of this paper was to present a general method for treating the electron-POP interaction in the semiclassical approximation of high-energy processes. In this framework we have derived a differential expression for the collision operator of the Boltzmann equation. The differential nature of the collision operators, which is similar to a Fokker-Planck expression, is well adapted to treat the stochastic processes of nonequilibrium phenomena. In this respect it is a better approximation than previous theories that exclude statistical considerations as well as realistic boundary conditions (neglected diffusion current). On the other hand, this method is less costly than numerical simulations. Specific simple examples have been treated, and closed forms for the distribution have been obtained. In each case, provided the electric field is considered as a perturbation, the time-dependent distribution and the space-dependent distribution have the same form, composed of a transient term and an asymptotic equilibrium term. The transient distribution is characterized by two fundamental parameters: the drift factor and the broadening factor. The former, given by $2\Gamma\beta\hbar\omega^2$ (temporal evolution) and $2\Gamma\beta^*\hbar\omega^2$ (spatial evolution), represents the net rate of phonon emission per unit time and unit distance, respectively. In our approximation it is independent of the temperature. The broadening factor is given by $4\hbar^2\omega^3\beta t$ (temporal evolution) and by $4\hbar^2\omega^3\beta^*x$ (spatial evolution). It is proportional to time and distance, respectively, as expected from the conventional diffusion theory, but it is also proportional to the drift parameter. The broadening factor is inversely proportional to the injection velocity $\sqrt{2\epsilon_0/m}$. Although the assumptions made to derive the collision operator are only justified for high-energy processes—because of the strong anisotropy of the transition probability of the electron-POP interaction—the method can be extended to low-energy situations, provided that the low-energy distribution function is the asymptotic solution of the problem. Under these conditions the mixed solution, including the transient distribution function (a solution of our high-energy differential operator) and the true asymptotic distribution function (a solution of the general low-energy Boltzmann equation), described the physical reality in a better way than the exact solution of our differential equation, which fails at low energy.

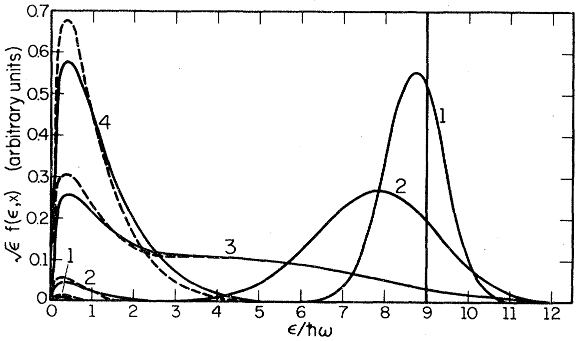

FIG. 4. Spatial evolution of the energy distribution function at $T=300$ K and for $E=0$. The starting distribution function (δ function) is represented by the vertical line at $\epsilon_0=9\hbar\omega$. (1) $\beta^*\omega x=0.25$, (2) $\beta^*\omega x=1$, (3) $\beta^*\omega x=4$, (4) $\beta^*\omega x=\infty$. For GaAs the $\beta^*\omega$ factor is 5.49×10^4 cm^{-1}. The solid line is for the equilibrium distribution given by Eq. (14); the dotted line is for the Maxwell-Boltzmann equilibrium distribution.

The simplicity of the solutions for the different problems treated in this paper arises from the assumption of the one-dimensional motion in $\vec{k}$ space and initial-energy δ function. This has the advantage of giving a simple picture of the temporal and spatial evolution of the distribution function and a first-principles theory of the various relaxation times. The results are directly applicable to transport in novel device structures such as planar diffused barriers and devices involving heterojunction structures.

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APPENDIX A

We want to evaluate the integral

$$I=\int_0^\infty d\mu\, C(\mu)\cos\left[\frac{\mu\epsilon}{\hbar\omega}\right]\exp(-\mu^2\beta\omega t) \tag{A1}$$

with the expression of $C(\mu)$

$$C(\mu)=\frac{1}{\pi^2}\left[\frac{\hbar^2}{2m}\right]^{3/2}\left[\frac{1}{\sqrt{\epsilon_0}}\exp\left[\frac{\Gamma\epsilon_0}{\hbar\omega}\right]\cos\left[\frac{\mu\epsilon_0}{\hbar\omega}\right]-2\pi\left[\frac{2m}{\hbar^2}\right]^{3/2}K(t)\frac{\Gamma}{\Gamma^2+\mu^2}\right]. \tag{A2}$$

This integral is composed of 2 parts:

$$I_1=\frac{1}{\pi^2}\left[\frac{\hbar^2}{2m}\right]^{3/2}\frac{1}{\sqrt{\epsilon_0}}\exp\left[\frac{\Gamma\epsilon_0}{\hbar\omega}\right]\int_0^\infty d\mu\cos\left[\frac{\mu\epsilon}{\hbar\omega}\right]\cos\left[\frac{\mu\epsilon_0}{\hbar\omega}\right]\exp(-\mu^2\beta\omega t) \tag{A3a}$$

and

$$I_2=\frac{2\Gamma}{\pi}K(t)\int_0^\infty\frac{d\mu}{\Gamma^2+\mu^2}\cos\left[\frac{\mu\epsilon}{\hbar\omega}\right]\exp(-\mu^2\beta\omega t)\,. \tag{A3b}$$

The first integral I_1 can be written

$$I_1=\frac{1}{\pi^2}\left[\frac{\hbar^2}{2m}\right]^{3/2}\frac{1}{\sqrt{\epsilon_0}}\exp\left[\frac{\Gamma\epsilon_0}{\hbar\omega}\right]\int_0^\infty\frac{d\mu}{2}\exp(-\mu^2\beta\omega t)\left[\cos\left[\frac{\mu}{\hbar\omega}(\epsilon_0+\epsilon)\right]+\cos\left[\frac{\mu}{\hbar\omega}(\epsilon-\epsilon_0)\right]\right] \tag{A4}$$

and evaluated

$$I_1=\left[\frac{\hbar^2}{4\pi m\beta[\epsilon_0(\hbar\omega)^2]^{1/3}\omega t}\right]^{3/2}\left[\exp-\left[\frac{(\epsilon+\epsilon_0)^2}{4\beta\hbar^2\omega^3 t}\right]+\exp\left[-\frac{(\epsilon-\epsilon_0)^2}{4\beta\hbar^2\omega^3 t}\right]\right]. \tag{A5}$$

The second integral I_2 has the expression

$$I_2=\frac{2\Gamma K(t)}{\pi}\exp(\Gamma^2\beta\omega t)\int_0^\infty d\mu\cos\left[\frac{\mu\epsilon}{\hbar\omega}\right]\int_0^\infty ds\exp[-(\Gamma^2+\mu^2)s]\,. \tag{A6}$$

Interchanging the integrals we obtain

$$I_2=\frac{\Gamma K(t)}{\sqrt{\pi}}\exp(\Gamma^2\beta\omega t)\int_{\beta\omega t}^\infty\frac{ds}{\sqrt{s}}\exp\left\{-\left[\Gamma^2 s+\left[\frac{\epsilon}{2\hbar\omega}\right]^2\frac{1}{s}\right]\right\}, \tag{A7}$$

or setting $s=z^2$

$$
\begin{aligned}
I_2 &= \frac{2\Gamma K(t)}{\sqrt{\pi}}\exp(\Gamma^2\beta\omega t)\left[\int_0^\infty - \int_0^{\sqrt{\beta\omega t}}\right]dz\,\exp\left[-\Gamma^2 z^2 - \left[\frac{\epsilon}{2\hbar\omega z}\right]^2\right] \\
&= \frac{2\Gamma K(t)}{\sqrt{\pi}}\exp(\Gamma^2\beta\omega t)\left\{\frac{\sqrt{\pi}}{2\Gamma}\exp(-\Gamma\epsilon) - \int_0^{\sqrt{\beta\omega t}} dz\,\exp\left[-(\Gamma z)^2 - \left[\frac{\epsilon}{2\hbar\omega z}\right]^2\right]\right\}, \qquad \text{(A8)}
\end{aligned}
$$

and finally

$$
\begin{aligned}
I\exp\left[-\left[\frac{\Gamma\epsilon}{\hbar\omega}+\Gamma^2\beta\omega t\right]\right] = \left[\frac{\hbar^2}{4\pi m\beta[\epsilon_0(\hbar\omega)^2]^{1/3}\omega t}\right]^{3/2} &\left[\exp\left[-\frac{(\epsilon-\epsilon_0+2\Gamma\beta\hbar\omega^2 t)^2}{4\beta\hbar^2\omega^3 t}\right]\right. \\
&\left.+\exp\left[\frac{2\Gamma\epsilon_0}{\hbar\omega}-\frac{(\epsilon+\epsilon_0+2\Gamma\beta\hbar^2\omega^3 t)^2}{4\beta h^2\omega^3 t}\right]\right] \\
-K(t)\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right] + \frac{2\Gamma}{\sqrt{\pi}}K(t)\exp\left[-\frac{2\Gamma\epsilon}{\hbar\omega}\right]& \\
\times \int_0^{\sqrt{\beta\omega t}} dz\,\exp\left[-\left[\Gamma z - \frac{\epsilon}{2\hbar\omega z}\right]^2\right]&, \qquad \text{(A9)}
\end{aligned}
$$

which yields Eq. (28) if we omit the second term in square brackets on the rhs, which is a negligible factor while $\epsilon_0 >> \hbar\omega$.

APPENDIX B

Equation (30) can be reduced to

$$\frac{\partial^2}{\partial\epsilon^2}\psi(\epsilon,x) - \left[\frac{\Gamma}{\hbar\omega}\right]^2\psi(\epsilon,x) - \frac{1}{\hbar^2\omega^3}\frac{1}{\beta^*}\frac{\partial}{\partial x}\psi(\epsilon,x) = e^{\Gamma\epsilon/\hbar\omega}F(\epsilon,x) \qquad \text{(B1)}$$

after the transformation

$$f(\epsilon,x) = e^{-\Gamma\epsilon/\hbar\omega}\psi(\epsilon,x) .$$

In terms of Green's functions Eq. (B1) can be written

$$\frac{\partial^2}{\partial\epsilon^2}G(\epsilon-\epsilon';x-x') - \left[\frac{\Gamma}{\hbar\omega}\right]^2 G(\epsilon-\epsilon';x-x') - \frac{1}{\beta^*\hbar^2\omega^3}\frac{\partial}{\partial x}G(\epsilon-\epsilon';x-x') = \delta(\epsilon-\epsilon')\delta(x-x') . \qquad \text{(B2)}$$

We can set $x'=0$ and $\epsilon'=0$; then the "initial" and boundary conditions are

$$G(\epsilon,x)=0 \quad \text{if } x<0 , \qquad \text{(B3a)}$$

and

$$G(\epsilon,x)=0 \quad \text{if } \epsilon<0 , \qquad \text{(B3b)}$$

respectively. By Fourier transforming in energy space we get

$$\delta(\epsilon) = \frac{1}{\pi}\int_0^\infty ds\,\cos(s\epsilon) , \qquad \text{(B4)}$$

$$G(\epsilon,x) = \frac{1}{\pi}\int_0^\infty ds\,\cos(s\epsilon)\widetilde{G}(s,x) . \qquad \text{(B5)}$$

Substituting the expressions in Eq. (B2), we find

$$-\left[s^2+\left[\frac{\Gamma}{\hbar\omega}\right]^2\right]\widetilde{G}(s,x) - \frac{1}{\beta^*\hbar^2\omega^3}\frac{\partial}{\partial x}\widetilde{G}(s,x) = \delta(x) \qquad \text{(B6)}$$

or

$$
\begin{aligned}
G(s,x) &= 0 \quad \text{if } x<0 \\
&= -\beta^*\hbar^2\omega^3\exp\{-[(sh\omega)^2+\Gamma^2]\beta^*\omega x\} \\
&\qquad \text{if } x>0 , \qquad \text{(B7)}
\end{aligned}
$$

which with Eq. (B5) yields the Green's function (36).

APPENDIX C

For the t-dependent solution the normalization constant of the energy distribution function given by the initial distribution is

$$A=\left[\int_0^\infty dk\,k^2\delta(\epsilon-\epsilon_0)\right]^{-1}=\frac{2}{\sqrt{\epsilon_0}}\left[\frac{\hbar^2}{2m}\right]^{2/3} \tag{C1}$$

with $k=\sqrt{2m\epsilon}/\hbar$. For the x-dependent solution the normalization constant of the distribution function is

$$\begin{aligned}A'&=\left[\int dk^3\delta(\epsilon-\epsilon_0)\delta(\cos\theta-1)\delta(\varphi)\right]^{-1}\\&=\frac{8}{\sqrt{\epsilon_0}}\left[\frac{\hbar^2}{2m}\right]^{3/2}\end{aligned} \tag{C2}$$

with

$$\int_0^\pi d\theta\,\sin\theta\,\delta(\cos\theta-1)=\int_0^{2\pi} d\varphi\,\delta(\varphi)=\tfrac{1}{2}\;, \tag{C3}$$

because only half of the δ function is included in the integration interval.

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