

¹See, e.g., F. Herman, R. L. Kortum, I. B. Ortenburger, and J. P. Van Dyke, *J. Phys. (Paris) Suppl.* **29**, 62 (1968).

²See, e.g., T. C. Collins, D. J. Stukel, and R. N. Euwema, *Phys. Rev. B* **1**, 724 (1970).

³See also, F. Herman, R. L. Kortum, C. D. Kuglin, and R. A. Short, *J. Phys. Soc. Japan Suppl.* **21**, 7 (1966).

⁴V. Heine, in *Solid State Physics*, Vol. 24, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1970), p. 1.

⁵M. L. Cohen and V. Heine, in Ref. 4, p. 38.

⁶See, e.g., W. Heitler, *The Quantum Theory of Radiation*, 3rd ed. (Oxford U. P., Oxford, 1954), Chap. III.

⁷H. A. Bethe and E. E. Salpeter, in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. XXXV, p. 136.

⁸A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1963), Vol. II, Chap. XX, Sec. V.

⁹E. O. Condon and G. H. Shortley, *The Theory Atomic*

Spectra (Cambridge U. P., Cambridge, 1935), p. 125ff.

¹⁰See Ref. 5, Eqs. (2.7) and (9.6).

¹¹G. Weisz, *Phys. Rev.* **149**, 504 (1966) [see Eq. (2.13) where U corresponds to W].

¹²P. J. Lin and L. Kleinman, *Phys. Rev.* **142**, 478 (1966) [see Eq. (5) where $V+V_R$ corresponds to W].

¹³Reference 12, Eq. (17). The extra factor α appearing in Eq. (17) of this reference has been introduced to account for the omission of the inner-core states in the summation over t .

¹⁴See Ref. 11, Eq. (3.11).

¹⁵J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960), Vol. 1, p. 369.

¹⁶S. Bloom and T. K. Bergstresser, *Solid State Commun.* **6**, 465 (1968).

¹⁷F. Herman and S. Skillman, *Atomic Energy Calculations* (Prentice-Hall, Englewood Cliffs, N. J., 1963), Chap. II. The values of $E_{1/2}^p - E_{3/2}^p$ for In and Sb were, respectively, obtained by averaging the values for Cd and Sn, and Sn and Te.

High-Field Distribution Functions of Carriers in Semiconductors

W. A. Wassef and K. C. Kao

Materials Research Laboratory,

Electrical Engineering Department, University of Manitoba, Winnipeg, Canada

(Received 10 November 1971)

On the basis of the principle of deriving the Fermi-Dirac distribution function, a general expression of the carrier distribution function taking into account the effect of applied electric field has been deduced. Theoretically, this general expression can be used to analyze any carrier transport phenomena in both nondegenerate and degenerate semiconductors with either parabolic or nonparabolic band structure. Using this general expression, the Boltzmann transport equation has been solved analytically for low and high temperatures. Some computed results are presented, and discussion and comparison with other available results are given.

I. INTRODUCTION

In the study of high-field transport phenomena the carrier distribution function f is one of the most important factors, which has to be determined first. f is governed by the applied fields, and the scattering of the carriers with the carriers and the phonons; and it is generally obtained by solving the Boltzmann transport equation with certain boundary conditions and some necessary assumptions. In the absence of external fields, f for nondegenerate semiconductors is usually assumed to be Maxwellian in thermal equilibrium. But in the presence of external fields the net carrier transport will disturb the equilibrium condition and hence f will be altered. At low fields the effect of all scatterings are usually treated by the relaxation-time approximation.¹ There are many shortcomings of the relaxation-time approximation and they have been discussed in detail by Law and Kao.² To avoid using the relaxation-time con-

cept, several investigators have used the variational method,^{3,4} iterative technique,⁵ Monte Carlo method,⁶⁻⁹ and self-consistent power series² to solve this problem. In this paper we present a new method for determining f as a function of applied electric field for fields of any strength. This method is based on the principle of deriving the Fermi-Dirac distribution function. With the general expression for f we have solved analytically the Boltzmann transport equation for low and high temperatures. We also present some computed results to show the field dependence of f , the effect of mixed scatterings, and the effect of temperature; and to compare our results with those calculated by other investigators.

II. GENERAL EXPRESSION OF DISTRIBUTION FUNCTION

With the flow of carriers in a semiconductor under the influence of applied fields, the carrier distribution function will depend on the applied field and temperature; and in the steady state it

will be formed under such a condition that the number of ways for arranging all carriers in all available energy states is a maximum.¹⁰ By taking into account the effect of applied electric field the carrier distribution function is derived as follows.

Suppose the energy states are divided into many compartments with N_1 electrons and G_1 states of energy E_1 in the first compartment, N_2 electrons and G_2 states of energy E_2 in the second compartment, N_i electrons and G_i states of energy E_i in the i th compartment, and so on. Then the number of ways for arranging the total N electrons in the total G states is given by

$$W = \prod_{i=1}^n \frac{G_i!}{N_i! (G_i - N_i)!} \quad (1)$$

The total number of electrons in the system is

$$N = \sum_{i=1}^n N_i, \quad (2)$$

and the total energy of the system is

$$E = \sum_{i=1}^n N_i E_i. \quad (3)$$

If there is a net carrier transport, an additional condition must be added, and it is

$$J = e \sum_{i=1}^n N_i V_{Fi}, \quad (4)$$

where J is the current density, e is the electronic charge, and V_{Fi} is the velocity of the carriers of the i th compartment in the direction of the applied electric field \vec{F} . In thermal equilibrium and in the absence of the applied electric field the conditions given in Eqs. (2) and (3) imply that the carriers in each compartment have the same energy and that all the compartments can be simply considered to be the constant energy surfaces in the momentum space. But in the presence of an external field these surfaces will be distorted, and for isotropic materials they will be symmetric around the direction of the field. In this case the carriers in each compartment may still have the same total energy, but their velocity components in the direction of the field would be different. For this reason we divide each compartment into many subcompartments in a way that in a given subcompartment, which is formed by the intersection of a cone with the constant energy surface within an angle θ from the direction of the field, the carriers have not only the same energy, but also the same velocity component in the direction of \vec{F} . Equation (3) is the necessary condition for a system to have a constant total energy, while Eq. (4) is the necessary condition for a system to have a steady current flow. Based on this argument the velocity component V_{Fi} in any subcompartment is thus given by

$$V_{Fi} = (\hbar k_i / m) \cos \theta, \quad (5)$$

where m is the effective mass, \hbar is Planck's constant divided by 2π , k_i is the magnitude of the wave vector \vec{k}_i , and θ is the angle between \vec{k}_i and \vec{F} , the latter being taken in the z direction only.

Using the method of Lagrange multipliers, the condition for the number of ways for arranging N electrons in G states to be a maximum is

$$\frac{d}{dN_i} [\ln W + \alpha (N - \sum_{i=1}^n N_i) + \beta (E - \sum_{i=1}^n N_i E_i) + \gamma (J - e \sum_{i=1}^n N_i V_{Fi})] = 0. \quad (6)$$

With the aid of Stirling's formula, the solution of Eq. (6) gives

$$\frac{N_i}{G_i} = \frac{1}{1 + \exp(\alpha + \beta E_i + \gamma e V_{Fi})}. \quad (7)$$

Hence the carrier distribution function is

$$f = \frac{1}{1 + \exp[\alpha + \beta E + (\gamma e \hbar k / m) \cos \theta]}. \quad (8)$$

This is a general expression for the carrier distribution function taking into account the effect of applied electric field. Thus γ must be field dependent and vanish when $\vec{F} = 0$. Since k is related to E through only the $E - k$ relationship for a given energy-band structure, Eq. (8) should be valid for both nondegenerate and degenerate semiconductors with either parabolic or nonparabolic band structure.

It is of interest to see how Eq. (8) can be reduced to the forms which have been used in the past. For nondegenerate semiconductors with a parabolic band structure, Eq. (8) can be approximated to

$$\begin{aligned} f &\approx \exp\left(-\alpha - \beta E - \frac{\gamma e \hbar k}{m} \cos \theta\right) \\ &\approx \exp\left[-\alpha + \frac{\gamma^2 e^2 \cos^2 \theta}{2\beta m} - \frac{\beta \hbar^2}{2m} \left(k + \frac{\gamma e \cos \theta}{\beta \hbar}\right)^2\right]. \end{aligned} \quad (9)$$

The first two terms in the exponential of Eq. (9) are independent of k . Equation (9) is generally referred to as the displaced Maxwellian distribution function¹¹ with the displacement vector given by

$$d = -\frac{\gamma e \cos \theta}{\beta \hbar}, \quad (10)$$

where $\beta = 1/k_B T$; k_B is the Boltzmann constant and T is the temperature of the electrons.

By rewriting Eq. (9) in the form

$$\begin{aligned} f &\approx e^{-\alpha - \beta E} e^{-(\gamma e \hbar k / m) \cos \theta} \\ &= f_0(E) e^{-(\gamma e \hbar k / m) \cos \theta} \\ &\approx f_0(E) [1 - (\gamma e \hbar k / m) \cos \theta] \\ &= f_0(E) + k_F g(E), \end{aligned} \quad (11)$$

with $f_0(E) = e^{-\alpha - \beta E}$, $k_F = k \cos \theta$, and $g = -f_0 \gamma e \hbar / m$. Equation (11) is the distribution function used by

Conwell and Vassell¹² for their study of transport phenomena, but they obtained this by expanding f in a series of Legendre polynomials and cutting off the series at $n=1$.

It is clear that both the displaced Maxwellian function and Eq. (11) are only approximations of Eq. (8), and they are definitely not accurate for high fields. In the following we shall determine the carrier distribution function based on the general expression given in Eq. (8) by solving the Boltzmann transport equation.

III. BOLTZMANN EQUATION AND SCATTERING MECHANISMS

The Boltzmann equation for a many-valley semiconductor is given by¹³

$$\frac{\partial f_i(\vec{k})}{\partial t} = \left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_F + \sum_j \left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_{ij}, \quad (12)$$

where i and j stand for the i th and the j th valley. The first term on the right-hand side is the rate of change of $f_i(\vec{k})$ due to the applied field, which is given by

$$\left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_F = -\frac{e}{\hbar} \vec{F} \cdot \nabla_{\vec{k}} f_i(\vec{k}). \quad (13)$$

The second term is the rate of change of $f_i(\vec{k})$ due to various scattering processes. To simplify the matter, we make the following assumptions: (a) The semiconductor is nondegenerate, so that the effect of carrier-carrier scattering can be ignored because the carrier concentration is so small that the carriers are mostly scattered by the lattice vibrations¹¹; (b) the energy-band structure is parabolic; and (c) \vec{F} is uniform across the sample. This means that the applied electric field is not high enough to cause space-charge effects such as the formation of domains. So we confine ourselves to scattering mechanisms due to phonons of different types denoted by s . Thus the second term on the right-hand side of Eq. (12) may be written in the form¹³

$$\begin{aligned} \left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_{ij} = & \int_j C_{ij}^{(s)}(\vec{k}, \vec{k}') \{ [N_s f_j(\vec{k}') - (N_s + 1) f_i(\vec{k})] \\ & \times \delta[E_i(\vec{k}) - E_j(\vec{k}') - \hbar\omega_s] - [N_s f_i(\vec{k}) - (N_s + 1) f_j(\vec{k}')] \\ & \times \delta[E_j(\vec{k}') - E_i(\vec{k}) - \hbar\omega_s] \} d\vec{k}'. \quad (14) \end{aligned}$$

The four terms in the integrand represent the transition from state \vec{k} in the i th valley to state \vec{k}' in the j th valley, and vice versa by emission and absorption of one phonon of type s with wave vector $\pm(\vec{k} - \vec{k}')$ and angular frequency ω_s . By assuming that the phonons remain in thermal equilibrium at the lattice temperature T_0 , the number of phonons of type s follows the Bose-Einstein statistics:

$$N_s = [\exp(\hbar\omega_s/k_B T_0) - 1]^{-1}. \quad (15)$$

The strength of the scattering is controlled by the function $C_{ij}^{(s)}$ which depends on the type of phonon and the magnitude $|\vec{k} - \vec{k}'|$. Therefore, $C_{ij}^{(s)}$ can be written in the form

$$C_{ij}^{(s)} = D_{ij}^{(s)} |\vec{k} - \vec{k}'|^r. \quad (16)$$

For different types of scatterings the (s) and r are changed as follows:

when $r = -2$, $(s) \rightarrow (o)$ for optical-mode scattering;

when $r = 1$, $(s) \rightarrow (a)$ for acoustic-mode scattering;

when $r = 0$, $(s) \rightarrow (ij)$ for intervalley scattering.

For mixed scattering, the parameter r would take a value between -2 and 1 , and the quantity $D_{ij}^{(s)}$ would be different from that for a single type of scattering.

The magnitude of the wave vector of the phonons may be written as

$$|\vec{k} - \vec{k}'| = (k^2 + k'^2 - 2kk'u)^{1/2}, \quad (17)$$

in which

$$u = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi - \phi'),$$

where k and k' are the magnitudes of wave vectors \vec{k} and \vec{k}' whose directions are θ and θ' from the z axis, and ϕ and ϕ' are the azimuthal angles about the z axis for k and k' . For mathematical simplicity, we divide the energy range of phonons into three regions as follows.

(i) *High-energy phonons.* For this case $\hbar\omega_s \gg k_B T_0$. Therefore, $N_s \ll 1$ and Eq. (14) reduces to

$$\left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_{ij}^{(s)} = \int_j C_{ij}^{(s)}(\vec{k}, \vec{k}') [f_j(\vec{k}') \delta_+ - f_i(\vec{k}) \delta_-] d\vec{k}', \quad (18)$$

with

$$\delta_+ = \delta[E_j(\vec{k}') - E_i(\vec{k}) - \hbar\omega_s]$$

and

$$\delta_- = \delta[E_i(\vec{k}) - E_j(\vec{k}') - \hbar\omega_s].$$

In this range of phonon energies, optical, polar-optical, and intervalley scatterings may play a role in the transport phenomena, and at very low temperatures the acoustic scattering may also become important. This case usually occurs at low temperatures.

(ii) *Low-energy phonons.* For this case $\hbar\omega_s \ll k_B T_0$. Therefore, $N_s \gg 1$ and Eq. (14) reduces to

$$\begin{aligned} \left(\frac{\partial f_i(\vec{k})}{\partial t} \right)_{ij}^{(s)} = & \int_j N_s C_{ij}^{(s)}(\vec{k}, \vec{k}') (\delta_+ + \delta_-) \\ & \times [f_j(\vec{k}') - f_i(\vec{k})] d\vec{k}', \quad (19) \end{aligned}$$

where

$$N_s \simeq k_B T_0 / \hbar \omega_s, \quad (20)$$

$$\omega_s \simeq |\vec{k} - \vec{k}'| v_s, \quad (21)$$

and v_s is the velocity of sound which may be considered to be constant for this case—the linear portion of the dispersion curve for phonons. This case usually occurs at high temperatures and the dominant scattering is of the acoustic type.

(iii) *Intermediate-energy phonons.* For this case $\hbar \omega_s \simeq k_B T_0$; no approximation can be made to simplify Eq. (14). This case is general and complicated, and will not be dealt in this paper.

We shall begin with case (i) for low temperature. Case (ii) for high temperature can be treated straightforwardly in the same way later.

$$\begin{aligned} \left(\frac{\partial f_i}{\partial t} \right)_{ij}^{(s)} = & - \sum_{n=0}^{\infty} \sum_{l=-n}^n \frac{4\pi}{2n+1} Y_n^{l*}(\theta, \phi) f_i(\vec{k}) \int_j a_n Y_n^l(\theta', \phi') \delta_+ k'^2 \sin \theta' d\theta' dk' d\phi' \\ & + \sum_{n=0}^{\infty} \sum_{l=-n}^n \frac{4\pi}{2n+1} Y_n^{l*}(\theta, \phi) \int_j a_n Y_n^l(\theta', \phi') f_j(\vec{k}') \delta_+ k'^2 \sin \theta' d\theta' dk' d\phi'. \end{aligned} \quad (24)$$

By denoting some integrals as follows:

$$W_n(k, k') = \int_{-1}^1 (k^2 + k'^2 - 2kk'u)^{r/2} P_n(u) du, \quad (25)$$

$$y_n^l = \int_0^{2\pi} \int_0^\pi \sin \theta' Y_n^l(\theta', \phi') d\theta' d\phi', \quad (26)$$

$$S_n(k)_{ij} = \int_j \delta_- W_n(k, k') k'^2 dk', \quad (27)$$

$$\begin{aligned} Z_n^l(k')_{ij} &= \int_0^{2\pi} \int_0^\pi \frac{\sin \theta' Y_n^l(\theta', \phi') d\theta' d\phi'}{1 + \exp[\alpha_j + \beta_j E_j + \gamma_j (e\hbar/m_j) k'_j \cos \theta']}, \end{aligned} \quad (28)$$

$$T_n^l(k)_{ij} = \int_j \delta_+ W_n(k, k') Z_n^l(k')_{ij} k'^2 dk', \quad (29)$$

it can be shown that the integrals $W_n(k, k')$ are appreciable only when $n=0$ and $n=1$ (see Appendix). Thus Eq. (24) takes the form

$$\begin{aligned} \left(\frac{\partial f_i}{\partial t} \right)_{ij}^{(s)} = & - 2\pi D_{ij}^{(s)} \left[f_i(\vec{k}) S_0(k)_{ij} - \frac{1}{(4\pi)^{1/2}} T_0^0(k)_{ij} \right. \\ & \left. - \left(\frac{3}{4\pi} \right)^{1/2} \cos \theta T_1^0(k)_{ij} \right]. \end{aligned} \quad (30)$$

The evaluation of the integrals defined in Eqs. (25)–(29) is given in the Appendix.

By substituting Eq. (8) into Eq. (13), we obtain

$$\begin{aligned} \left(\frac{\partial f_i}{\partial t} \right)_F = & \frac{e}{\hbar} F \left(\frac{\gamma_i e\hbar}{m_i} + \beta_i \hbar^2 \frac{k - K_i}{m_i} \cos \theta \right) \\ & \times [1 - f_i(\vec{k})] f_i(\vec{k}), \end{aligned} \quad (31)$$

and by substituting Eqs. (30) and (31) into Eq. (11) we obtain the general Boltzmann equation

A. High-Energy Phonons

The function $C_{ij}^{(s)}$ may be expanded in a series of Legendre polynomials $P_n(u)$ as

$$\begin{aligned} C_{ij}^{(s)} = & D_{ij}^{(s)} (k^2 + k'^2 - 2kk'u)^{r/2} \\ = & \sum_{n=0}^{\infty} a_n P_n(u). \end{aligned} \quad (22)$$

The coefficients a_n can be determined by the following relation:

$$a_n(k, k') = \frac{1}{2} (2n+1) D_{ij}^{(s)} \int_{-1}^1 (k^2 + k'^2 - 2kk'u)^{r/2} P_n(u) du. \quad (23)$$

Using the addition theorem of the spherical harmonics, Eq. (18) becomes

$$\begin{aligned} \frac{e}{\hbar} F \left(\frac{\gamma_i e\hbar}{m_i} + \beta_i \hbar^2 \frac{k - K_i}{m_i} \cos \theta \right) [1 - f_i(\vec{k})] f_i(\vec{k}) \\ - 2\pi \sum_j D_{ij}^{(s)} \left[f_i(\vec{k}) S_0(k)_{ij} - \frac{1}{(4\pi)^{1/2}} T_0^0(k)_{ij} \right. \\ \left. - \left(\frac{3}{4\pi} \right)^{1/2} \cos \theta T_1^0(k)_{ij} \right] = 0, \end{aligned} \quad (32)$$

where K_i is the reciprocal-lattice vector of the i th subband.

B. Low-Energy Phonons

Following the same procedure, we can obtain the general Boltzmann equation for low-energy phonons as follows:

$$\begin{aligned} \frac{e}{\hbar} F \left(\frac{\gamma_i e\hbar}{m_i} + \beta_i \hbar^2 \frac{k - K_i}{m_i} \cos \theta \right) [1 - f_i(\vec{k})] f_i(\vec{k}) \\ - 2\pi \sum_j D_{ij}^{(s)} \left[f_i(\vec{k}) S'_0(k)_{ij} - \frac{1}{(4\pi)^{1/2}} T'_0{}^0(k)_{ij} \right. \\ \left. - \left(\frac{3}{4\pi} \right)^{1/2} \cos \theta T'_1{}^0(k)_{ij} \right] = 0, \end{aligned} \quad (33)$$

where

$$D_{ij}^{(s)} = D_{ij}^{(s)} k_B T / \hbar v_s, \quad (34)$$

$$S'_n(k)_{ij} = \int_j (\delta_+ + \delta_-) W'_n(k, k') k'^2 dk', \quad (35)$$

$$W'_n(k, k') = \int_{-1}^1 [k^2 + k'^2 - 2kk'u]^{(r-1)/2} P_n(u) du, \quad (36)$$

$$T'_n{}^l(k)_{ij} = \int_j (\delta_+ + \delta_-) W'_n(k, k') Z_n^l(k')_{ij} k'^2 dk'. \quad (37)$$

IV. ANALYTICAL SOLUTION

For the case of high-energy phonons (or at low temperatures), it is clear that Eq. (32) with the integrals given in the Appendix has no simple solution. To obtain an analytical solution, we make the following assumptions:

$$(i) \quad f_i(\vec{k}) \ll 1; \quad (38)$$

this condition is well satisfied, since for nondegenerate semiconductors $\exp[\alpha + \beta E + (\gamma e \hbar k/m) \cos \theta] \gg 1$;

$$(ii) \quad |2\gamma_j e \hbar k_j^*/m_j| \ll 1, \quad (39)$$

where k_j^* is defined by Eq. (A16) in the Appendix. This condition is equivalent to

$$|\gamma_j| \ll 1/2eV_j^*.$$

Therefore,

$$|\gamma_j| \ll 1/2e\mu_j^*F, \quad (40)$$

where $V_j^* = \hbar k_j^*/m_j = \mu_j^*F$, and μ_j^* is the electron mobility in the j th subband. This condition can be applied for $|\gamma_j| = 0$ corresponding to $\vec{F} = 0$ up to high values of $|\gamma_j|$ for any desired values of \vec{F} .

From Eqs. (38) and (39) we obtain the following relation:

$$\begin{aligned} & \frac{\pi^{1/2} m_i}{e \hbar \gamma_j k_j^*} \ln \left[\exp\left(\frac{2e \hbar \gamma_j k_j^*}{m_j}\right) \frac{1 + \exp[\alpha_j + \beta_j(E + \hbar \omega_s) - (e \hbar/m_j) \gamma_j k_j^*]}{1 + \exp[\alpha_j + \beta_j(E + \hbar \omega_s) + (e \hbar/m_j) \gamma_j k_j^*]} \right] \\ &= \frac{\pi^{1/2} m_i}{e \hbar \gamma_j k_j^*} \ln \left\{ 1 + \left[\exp\left(\frac{2e \hbar \gamma_j k_j^*}{m_j}\right) - 1 \right] f_j(E + \hbar \omega_s) \right\} \approx 2\pi^{1/2} f_j(E + \hbar \omega_s). \end{aligned} \quad (41)$$

Using Eq. (41), the integrals $T_0^0(k)_{ij}$ and $T_1^0(k)_{ij}$ reduce to (see also the Appendix)

$$\begin{aligned} T_0^0(k)_{ij} \approx f_j(E + \hbar \omega_s) \pi^{1/2} \frac{(2m_i/\hbar^2) k_j^{*2}}{k_j^* - K_j} \left(\sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+1) (\frac{1}{2}+p)} \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p} \right. \\ \left. \times \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p} \right) \end{aligned} \quad (42)$$

and

$$\begin{aligned} T_1^0(k)_{ij} = f_j(E + \hbar \omega_s) \frac{(3\pi)^{1/2} (2m_j/\hbar^2) k_j^{*2}}{k_j^* - K_j} \cos \theta \left(\sum_{p=0}^{\infty} \frac{\Gamma(2p+1 - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+2) (\frac{3}{2}+p)} \right. \\ \left. \times \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p-1} \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p+1} \right). \end{aligned} \quad (43)$$

Thus Eq. (32) takes the form

$$L_i(E) f_i(E) = \sum_j H_{ij}(E) f_j(E + \hbar \omega_s), \quad (44)$$

where

$$L_i(E) = \frac{e}{\hbar} F \left(\frac{\gamma_i e \hbar}{m_i} + \beta_i \hbar^2 \frac{k - K_i}{m_i} \cos \theta \right) - 2\pi \sum_j D_{ij}^{(s)} S_0(k)_{ij}, \quad (45)$$

$$\begin{aligned} H_{ij}(E) = -\pi D_{ij}^{(s)} \frac{(2m_j/\hbar^2) k_j^{*2}}{k_j^* - K_j} \left(\sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+1) (\frac{1}{2}+p)} \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p} \right. \\ \left. \times \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p} \right) - 3\pi D_{ij}^{(s)} \frac{(2m_j/\hbar^2) k_j^{*2}}{k_j^* - K_j} \cos^2 \theta \left(\sum_{p=0}^{\infty} \frac{\Gamma(2p+1 - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+2) (\frac{3}{2}+p)} \right. \\ \left. \times \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p-1} \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p+1} \right), \end{aligned} \quad (46)$$

and

$$E - \Delta_i = \hbar^2(k - K_i)^2/2m_i, \quad (47)$$

where Δ_i is the minimum energy at the edge of the i th subband.

In this paper we shall treat the case with only two conduction subbands. The treatment for cases with more conduction subbands presents no formal problem, except that the amount of calculations will be enormously increased. By denoting the lower subband with the subscript 1 and the higher subband with the subscript 2, Eq. (44) becomes

$$L_1(E)f_1(E) = H_{11}(E)f_1(E + \hbar\omega_s) + H_{12}(E)f_2(E + \hbar\omega_s), \quad (48)$$

$$L_2(E)f_2(E) = H_{21}(E)f_1(E + \hbar\omega_s) + H_{22}(E)f_2(E + \hbar\omega_s).$$

Therefore we have

$$\begin{bmatrix} f_1(E + \hbar\omega_s) \\ f_2(E + \hbar\omega_s) \end{bmatrix} = \begin{bmatrix} J_{11}(E) & J_{12}(E) \\ J_{21}(E) & J_{22}(E) \end{bmatrix} \begin{bmatrix} L_1(E)f_1(E) \\ L_2(E)f_2(E) \end{bmatrix}, \quad (49)$$

where

$$[J_{ij}] = [H_{ij}]^{-1}. \quad (50)$$

Thus the carrier distribution function for the first subband is

$$f_1(E + \hbar\omega_s) = J_{11}(E)L_1(E)f_1(E) + J_{12}(E)L_2(E)f_2(E). \quad (51)$$

This difference equation is simply a mathematical expression of the physical process that the change of the electron energy E by $\pm\hbar\omega_s$ through the absorption or emission of a phonon of energy $\hbar\omega_s$ causes a corresponding change of the values of the carrier distribution function. This is of course a natural consequence. In the above mathematical treatment we use the energy rather than the wave vector in the argument of f because it is convenient to express the change of the electron energy by a discrete interval $\pm\hbar\omega_s$. Furthermore, f in Eq. (8) with the energy in the argument enables an easy solution of Eq. (14) and an easy calculation of the quantities $T_0^0(k)_{ij}$ and $T_1^0(k)_{ij}$ given by Eqs. (42) and (43), which lead to the conversion of the Boltzmann equation into the difference equations.

If we confine ourselves to the electron energy $\Delta_1 < E < \Delta_2$, then $f_2(E) = 0$. This implies that the distribution function diminishes at $E = \Delta_2$. For this case Eq. (51) becomes

$$f_1(E + \hbar\omega_s) = J_{11}(E)L_1(E)f_1(E). \quad (52)$$

By denoting

$$x = E/\hbar\omega_s, \quad (53)$$

Eq. (52) becomes

$$f_1(x+1) = J_{11}(x)L_1(x)f_1(x). \quad (54)$$

This is a difference equation, which has the following solution:

$$f_1(x) = A \exp\{(1/\square)\ln[J_{11}(x)L_1(x)]\}, \quad (55)$$

where \square is the difference operator. Thus by combining Eqs. (8) and (55) we obtain

$$\begin{aligned} \ln A + (1/\square)[J_{11}(x)L_1(x)] &= -\alpha_1 - \beta_1\hbar\omega_s x \\ &- \frac{\gamma_1 e\hbar}{m_1} \cos\theta \left[\left(\frac{2m_1\hbar\omega_s}{\hbar^2} \right)^{1/2} \left(x - \frac{\Delta_1}{\hbar\omega_s} \right)^{1/2} + K_1 \right], \end{aligned} \quad (56)$$

which gives

$$\begin{aligned} (x - \Delta_1/\hbar\omega_s) \ln[J_{11}(x)L_1(x)] \\ = -\beta_1 E - \frac{1}{2} \frac{\gamma_1 e\hbar k}{m_1} \cos\theta + \beta_1 \Delta_1 + \frac{1}{2} \frac{\gamma_1 e\hbar k_1}{m_1} \cos\theta. \end{aligned} \quad (57)$$

If we choose the coordinates of the $E - k$ relationship such that $\Delta_1 = 0$ and $K_1 = 0$, we obtain finally

$$\exp\left(-\beta_1 E - \frac{1}{2}\gamma_1 \frac{e\hbar k}{m_1} \cos\theta\right) = [J_{11}(E)L_1(E)]^{E/\hbar\omega_s}. \quad (58)$$

Since $f_1(E) \simeq \exp[-\alpha_1 - \beta_1 E - (\gamma_1 e\hbar k/m_1)\cos\theta]$, the carrier distribution function can be written as

$$f_1(E) = e^{-\alpha_1} [J_{11}(E)L_1(E)]^{nE/\hbar\omega_s}, \quad (59)$$

where n is a factor taking a value between 1 and 2 depending on whether $\beta_1 E$ is larger or smaller than $(\gamma_1 e\hbar k/m_1)\cos\theta$. At low temperatures n is expected to be approximately equal to 1.

By applying the same argument in determining $L_1(E)$, we obtain the following relation for small values of θ :

$$\begin{aligned} e^{\alpha_1} f_1(E) - \left[\frac{H_{22}}{H_{11}H_{22} - H_{12}H_{21}} \left(-\frac{2eF}{\hbar} \frac{\ln[e^{\alpha_1} f_1(E)]}{(2m_1 E/\hbar^2)^{1/2} \cos\theta} \right. \right. \\ \left. \left. - 2\pi \sum_j D_{1j}^{(s)} S_0(E)_{1j} \right) \right]^{nE/\hbar\omega_s} = 0. \end{aligned} \quad (60)$$

For large values of θ , Eq. (8) reduces to the Fermi-Dirac distribution function.

For the case of low-energy phonons (or at high temperatures) Eq. (48) becomes

$$\begin{aligned} L_1'(E)f_1(E) &= H_{11}(E)f_1(E + \hbar\omega_s) + H_{12}(E)f_2(E + \hbar\omega_s) \\ &+ H_{11}'(E)f_1(E - \hbar\omega_s) + H_{12}'(E)f_2(E - \hbar\omega_s), \\ L_2'(E)f_2(E) &= H_{21}(E)f_1(E + \hbar\omega_s) + H_{22}(E)f_2(E + \hbar\omega_s) \\ &+ H_{21}'(E)f_1(E - \hbar\omega_s) + H_{22}'(E)f_2(E - \hbar\omega_s), \end{aligned} \quad (61)$$

where

$$L_i'(E) = \frac{eF}{\hbar} \left(\frac{\gamma_i e\hbar}{m_i} + \beta_i \hbar^2 \frac{k - K_i}{m_i} \cos\theta \right) - 2\pi \sum_j D_{ij}^{(s)} S_0'(k)_{ij}, \quad (62)$$

and $H_{ij}'(E)$ can be obtained from Eq. (46) by replacing r with $r - 1$, and k_j^+ with k_j^- , which is given

by

$$k_j^* = (2m_j/\hbar^2)^{1/2} (E - \hbar\omega_s - \Delta_j)^{1/2} + K_j. \quad (63)$$

In the energy range $\Delta_1 < E < \Delta_2$ we can set $f_2(E) = 0$ and $f_2(E - \hbar\omega_s) = 0$. Thus Eq. (62) reduces to

$$L_1'(E)f_1(E) = \left(H_{11}(E) - \frac{H_{12}(E)H_{21}(E)}{H_{22}(E)} \right) f_1(E + \hbar\omega_s) \\ + \left(H_{11}'(E) - \frac{H_{12}(E)H_{21}'(E)}{H_{22}(E)} \right) f_1(E - \hbar\omega_s). \quad (64)$$

If $f_1(E/\hbar\omega_s)$ is assumed to be in the form

$$f_1(E/\hbar\omega_s) = e^{\lambda E/\hbar\omega_s}, \quad (65)$$

it can be shown that the solution of Eq. (64) is given by

$$f_1(E) - \left\{ L_1(E) \pm \left[L_1'^2(E) - 4 \left(H_{11}(E) - \frac{H_{12}(E)H_{21}(E)}{H_{22}(E)} \right) \right. \right. \\ \left. \left. \times \left(H_{11}'(E) - \frac{H_{12}(E)H_{21}'(E)}{H_{22}(E)} \right) \right]^{1/2} \right\} e^{\lambda E/\hbar\omega_s} \\ \times \left[2 \left(H_{11}(E) - \frac{H_{12}(E)H_{21}(E)}{H_{22}(E)} \right) \right]^{-1} = 0. \quad (66)$$

V. COMPUTED RESULTS AND DISCUSSION

By solving Eq. (60) for $e^{\alpha_1} f_1(E)$, we obtain

$$e^{\alpha_1} f_1(E) = f'(E) + C, \quad (67)$$

where C is a constant which depends on the applied field and can be determined by employing the following boundary condition:

$$f_1(E) \rightarrow 0 \text{ as } E \rightarrow \infty. \quad (68)$$

In this section we shall confine ourselves to the case for high-energy phonons (i. e., $\hbar\omega_s > k_B T$), since it is of direct interest to the study of electron transfer between conduction subbands in multi-valley semiconductors.

To show the possible carrier distribution functions under various conditions based on the analysis given in Secs. II-IV, we choose n -type GaAs as an example. In this semiconductor the bottom of the first valley in the conduction band is located at (000) in k space with the electron effective mass $m_1 = 0.067m_0$, and that of the second valley at (100) with $m_2 = 0.35m_0$, where m_0 is the rest mass of the electron, the energy separation between these two valleys $\Delta_2 - \Delta_1$ being 0.36 eV. By assuming the band structure of the semiconductor to be parabolic for simplicity, $f'(E)$ has been computed under various conditions, and the results are presented and discussed as follows.

The values of $D_{ij}^{(0)}$ and $D_{ij}^{(ij)}$ for n -GaAs are given¹³ by

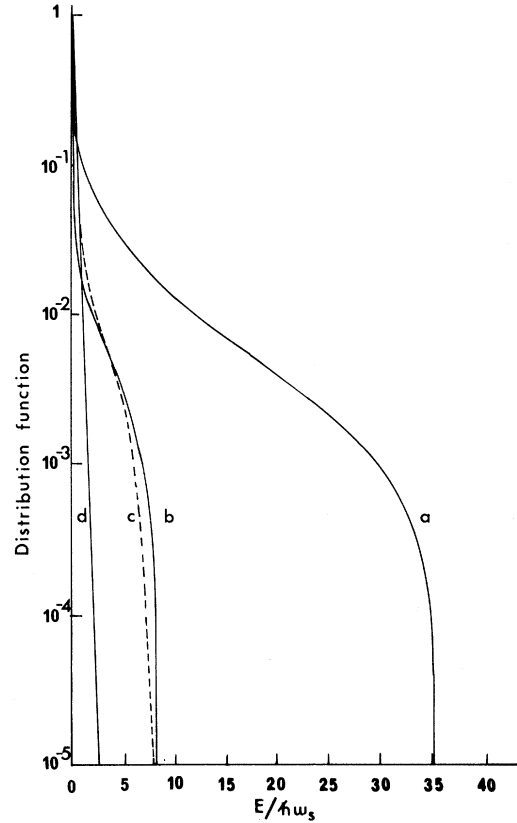


FIG. 1. Distribution function of electrons in the (000) valley in n -GaAs for $C_{ij} = 2 \times 10^{-18} |\vec{k} - \vec{k}'|^{-2}$ and $\theta = 0^\circ$. (a) $F = 2$ kV/cm, $n = 1$; (b) $F = 1$ kV/cm, $n = 1$; (c) $F = 1$ kV/cm, $n = 1.02$; (d) Maxwellian distribution at $F = 0$ and $T = 30^\circ\text{K}$ for comparison purposes.

$$D_{ij}^{(0)} = \frac{e^2 \omega_0}{2\pi} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \approx 10^{-15} \text{ mks units}$$

and

$$D_{ij}^{(ij)} = \frac{\bar{D}_{ij}^2}{8\pi^2 \rho \omega_{ij}} \approx 10^{-22} \text{ mks units},$$

where ω_0 is the angular frequency of optical phonons; ϵ_∞ and ϵ_0 are, respectively, the dielectric constants at zero and infinite frequencies; \bar{D}_{ij} is the deformation potential field for the ij phonons,¹⁴ which is taken to be 5×10^8 eV cm⁻¹; ρ is the density of the semiconductor; and ω_{ij} is the phonon frequency at $K_i - K_j$. We choose the value of the order of 10^{-18} mks units for D_{ij} in order to examine the effect of mixed optical and intervalley scatterings. A decrease of D_{ij} corresponds to an increase in weight of the intervalley scattering, and in turn corresponds to an increase of electron transfer from the lower to the upper valley and consequently leads to current instabilities.

Figure 1 shows the carrier distribution function as a function of $E/\hbar\omega_s$ for the applied electric fields

of 1 and 2 kV/cm. The case for $n=1$ corresponds to that for $T=0^\circ\text{K}$, and the case for $n=1.02$ corresponds to that for $T=30^\circ\text{K}$ and the phonon energy $\hbar\omega_s=0.01$ eV. The tail of curve (c) is clearly parallel to the Maxwellian distribution curve (d) for the same temperature and phonon energy. By comparing curve (a) with curves (b) and (d) it is clear that the higher the applied electric field, the more electrons have higher energies.

Figure 2 shows that if the value $C_{ij}=2\times 10^{-18} \times |\vec{k}-\vec{k}'|^{-2}$ is replaced with $C_{ij}=1\times 10^{-18} |\vec{k}-\vec{k}'|^{-2}$, the distribution decreases with increasing applied field throughout the whole energy range. This trend is just opposite to that shown in Fig. 1, indicating that there is a critical value of D_{ij} , below which the distribution function reverses its trend of response to the applied field.

Figure 3 shows the effect of the parameter r . By changing r from -2 to -1.98 so that the scattering is a mixed scattering, and comparing the results with those in Fig. 2, it can be seen that the distribution increases with decreasing value of r , particularly in the low-energy region. This indicates the importance of the mixture of several dif-

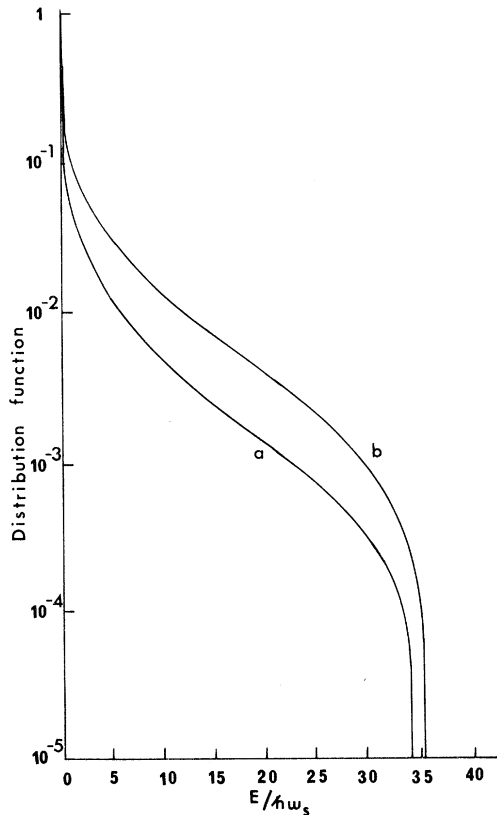


FIG. 2. Distribution function of electrons in the (000) valley in n -GaAs for $C_{ij}=1\times 10^{-18} |\vec{k}-\vec{k}'|^{-2}$ and $\theta=0^\circ$. (a) $F=2$ kV/cm, $n=1$; (b) $F=1$ kV/cm, $n=1$.

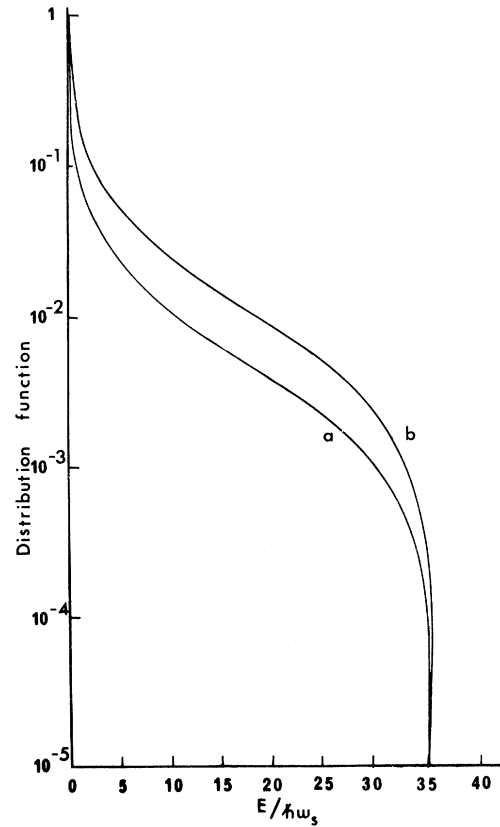


FIG. 3. Distribution function of electrons in the (000) valley in n -GaAs for $C_{ij}=1\times 10^{-18} |\vec{k}-\vec{k}'|^{-1.98}$ and $\theta=0^\circ$. (a) $F=2$ kV/cm, $n=1$; (b) $F=1$ kV/cm, $n=1$.

ferent types of scatterings.

Figure 4 shows the effect of the angle θ . It is clear that the distribution function is not sensitive to a small variation of θ . But for large θ , the distribution function will greatly decrease, and for $\theta=\pi/2$, the distribution function becomes Maxwellian.

Figure 5 gives the comparison between our result and that of Vassell and Conwell¹⁴ for $F=2.4$ kV/cm. In order to use the mixed scattering approximately similar to that used by Vassell and Conwell, we use $C_{ij}=2\times 10^{-18} |\vec{k}-\vec{k}'|^{-2}$, $\theta=0^\circ$, and $n=1.05$, which corresponds to $T=293^\circ\text{K}$. Our result deviates from the Maxwellian in the high-energy region much more than that of Vassell and Conwell. Based on Fig. 5 at the field of 2.4 kV/cm, an appreciable portion of electrons have energies extending to the bottom of the upper subband.

ACKNOWLEDGMENT

The authors wish to thank the National Research Council of Canada for the research support under Grant No. A-3339.

APPENDIX: EVALUATION OF INTEGRALS DEFINED IN EQS. (25)-(29)

(a) The integral $W_n(k, k')$ can be put in the form

$$W_n(k, k') = (k^2 + k'^2)^{r/2} \int_{-1}^1 \left[1 - \left(\frac{2kk'}{k^2 + k'^2} \right) u \right]^{r/2} P_n(u) du. \quad (\text{A1})$$

Since $[2kk'/(k^2 + k'^2)]u$ is always less than unity, we can write

$$\begin{aligned} \left[1 - \left(\frac{2kk'}{k^2 + k'^2} \right) u \right]^{r/2} &= 1 - \frac{1}{2} r \left(\frac{2kk'}{k^2 + k'^2} \right) u + \frac{\frac{1}{2} r (\frac{1}{2} r - 1)}{2!} \left(\frac{2kk'}{k^2 + k'^2} \right)^2 u^2 - \frac{\frac{1}{2} r (\frac{1}{2} r - 1) (\frac{1}{2} r - 2)}{3!} \left(\frac{2kk'}{k^2 + k'^2} \right)^3 u^3 + \dots \\ &= \sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 1)} \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p} u^{2p} + \sum_{p=0}^{\infty} \frac{\Gamma(2p + 1 - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 2)} \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p+1} u^{2p+1}. \end{aligned} \quad (\text{A2})$$

Legendre function $P_n(u)$ is an even or odd function according to whether n is even or odd integer, respectively. Therefore, the integration in Eq. (A1) will be twice the integration from 0 to 1 if we take the first summation on the right-hand side of Eq. (A2) with $P_{n \text{ even}}$ and the second summation on the right-hand side of Eq. (A2) with $P_{n \text{ odd}}$ such that the integrand in Eq. (A1) is always an even function; otherwise the integration will vanish.

Therefore, if q is a positive integer, we get

$$W_{2q}(k, k') = (k^2 + k'^2)^{r/2} \sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 1)} \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p} \frac{(-1)^q \Gamma(q - p) \Gamma(\frac{1}{2} + p)}{\Gamma(-p) \Gamma(q + \frac{3}{2} + p)}, \quad (\text{A3})$$

$$W_{2q+1}(k, k') = (k^2 + k'^2)^{r/2} \sum_{p=0}^{\infty} \frac{\Gamma(2p + 1 - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 2)} \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p+1} \frac{(-1)^q \Gamma(q - p) \Gamma(\frac{3}{2} + p)}{\Gamma(q + \frac{5}{2} + p) \Gamma(-p)}. \quad (\text{A4})$$

As a special case we examine the behavior of the integrals W_n for polar-optical scattering^{15,16} for which $r = -2$:

$$\begin{aligned} W_n(k, k') &= \frac{1}{2kk'} \sum_{m=0}^{\infty} (2m + 1) Q_m \left(\frac{k^2 + k'^2}{2kk'} \right) \\ &\quad \times \int_{-1}^1 P_m(u) P_n(u) du \\ &= \frac{1}{kk'} Q_n \left(\frac{k^2 + k'^2}{2kk'} \right), \end{aligned} \quad (\text{A5})$$

where Q_n are Legendre functions of the second kind. From the characteristics of $Q_n((k^2 + k'^2)/2kk')$ for $(k^2 + k'^2)/2kk' > 1$ it can be shown¹⁷ that we need consider only W_0 and W_1 , since the value of W_n decreases rapidly for n greater than 1. In general cases in which r is arbitrary, the integrals W_{2q} and W_{2q+1} given in Eqs. (A3) and (A4) have the same features as the aforementioned case, and therefore we consider only W_0 and W_1 . These are given by

$$\begin{aligned} W_0(k, k') &= (k^2 + k'^2)^{r/2} \sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 1) (\frac{1}{2} + p)} \\ &\quad \times \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p} \end{aligned} \quad (\text{A6})$$

and

$$\begin{aligned} W_1(k, k') &= (k^2 + k'^2)^{r/2} \sum_{p=0}^{\infty} \frac{\Gamma(2p + 1 - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 2) (\frac{3}{2} + p)} \\ &\quad \times \left(\frac{2kk'}{k^2 + k'^2} \right)^{2p+1}. \end{aligned} \quad (\text{A7})$$

This shows that the summation over n for the scattering term in Eq. (24) will contain only the first two terms: $n=0$ ($l=0$) and $n=1$ ($l=-1, 0, 1$). Therefore, in the following integrals we shall consider these two values of n only.

(b) The integrals y_n^l can be readily obtained if only the values 0 and 1 for n are considered. The results are

$$y_0^0 = 2\pi^{1/2}, \quad (\text{A8})$$

$$y_1^{-1} = 0, \quad (\text{A9})$$

$$y_1^0 = 0, \quad (\text{A10})$$

$$y_1^1 = 0. \quad (\text{A11})$$

(c) Since the integrals y_n^l are multiplied by $S_n(k)_{ij}$ in Eq. (24) and from the results given by Eqs. (A8)-(A11), we conclude that it is necessary only to calculate $S_0(k)_{ij}$. The result is given by

$$S_0(k)_{ij} = \frac{1}{2} \frac{(2m_j/\hbar^2)^{1/2}}{(E - \hbar\omega_s - \Delta_j)^{1/2}} \left[\left(\frac{2m_j}{\hbar^2} \right)^{1/2} (E - \hbar\omega_s - \Delta_j)^{1/2} + K_j \right]^2 \sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2} r)}{\Gamma(-\frac{1}{2} r) \Gamma(2p + 1) (\frac{1}{2} + p)}$$

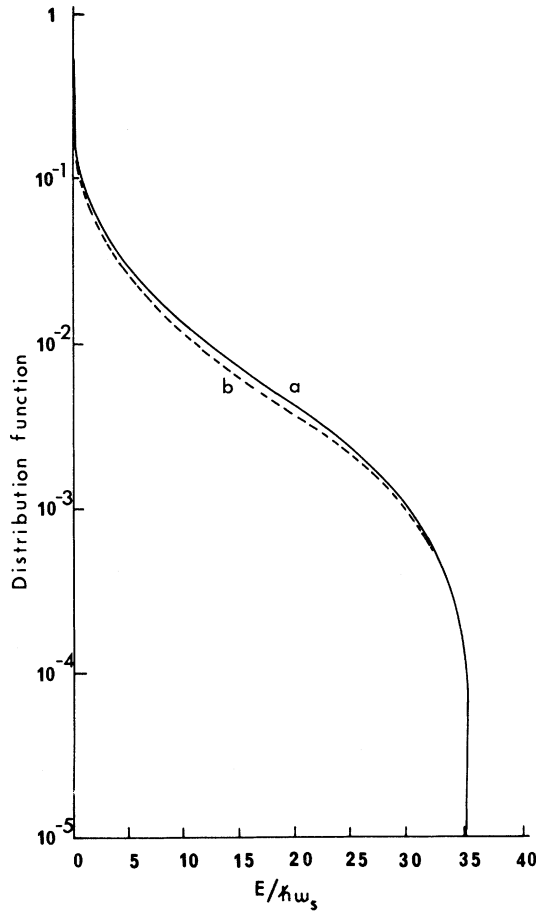


FIG. 4. Distribution function of electrons in the (000) valley in n -GaAs for $C_{ij} = 1 \times 10^{-18} |\vec{k} - \vec{k}'|^{-2}$, $F = 1$ kV/cm, and $n = 1$. (a) $\theta = 0^\circ$; (b) $\theta = 10^\circ$.

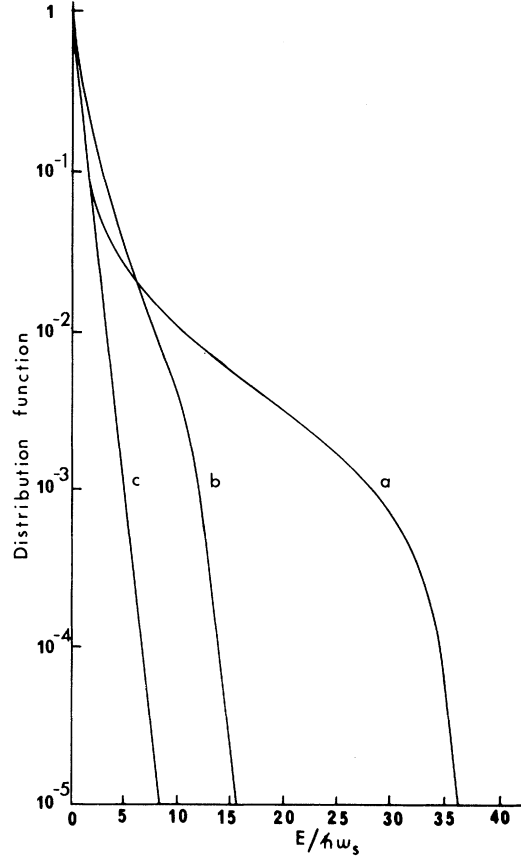


FIG. 5. Distribution function of electrons in the (000) valley in n -GaAs for $C_{ij} = 2 \times 10^{-18} |\vec{k} - \vec{k}'|^{-2}$, $F = 2.4$ kV/cm, $n = 1.05$, and $\theta = 0^\circ$. (a) Wassef and Kao; (b) Vassell and Conwell (Ref. 14); (c) Maxwellian distribution at $F = 0$ and $T = 293^\circ \text{K}$ corresponding to $n = 1.05$ for comparison purposes.

$$\times \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + \left[\left(\frac{2m_j}{\hbar^2} \right)^{1/2} (E - \hbar\omega_s - \Delta_j)^{1/2} + K_j \right]^2 \right\}^{r/2-2p} \\ \times \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] \left[\left(\frac{2m_j}{\hbar^2} \right)^{1/2} (E - \hbar\omega_s - \Delta_j)^{1/2} + K_j \right] \right\}^{2p}. \quad (\text{A12})$$

(d) The integral $Z_n^l(k')_{ij}$ for $n = 0$ and $l = 0$ is

$$Z_0^0(k')_{ij} = \frac{\pi^{1/2} m_j}{e \hbar \gamma_j k'} \ln \left(e^{2e \hbar \gamma_j k' / m_j} \frac{1 + \exp(\alpha_j + \beta_j E' - e \hbar \gamma_j k' / m_j)}{1 + \exp(\alpha_j + \beta_j E' + e \hbar \gamma_j k' / m_j)} \right). \quad (\text{A13})$$

The integrals $Z_1^{+1}(k')_{ij}$ will vanish owing to the integration over the angle ϕ' . The remainder integration of this group is

$$Z_1^0(k')_{ij} = (3\pi)^{1/2} \left(\frac{m_j}{e \hbar \gamma_j k'} \right)^2 \left\{ 2(\alpha_j + \beta_j E') \left(\frac{e \hbar \gamma_j k'}{m_j} \right) - \left[\sum_{t=0}^{\infty} \frac{2(-1)^t}{t^2 t!} e^{-t(\alpha_j + \beta_j E')} \left([1 + t(\alpha_j + \beta_j E')] \sinh \frac{te \hbar \gamma_j k'}{m_j} \right. \right. \right. \\ \left. \left. \left. - \frac{te \hbar \gamma_j k'}{m_j} \cosh \frac{te \hbar \gamma_j k'}{m_j} \right) \right] - (\alpha_j + \beta_j E') \ln \left(e^{2e \hbar \gamma_j k' / m_j} \frac{1 + \exp(\alpha_j + \beta_j E' - e \hbar \gamma_j k' / m_j)}{1 + \exp(\alpha_j + \beta_j E' + e \hbar \gamma_j k' / m_j)} \right) \right\}. \quad (\text{A14})$$

(e) The integral $T_n^l(k)_{ij}$ for $n = 0$ and $l = 0$ is

$$T_0^0(k)_{ij} = \frac{1}{2} \frac{2m_j / \hbar^2}{k_j^* - K_j} k_j^{*2} \frac{\pi^{1/2} m_j}{e \hbar \gamma_j k_j^*} \ln \left(e^{2e \hbar \gamma_j k_j^* / m_j} \frac{1 + \exp[\alpha_j + \beta_j (E + \hbar\omega_s) - e \hbar \gamma_j k_j^* / m_j]}{1 + \exp[\alpha_j + \beta_j (E + \hbar\omega_s) + e \hbar \gamma_j k_j^* / m_j]} \right)$$

$$\times \sum_{p=0}^{\infty} \frac{\Gamma(2p - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+1) (\frac{1}{2}+p)} \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p} \\ \times \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p}, \quad (\text{A15})$$

where

$$k_j^* = (2m_j/\hbar^2)^{1/2} (E + \hbar\omega_s - \Delta_j)^{1/2} + K_j \quad (\text{A16})$$

The integrals $T_1^{*1}(k)_{ij}$ will vanish since $Z_1^{*1}(k')_{ij} = 0$. Therefore, the last integral in this group is given by

$$T_1^0(k)_{ij} = \frac{1}{2} \frac{(2m_j/\hbar^2) k_j^{*2}}{k_j^* - K_j} \left(\sum_{p=0}^{\infty} \frac{\Gamma(2p+1 - \frac{1}{2}r)}{\Gamma(-\frac{1}{2}r) \Gamma(2p+2) (\frac{3}{2}+p)} \left\{ \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right]^2 + k_j^{*2} \right\}^{r/2-2p-1} \right. \\ \times \left. \left\{ 2 \left[\left(\frac{2m_i}{\hbar^2} \right)^{1/2} (E - \Delta_i)^{1/2} + K_i \right] k_j^* \right\}^{2p+1} \right) (3\pi)^{1/2} \left(\frac{m_j}{e\hbar\gamma_j k_j^*} \right)^2 \left\{ 2 [\alpha_j + \beta_j(E + \hbar\omega_s)] \frac{e\hbar\gamma_j k_j^*}{m_j} \right. \\ \left. - \left[\sum_{t=0}^{\infty} \frac{2(-1)^t}{t^2 t!} e^{-t[\alpha_j + \beta_j(E + \hbar\omega_s)]} \left(\{1 + t[\alpha_j + \beta_j(E + \hbar\omega_s)]\} \sinh \frac{te\hbar\gamma_j k_j^*}{m_j} - \frac{te\hbar\gamma_j k_j^*}{m_j} \cosh \frac{te\hbar\gamma_j k_j^*}{m_j} \right) \right] \right. \\ \left. - [\alpha_j + \beta_j(E + \hbar\omega_s)] \ln \left(e^{2e\hbar\gamma_j k_j^*/m_j} \frac{1 + \exp[\alpha_j + \beta_j(E + \hbar\omega_s) - e\hbar\gamma_j k_j^*/m_j]}{1 + \exp[\alpha_j + \beta_j(E + \hbar\omega_s) + e\hbar\gamma_j k_j^*/m_j]} \right) \right\}. \quad (\text{A17})$$

¹E. M. Conwell, in *Solid State Physics*, edited by F. Seitz and Turnbull (Academic, New York, 1967), Suppl. 9.

²H. C. Law and K. C. Kao, *Phys. Rev. B* **4**, 2524 (1971).

³D. J. Howarth and E. H. Sandheimer, *Proc. Roy. Soc. (London)* **A219**, 53 (1953).

⁴H. Ehrenreich, *J. Phys. Chem. Solids* **9**, 129 (1959).

⁵D. L. Rode, *Phys. Rev. B* **2**, 1012 (1970).

⁶K. Kurosawa, *J. Phys. Soc. Japan Suppl.* **21**, 424 (1966).

⁷P. J. Price (private communication).

⁸H. D. Rees, *J. Phys. Chem. Solids* **30**, 643 (1969).

⁹W. Fawcett, A. D. Boardman, and S. Swain, *J. Phys. Chem. Solids* **31**, 1963 (1970).

¹⁰K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

¹¹H. Frohlich and B. V. Paranjape, *Proc. Phys. Soc. (London)* **69B**, 21 (1956).

¹²E. M. Conwell and M. O. Vassell, *Trans. IEEE* **ED13**, 22 (1966).

¹³P. N. Butcher, *Rept. Progr. Phys.* **30**, 97 (1967).

¹⁴M. O. Vassell and E. M. Conwell, *Phys. Letters* **21**, 612 (1966).

¹⁵P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. I.

¹⁶E. M. Conwell and M. O. Vassell, *Phys. Rev.* **166**, 797 (1968).

¹⁷*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).