Hot-Carrier Distribution Function in Degenerate Nonparabolic Semiconductors

M. S. Sodha, U. P. Phadke, and A. K. Chakravarti
Department of Physics, Indian Institute of Technology, New Delhi-29, India
(Received 19 October 1970)

An expression for the energy distribution function of hot carriers in III-V compounds (viz., InSb, InAs, etc.) in the presence of arbitrary dc electric and magnetic fields has been derived for degenerate transport carriers, taking into account the more accurate forms of wave functions and nonparabolicity. The screened polar optical mode of the carrier-lattice interaction has been taken as the dominant scattering mechanism; this is justified for high electric fields and/or for lattice temperatures where the relaxation-time approximation is valid.

There are two approaches to the investigation of hot-carrier transport phenomena in nonparabolic polar semiconductors[1,2] which at high temperatures, since the carrier concentration in doped samples is large, should incorporate Pauli's exclusion principle and hence degeneracy. The effective-temperature model (ETM) suffers from the weakness of its basic assumption that the isotropic part of the distribution function remains unchanged in its form by the application of an electric field[1]; further, the effects of nonparabolicity are brought out only after a great deal of computational work. The second approach, i.e., the Boltzmann-equation solution (BES) has been used by Sodha and Gupta[3] to calculate the distribution function for a degenerate sample using an approximate form of nonparabolicity and carrier wave function. The more rigorous treatment of hot carriers in these semiconductors necessitates the appropriate energy-band shapes in various samples under investigation and more accurate wave functions[4] than plane waves. Matz[5,6] has given an elegant treatment for a few III-V compounds but has overlooked the degeneracy of carriers at high temperatures.

Since it is well established that the BES gives better agreement with the experimental results than the ETM approach,[1] in this paper, we have derived an expression for the energy distribution function of hot carriers in III-V compounds (viz., InSb, InAs, etc.) in the presence of a dc field arbitrarily oriented with respect to a magnetic field. More rigorous forms of wave functions and nonparabolicity of the conduction band and the degeneracy of transport carriers have been incorporated in the treatment. The polar optical mode of the carrier-lattice interaction has been taken as the dominant scattering mechanism at electric fields and/or lattice temperatures high enough to justify the relaxation-time approximation.[5] At these electronic temperatures, because of the strong interaction between electrons and optical phonons, other interactions (viz., acoustic, carrier-carrier scatterings, etc.) may be neglected in explaining the observed behavior adequately in these semiconductors. To make a consistent interpretation of the samples with different carrier concentrations, screening of the electron optical-phonon interaction has been included in this analysis.

It is convenient to define an arbitrary function of energy $\gamma(\mathcal{E})$ in terms of the carrier Bloch vector $\vec{k}$ as

$$\gamma(\mathcal{E}) = \frac{\hbar^2 k^2}{2m_n} , \tag{1}$$

where m_n is the carrier effective mass at the band edge. For a few specific III-V compounds (viz., InSb, InAs, etc.) $\gamma(\mathcal{E})$, following Kane's model, can be written as[6]

$$\gamma(\mathcal{E}) = \frac{\mathcal{E}(\mathcal{E}+\mathcal{E}_g)(\mathcal{E}+\mathcal{E}_g+\Delta)(\mathcal{E}_g+\frac{2}{3}\Delta)}{\mathcal{E}_g(\mathcal{E}_g+\Delta)(\mathcal{E}+\mathcal{E}_g+\frac{2}{3}\Delta)} , \tag{2}$$

where $\mathcal{E}_g$ is the band gap and Δ is the spin-orbit splitting of the valence band.

The time-independent Boltzmann equation can be written in the tensorial notation, as

$$-\frac{e}{\hbar} E_i \frac{\partial f}{\partial k_i} + \epsilon_{ijk}\Omega_j k_k \frac{\partial f}{\partial k_i} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} , \tag{3a}$$

where

$$\Omega_j = eH_j/m^* c . \tag{3b}$$

The momentum effective mass m^* is related to $\gamma(\mathcal{E})$ by the relation

$$m^* = m_n \frac{d\gamma}{d\mathcal{E}} = m_n \gamma' . \tag{3c}$$

Since the drift energy is assumed to be much smaller than the thermal energy in the present case, we can expand the distribution function in spherical harmonics and retain only the first two terms of the expansion,

$$f(k_i) = \sum_{l=0}^{l=\infty} P_l\left(\frac{k_i}{k}\right) f_i^l , \tag{4a}$$

$$F(k_i) \simeq f^0 + \frac{k_i}{k} f_i^1 . \tag{4b}$$

Substituting relation (4b) in Eq. (3a) and going through the usual procedure,[2] we obtain the following set of coupled equations for isotropic and anisotropic parts of the distribution function:

$$-\frac{2}{3}\frac{e}{(2m_n\gamma)^{1/2}}\frac{1}{\gamma'}\frac{\partial}{\partial\mathcal{E}}(\gamma E_i f_i^1)=\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}}, \quad (5)$$

$$\frac{f_i^1}{\tau}-\frac{2e}{(2m_n)^{1/2}}\frac{\gamma^{1/2}}{\gamma'}E_i\frac{\partial f^0}{\partial\mathcal{E}}-\epsilon_{ijk}\Omega_j f_k^1=0, \quad (6)$$

where τ is the momentum relaxation time for the polar optical mode of scattering. The relaxation-time approximation which is usually invalid for inelastic scattering (especially polar optical mode) is justified here because the electron temperature is greater than the Debye temperature, and further the nonparabolicity of the conduction band restricts any large changes in electron energy.[5]

Solving Eq. (6) for f_i^1 and substituting in Eq. (5) we have

$$-\frac{2e^2E^2}{3m_n}\frac{1}{\gamma'}\frac{1}{\gamma^{1/2}}\frac{\partial}{\partial\mathcal{E}}\left[\frac{\gamma^{3/2}}{\gamma'}\tau\left(\frac{1+\Omega^2\tau^2\cos^2\alpha}{1+\Omega^2\tau^2}\right)\frac{\partial f^0}{\partial\mathcal{E}}\right]=\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}}, \quad (7)$$

where α is the angle between $\vec{E}$ and $\vec{H}$.

After incorporating Pauli's exclusion principle,[3] screening of electron polar-phonon scattering[7] and more accurate carrier wave functions, the symmetrical part of the collision term of a degenerate sample, $(\partial f^0/\partial t)_{\text{coll}}$, can be expressed as[5]

$$\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}}=\frac{V}{2\pi\hbar}\iint dy\,dk'\,(k')^2B(k;|\vec{k}-\vec{k}'|)\Big(\{f^0(k)[1-f^0(\vec{k}')]N-f^0(\vec{k}')[1-f^0(k)](N+1)\}\delta(\mathcal{E}(\vec{k}')-\mathcal{E}(\vec{k})-k_0\Theta)$$
$$+\{f^0(k)[1-f^0(\vec{k}')](N+1)-f^0(\vec{k}')[1-f^0(k)]N\}\delta(\mathcal{E}(\vec{k}')-\mathcal{E}(\vec{k})+k_0\Theta)\Big), \quad (8a)$$

where N is the number of phonons with wave number $|\vec{k}-\vec{k}'|$, V is the volume, and $B(k;|\vec{k}-\vec{k}'|)$ the square of the interaction matrix element is given by[6]

$$B(k;|\vec{k}-\vec{k}'|)=\frac{2\pi e^2k_0\Theta}{V}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\times\frac{|\vec{k}-\vec{k}'|^2}{(|\vec{k}-\vec{k}'|^2+1/\lambda^2)^2}\,\mathcal{G}(k,k',y), \quad (8b)$$

where

$$\lambda^2=k_0T\epsilon_0/4\pi ne^2, \quad (8c)$$

$$\mathcal{G}(k,k',y)=\frac{1}{2}\sum_{\mu\mu'}\left|\int\phi^*_{\mu',k'}(\vec{r})\,\phi_{\mu k}(\vec{r})\,d^3r\right|^2, \quad (8d)$$

ϵ_∞ and ϵ_0 are the high-frequency and static dielectric constants, y is the cosine of the angle between $\vec{k}$ and $\vec{k}'$, $\phi_{\mu',k'}$ and $\phi_{\mu k}$ are the more accurate wave functions[4] usually approximated, in the majority of treatments, by plane waves, and n is the carrier concentration. The assumption of Debye screening of carrier polar phonon interaction in the derivation of Eq. (8b) is necessary to facilitate calculation because an exact treatment of screening in nonequilibrium solid-state plasmas is not known.

From Eqs. (8) by a standard and straightforward procedure[3,6] we obtain

$$\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}}=\frac{1}{(2m_n\gamma)^{1/2}}\frac{1}{\gamma}\sum_n\frac{P_n}{Q_n}\times\frac{d}{d\mathcal{E}}\left[(\gamma'Q_n)^2G_{n1}\left(f^0(1-f^0)+\eta\frac{df^0}{d\mathcal{E}}\right)\right], \quad (9a)$$

where

$$\mathcal{G}(q,\mathcal{E},\mathcal{E}\pm k_0\Theta)=\textstyle\sum_n P_n(\mathcal{E})\,Q_n(\mathcal{E}\pm k_0\Theta)\,R_n(q), \quad (9b)$$

$$\eta=k_0\Theta(N+\tfrac{1}{2}), \quad (9c)$$

$$G_{n1}=eF_0k_0\Theta\int_u^\varphi\frac{q^3}{(q^2+\gamma^2)^2}R_n(q)\,dq, \quad (9d)$$

in which

$$u=k_0\Theta\gamma'/2\gamma^{1/2}, \quad (9e)$$

$$\varphi=2\gamma^{1/2}, \quad (9f)$$

$$\gamma^2=\hbar^2/2m_n\lambda^2, \quad (9g)$$

$$F_0=\frac{ek_0\Theta m_n}{\hbar^2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right). \quad (9h)$$

Equations (9) differ from the expression obtained by Matz[6,7] in that f^0 is replaced by $f^0(1-f^0)$ inside the square brackets. This then is the only change in the collision term due to degeneracy.[8]

Combining Eqs. (9) and (7) and proceeding along the same lines as Matz[6] and Sodha and Gupta,[3] one finally obtains

$$f^0=[1+A(E)\exp I(\mathcal{E},E)]^{-1}, \quad (10a)$$

where $A(E)$ is a normalization constant to be determined from the condition

$$\frac{(2m_n)^{3/2}}{2\pi^2\hbar^3}\int_0^\infty\gamma^{1/2}\gamma' f^0\,d\mathcal{E}=\text{carrier density}, \quad (10b)$$

$$I(\mathcal{E}, E) = \eta^{-1} \int \left[1 + \frac{2}{3} \frac{E^2}{F_0^2} \frac{\gamma^2}{\gamma'^4} \frac{2\gamma}{G_0 G_1 \eta^2} \times \left(\frac{1+\Omega^2\tau^2\cos^2\alpha}{1+\Omega^2\tau^2}\right)\right]^{-1} d\mathcal{E} , \quad (11a)$$

in which

$$G_0 = A_1 - (1/\gamma)[(1-a_k^2) + (\sqrt{2}\, b_k c_k - \tfrac{1}{2} b_k^2)^2] A_2 + (1/4\gamma^2) \times [(1-a_k^2)^2 - (\sqrt{2}\, b_k c_k - \tfrac{1}{2} b_k^2)^2] A_3 , \quad (11b)$$

$$G_1 = A_2 - (1/\gamma)[(1-a_k^2) + (\sqrt{2}\, b_k c_k - \tfrac{1}{2} b_k^2)^2] A_3 + (1/4\gamma^2)[(1-a_k^2)^2 - (\sqrt{2}\, b_k c_k - \tfrac{1}{2} b_k^2)^2] A_4 , \quad (11c)$$

$$\frac{1}{\tau} = \frac{eF_0(2N+1)\gamma' G_1}{2\gamma(2m_n\gamma)^{1/2}} . \quad (11d)$$

A_1, A_2, A_3, and A_4 are defined as

$$A_1 = \left(\ln(q^2+r^2)^{1/2} + \frac{r^2}{2(q^2+r^2)}\right)_{q=u}^{q=\varphi} , \quad (11e)$$

$$A_2 = \frac{1}{2}\left((q^2+r^2) - 2r^2\ln(q^2+r^2) - \frac{r^4}{(q^2+r^2)}\right)_{q=u}^{q=\varphi} , \quad (11f)$$

$$A_3 = \frac{1}{2}\left(\frac{1}{2}(q^2+r^2)^2 - 3r^2(q^2+r^2) + 3r^4\ln(q^2+r^2) + \frac{r^6}{q^2+r^2}\right)_{q=u}^{q=\varphi} , \quad (11g)$$

$$A_4 = \left(\frac{1}{6}(q^2+r^2)^3 - r^2(q^2+r^2)^2 + 3r^4(q^2+r^2) - 2r^6\ln(q^2+r^2) - \frac{1}{2}\frac{r^6}{q^2+r^2}\right)_{q=u}^{q=\varphi} . \quad (11h)$$

a_k, b_k, and c_k are given by Kane.[4] In the limit $E \to 0$, $I(\mathcal{E}, 0) \simeq \mathcal{E}/k_0T$ and the distribution function reduces to the Fermi-Dirac distribution. $A(0)$ can be interpreted as $\exp(-\mathcal{E}_F/k_0T)$, where $\mathcal{E}_F$ is the Fermi energy, to be determined by Eq. (10b). In the absence of a magnetic field and screening of the carrier-lattice interaction, Eq. (10a), for a nondegenerate sample, reduces to the distribution function obtained by Matz,[6] and also modifies to the expression obtained by Sodha and Gupta[3] if the more accurate wave functions are approximated by plane waves.

At this stage, it is worthwhile to discuss the validity of the above analysis. First since the relaxation-time model has been used for polar optical scattering, the present formulation is expected to give quantitatively correct results only above the Debye temperature. Second, for increasing electron concentration and consequently increasing degeneracy, one usually expects the electron-electron interaction to become important, thus questioning the validity of the above approach. For this case, recourse is made to the ETM by various workers,[9,10] which assumes that the electron-electron (el-el) scattering is strong enough to enforce a Fermi-Dirac distribution. This assumption has not been proved because of the difficulty of solving the transport equation for arbitrary electric and magnetic fields in the presence of el-el collisions. Recently, Crandall[1] has shown that even for electron concentrations three or four orders of magnitude above the critical electron concentration necessary for ETM to be valid,[2] the el-el interaction is unable to enforce a shifted Fermi distribution. This establishes that the true distribution is much closer to the BES (incorporating Pauli's exclusion principle and screening of electron optical-phonon scattering) than the ETM at high electron concentrations, and thus justifies the use of the BES. Physically, the el-el interaction represents a redistribution between the electrons of the energy that they receive from the electric field. Consequently, the fast electrons should be able to acquire smaller momenta by transferring some of their energy to the slower electrons. However, this process will not reduce the high-energy tail of the true distribution function, since it arises because the mean free time between collisions increases faster with increasing energy than does the energy-loss rate; as energy increases, the scattering rate for el-el collisions decreases. Furthermore, since all the scattered electrons have the same wave vector governed by the Fermi energy, the role of el-el scattering in heavily doped semiconductors should not be important.[11] From the foregoing discussion, we conclude that the present treatment should be valid for all electron concentrations and hence for an arbitrary degree of degeneracy of electrons, if the el-el interaction is negligible as compared to polar optical scattering. On the other hand, as there is no theoretical or experimental evidence which conclusively proves that el-el scattering can be completely neglected in comparision with polar optical scattering for all electron concentrations, we expect that the present distribution function would give quantitatively correct results at least up to the electron concentration $n \sim 10^{19}$ cm^{-3}: Even for $n > 10^{19}$ cm^{-3}, qualitatively correct results are expected.

The present distribution function of carriers is

expected to enhance our understanding of the transport phenomena in III-V nonparabolic semiconductors. To test the validity of the present theory, it is suggested that hot-electron effects in n-type InSb or InAs with carrier concentration $n \lesssim 10^{19}$ cm^{-3} should be studied in the temperature range $300 \lesssim T \lesssim 500$ °K so that the screened polar optical mode of carrier-lattice interaction is the only dominant scattering mechanism.[4] Electric fields should be limited below ~ 350 V/cm and should be applied in the form of very short voltage pulses (duration ~ 10^{-10} sec) and at low-repetition rates in order to avoid impact ionization and heating of the lattice.[12,13] With little impact ionization one need not consider pinching and electron-hole scattering.[7] Calculations for the actual comparison with limited available experimental results are in progress and will be reported soon.

The present investigation was supported by Environmental Scientific Services Administration, Boulder, Colo. and Council of Scientific and Industrial Research, India.

[1]R. S. Crandall, J. Phys. Chem. Solids 31, 771 (1970).
[2]E. M. Conwell, *High Field Transport in Semiconductors* (Academic, New York, 1967).
[3]M. S. Sodha and B. M. Gupta, Phys. Rev. B 2, 3249 (1970).
[4]E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957); H. Ehrenreich, *ibid.* 2, 131 (1957).
[5]D. Matz, J. Phys. Chem. Solids 28, 373 (1967).
[6]D. Matz, Phys. Rev. 168, 843 (1968).
[7]B. C. Burkey and D. Matz., Phys. Rev. B 1, 4753 (1970).
[8]M. Saitoh, Progr. Theoret. Phys. (Kyoto) 43, 562 (1970).
[9]P. Das and V. Sahni, J. Phys. C 1, 1398 (1968).
[10]M. S. Sodha, J. Kamal, and P. K. Dubey, J. Phys. Soc. Japan 28, 1461 (1970).
[11]V. J. Fistul', *Heavily Doped Semiconductors* (Plenum, New York, 1969), p. 96.
[12]A. C. Prior, J. Electron. Control 4, 165 (1958).
[13]J. C. McGroddy and M. I. Nathan, J. Phys. Soc. Japan Suppl. 21, 437 (1966).