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Corrections to conductivity caused by a constant-field influence on the scattering processes in semiconductors

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Abstract. The constant-field influence on the electron scattering processes in semiconductors is shown to lead to correction of the static conductivity. This correction is non-zero in particular for the absence of electron heating. In the case of acoustic phonon scattering, the correction is small. For optic phonon scattering and ionised impurity scattering, the corrections can be of the order of a few per cent and 10–20%, respectively.

1. Introduction

In recent years the problem of correction of the Boltzmann equation for free-charge carriers in semiconductors under a strong uniform electric field has been intensively discussed [1–15]. The quantum kinetic equation in the presence of a constant electric field acting on the electron scattering processes has been derived by the Green function technique [3, 10, 15] and by use of the generalised kinetic equations [1, 2, 16, 17]. The kinetic equation for electrons with the Airy wavefunction is also considered [4, 5]. The possible corrections of the Boltzmann equation due to non-zero scattering time and non-zero de Broglie wavelength of electron have been discussed [3, 6–9, 11]. The change in scattering cross section in the presence of a constant external field has been explored as a rule in the strong-field approximation. The corresponding correction has been found to be non-linear in the electric field and estimated to have an order of magnitude of both 10% [3, 7, 8] and 0.1 or 0.001% [11, 12].

In this paper the balance equation for the electron temperature T_e and drift momentum $\hbar k_0$ using the displaced Maxwell distribution function are obtained on the basis of the kinetic equation taking into account the collision integral dependence on the constant electric field E . The solution of these equations in the case of small anisotropy has shown the existence of corrections Γ and β in the current:

$$j = \frac{j_0(1 + \Gamma)}{(1 + \beta)} \quad \Gamma = \sum_i \Gamma_i(1 + \eta_i)$$

where j_0 is the current obtained with the usual collision integral (i indicates the scattering types). The appearance of these corrections is caused by the collision integral dependence on the field E , which distorts the conventional δ -form of energy conservation in collision. For $E \rightarrow 0$ the quantities β and η_i tend to zero. The quantities Γ_i depend on

the field via T_e and differ from zero also without heating of electrons (T_e is measured in energy units).

We are concerned with the physical sense of these corrections in the limit $\hbar \rightarrow 0$ for ionised impurity scattering, in the classical analogue case, i.e. gas plasma. At $\hbar \rightarrow 0$ we obtain $\Gamma_{im} = -e^2/6\epsilon_0 r_D T_e$ (ϵ_0 is the static permittivity of lattice and r_D is the Debye radius) which exactly agrees with the case of gas plasma [18, p 260]. Thus the quantity Γ_i is proportional to the ratio of the interaction electron energy with the scatterer to the electron kinetic energy. In the region of temperatures and charge carrier concentrations where the de Broglie wavelength is of the order of r_D , the behaviour of Γ_{im} differs essentially from that for $\hbar \rightarrow 0$. In this classical limit we obtain $\eta_{im} = -\frac{2}{3}(eEr_D/T_e)^2$, i.e. η_{im} is proportional to the square of the electron energy due to the external field during the collision time. At $\hbar \rightarrow 0$ for impurity scattering we get $\beta \sim (eEr_D/T_e)^2$; however, the proportional coefficient tends to zero in this limit.

2. Balance equations and corrections to conductivity

The kinetic equation for non-degenerate electrons interacting with phonons and chaotic ionised impurities in the presence of a uniform constant external field E is given by

$$\begin{aligned}
 eE \frac{\partial f}{\partial k} = & 2 \sum_i \int \frac{d^3 q}{(2\pi)^3} |g_i(q)|^2 \int_0^\infty d\tau \left\{ [(1 + N_q^{(i)})f(\mathbf{k} + \mathbf{q} - eE\tau) \right. \\
 & - N_q^{(i)}f(\mathbf{k} - eE\tau)] \cos \left[\tau \left(\epsilon_k - \epsilon_{\mathbf{k}+\mathbf{q}} + \hbar\omega_q^{(i)} + \frac{\hbar^2}{2m} \tau eE\mathbf{q} \right) \right] \\
 & - [(1 + N_q^{(i)})f(\mathbf{k} - eE\tau) - N_q^{(i)}f(\mathbf{k} + \mathbf{q} - eE\tau)] \\
 & \left. \times \cos \left[\tau \left(\epsilon_k - \epsilon_{\mathbf{k}+\mathbf{q}} - \hbar\omega_q^{(i)} + \frac{\hbar^2}{2m} \tau eE\mathbf{q} \right) \right] \right\} \quad (1)
 \end{aligned}$$

where $\epsilon_k = \hbar^2 k^2/2m$, \mathbf{k} and \mathbf{q} are wavevectors, $\hbar\omega_q$ is the phonon energy, N_q is the phonon distribution function, $g_i(q)$ is interaction constant for the scattering mechanism i (for an impurity, $N_q = \hbar\omega_q = 0$). This equation has been derived by different methods [3, 17]; it also follows from the generalised equation [16]. At $\hbar \rightarrow 0$, for impurity scattering, equation (1) transforms to the classical kinetic equation taking into account the field dependence of the collision process. The latter equation can be obtained independently by methods of classical statistical mechanics and from it the above-mentioned classical correction Γ_{im} to conductivity follows.

The analysis of equation (1) is difficult because of the term $eE\tau$ in the argument of the distribution function. From the derivation of the balance equations, it follows, however, that the elimination of this term compared with \mathbf{k} leads in particular to a change in the sign of Γ_i and thus to a contradiction with the result for gas plasma. Therefore it is convenient to take the model distribution function to produce the balance equations for energy and momentum, because the field dependence of the collision integral in these equations can be included sufficiently correctly. The displaced Maxwell distribution leads to a rather complex system of equations for T_e and $\hbar k_0$ which is not interpretable obviously. So the small-anisotropy approximation has been chosen for

simplicity: $f(\mathbf{k}) = f_0(k)(1 + 2\lambda^2 \mathbf{k} \mathbf{k}_0)$, $f_0(k) \sim \exp(-\varepsilon_k/T_e)$, $\lambda = \hbar/\sqrt{2mT_e}$. In this approximation the momentum balance equation is as follows:

$$\frac{eE\lambda}{T_e} = \frac{1}{\pi^2 \lambda^3 T_e^2} \sum_i \int_0^\infty dx x \left| g_i \left(\frac{x}{\lambda} \right) \right|^2 \{ (1 + N_q^{(i)}) [I_1(x, \alpha, \gamma_i) + 2\lambda k_0 I_2(x, \alpha, \gamma_i) + 2\lambda k_0 x^2 I_3(x, \alpha, \gamma_i)] + N_q^{(i)} [\gamma_i \rightarrow -\gamma_i] \} \quad (2)$$

where $q = x/\lambda$, $\alpha = eE\lambda/T_e$, $\gamma_i = \hbar\omega_q^{(i)}/T_e$,

$$I_1 = -\frac{1}{2\alpha^2} \int_0^\infty \frac{dy}{y} \exp(-x^2 y^2) \sin[y(x^2 + \gamma_i)] \frac{d}{dy} \frac{\sin(\alpha x y^2)}{y^2}$$

$$I_2 = \frac{1}{\alpha^3} \int_0^\infty \frac{dy}{y^2} \exp(-x^2 y^2) \sin[y(x^2 + \gamma_i)] \frac{d}{dy} \frac{\sin(\alpha x y^2)}{y^2}$$

$$I_3 = \frac{1}{\alpha} \int_0^\infty \frac{dy}{y} \exp(-x^2 y^2) \sin[y(x^2 + \gamma_i)] \sin(\alpha x y^2).$$

In equation (2), for polar optical scattering ($i \equiv \text{po}$), $|g_{\text{po}}(q)|^2 = 2\pi e^2 \hbar \omega / \bar{\varepsilon} q^2$ and $\bar{\varepsilon}^{-1} = \varepsilon_\infty^{-1} - \varepsilon_0^{-1}$, for deformation optical scattering ($i \equiv \text{do}$), $|g_{\text{do}}(q)|^2 = \hbar D^2 / 2\rho\omega$ and for ionised impurity scattering ($i \equiv \text{im}$), $|g_{\text{im}}(q)|^2 = n_{\text{im}} T_e^2 / n^2 (1 + q^2 r_D^2)^2$, where D is the coupling constant, ρ is the density, n_{im} is the impurity concentration, n is the free charge carrier concentration and ω is the optical phonon frequency. To obtain the balance equation (2) the displaced Maxwell distribution function may be used with subsequent expansion of λk_0 in the first order. We do not write the energy balance equation in this work, because it is necessary to evaluate T_e only. Direct expansion I_j ($j = 1, 2, 3$) over α to high orders gives at $x \rightarrow 0$ either a divergence term in (2) (for deformation acoustical or impurity scattering) or a series for which the convergence is difficult to prove (for polar optical or deformation optical scattering), but the upper estimation and different representations of the Dirac δ -function allows us to show that the behaviour of I_j for $x \rightarrow 0$ and $x \rightarrow \infty$ is that the integral over x in (2) converges for $\alpha \neq 0$ and is restricted for $\alpha \rightarrow 0$. In the lowest order the expansion I_j over α leads to $I_1(\alpha \rightarrow 0) = I'_1 \sim \alpha$, $I_j(\alpha \rightarrow 0) = I'_j = I_j(x, 0, \gamma_i)$ ($j = 2, 3$). Direct calculation shows convergence of I'_j ($j = 1, 2, 3$) on integration of x in (2). The above-mentioned results mean that the integral $I_j - I'_j$ of x converges and that $I_j - I'_j \rightarrow 0$ at $\alpha \rightarrow 0$. By calculating the limit $(I_j - I'_j)/\alpha^m$ for $\alpha \rightarrow 0$ it can be proved that $I_j - I'_j \sim \alpha^2 I'_j$ when $\alpha \ll 1$. Therefore, at $\alpha \ll 1$, I'_j ($j = 1, 2, 3$) gives the main contribution to the momentum balance equation and to the current density. The calculation of I'_j and $I_j - I'_j$ at $\alpha \ll 1$ leads to the following expression for the current density:

$$\mathbf{j} = ne \frac{\hbar \mathbf{k}_0}{m} = \frac{ne^2}{m\nu} \frac{1 + \Gamma}{1 + \beta} \mathbf{E} \quad \nu = \sum_i \nu_i$$

$$\beta = \nu^{-1} \sum_j \beta_j(\alpha) \quad \Gamma = \sum_i \Gamma_i [1 + \eta_i(\alpha)]$$

where ν_i is the corresponding collision rate. By introducing the functional $F(\lambda, \gamma_i)$ of the function $f(x, \gamma_i)$ according to the rule

$$F(\lambda, \gamma_i)[f(x, \gamma_i)] = \frac{1}{\pi^2 \lambda^3 T_e^2} \int_0^\infty dx \left| g_i \left(\frac{x}{\lambda} \right) \right|^2 [(1 + N_q^{(i)})p(\gamma_i)f(x, \gamma_i) + N_q^{(i)}p(-\gamma_i)f(x, -\gamma_i)]$$

we can write

$$\nu_i = (\sqrt{\pi}/3)(T_e/\hbar)F(\lambda, \gamma_i)\{x \exp[-p^2(\gamma_i)]\} \quad (3)$$

$$\Gamma_i = -\frac{1}{3}F(\lambda, \gamma_i)[x {}_1F_1(2, \frac{3}{2}; -p^2(\gamma_i))] \quad (4)$$

$$\eta_i(\alpha) = (\alpha^2/5\Gamma_i)F(\lambda, \gamma_i)[(1/x) {}_1F_1(4, \frac{3}{2}; -p^2(\gamma_i))] \quad (5)$$

$$\beta_i(\alpha) = -(3\sqrt{\pi}/8)\alpha^2(T_e/\hbar)F(\lambda, \gamma_i)\{\exp[-p^2(\gamma_i)] [1 - \frac{4}{3}p^2(\gamma_i) + \frac{4}{15}p^4(\gamma_i)]\} \quad (6)$$

where ${}_1F_1$ is the degenerate hypergeometric function [19], $p(\gamma) = (x^2 + \gamma)/2x$. For impurity scattering in equations (3)–(6), $N_q = \gamma = 0$. In the cases of optic and impurity scattering the integrals (4)–(6) can be calculated analytically. The result is represented for Γ_i and η_{im} as follows:

$$\Gamma_{do} = \frac{1}{12}\sqrt{2}/\pi(D^2/\rho\hbar)(m/T_e)^{3/2}(1 + N_\omega) \exp(-\gamma/2)[\gamma I_0(\gamma/2) - (1 + \gamma)I_1(\gamma/2)]$$

$$\Gamma_{po} = (\sqrt{\pi}/6)(\omega e^2/\varepsilon T_e)(2m/T_e)^{1/2}(1 + N_\omega) \exp(-\gamma/2)[(\gamma - 1)I_0(\gamma/2) - \gamma I_1(\gamma/2)]$$

$$\Gamma_{im} = -(e^2/6\varepsilon_0 T_e r_D)(n_{im}/n)[1 + a - \sqrt{a}(a + \frac{3}{2}) \exp a \sigma(a)]$$

$$\eta_{im} = (eEr_D/T_e)^2(e^2\Gamma_{im}^{-1}/16\varepsilon_0 T_e r_D)(n_{im}/n)(1/\sqrt{a})[\sqrt{\pi}/2 + (\sqrt{a}/15)(g - 5ga - 36a^2 - 4a^3) - \exp a \sigma(a)\frac{1}{30}(15 - 15a - 150a^2 - 76a^3 - 8a^4)]$$

where

$$\sigma(a) = \int_a^\infty dx \exp(-x) x^{-1/2}$$

$a = (\lambda/2r_D)^2$ and $I_n(x)$ is the modified Bessel function of the first kind [19]. $N_q = N_\omega$ is supposed to be equilibrium.

When $\hbar \rightarrow 0$ the limit of Γ_{im} is obvious and it has been written above. The quantity η_{im} at $\hbar \rightarrow 0$ may be expressed via $\tau_0 = r_D/v$ ($v = \sqrt{3T_e/m}$), where τ_0 is the time of flight of the electron across the Debye radius:

$$\eta_{im}(\hbar \rightarrow 0) = -\frac{3}{8}(eEr_D/T_e)^2 = -\frac{3}{8}e^2 E^2 \tau_0^2 / m T_e.$$

Generalising this relation to the quantum case we get the following expression for the interaction time τ_{im} with impurity centre:

$$\tau_{im} = [-\frac{5}{9}(mT_e/e^2 E^2)\eta_{im}]^{1/2}$$

which depends on E only via T_e . When $a \gg 1$ we obtain $\tau_{im} = \tau_0 a^{3/2} (5\sqrt{\pi}/2)^{1/2}$. To save space, we shall not write the expressions for (known) ν_i , β_i and η_i for phonon scattering. The quantity Γ_{da} cannot be calculated analytically and the computation result for n-Ge is $\Gamma_{da} \sim 10^{-4}$. In this case the integration of x in the spontaneous acoustic phonon emission term of equation (4) must be limited by the phonon maximum wavevector.

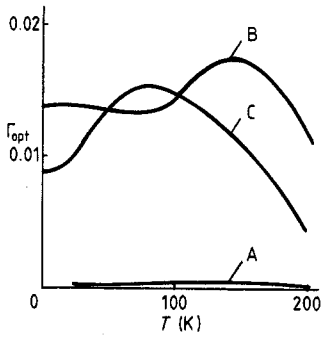


Figure 1. The value of the correction to conductivity for optical phonon scattering: curve A, n-Ge; curve B, p-Ge; curve C, n-GaAs.

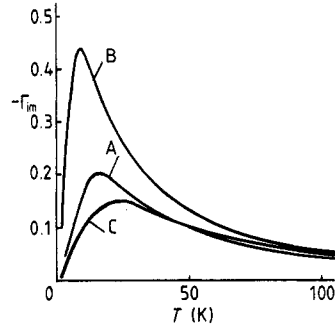


Figure 2. The value of the correction to conductivity for ionised impurity scattering as a function of temperature at $n = n_{im} = 10^{16} \text{ cm}^{-3}$: curve A, n-Ge; curve B, p-Ge; curve C, n-GaAs.

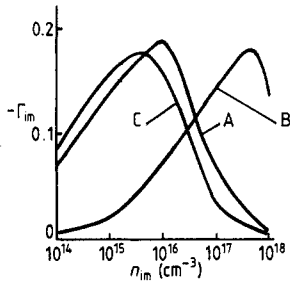


Figure 3. The value of the correction to conductivity for ionised impurity scattering as a function of $n (=n_{im})$ concentration: curve A, n-Ge, T (K) = 20 K; curve B, p-Ge, T (K) = 80 K; curve C, n-GaAs, T (K) = 20 K.

The energy balance equation has been solved to evaluate α and the dependence $T_e(E)$ for n-Ge ($n = 10^{16} \text{ cm}^{-3}$ and $T(\text{K}) = T/k_B = 4$ or 20 K) has been found (k_B is the Boltzmann constant). This computation leads to $\alpha^2 \leq 10^{-5}$ for any value of E ; this does not contradict the model used for the distribution function. It has also been found that the value of T_e is only weakly influenced (by a few per cent) by the corrections arising from the explicit field dependence of collision integral. By calculating integrals (3)–(6) the following estimates can be obtained (for n-Ge): $|\beta| \leq 10^{-4}$ and $\sum_i |\Gamma_i \eta_i| \leq 10^{-5}$ which agrees with [12].

3. Numerical results and conclusions

Numerical results of the Γ_i calculation for the non-heating field case ($T_e = T$) are shown in figures 1–3 for three semiconductors: n-Ge, p-Ge (only the heavy holes have been taken into account) and n-GaAs. For n-Ge we have used $D \approx 4 \times 10^8 \text{ eV cm}^{-1}$ and for p-Ge $D \approx 1.19 \times 10^9 \text{ eV cm}^{-1}$ [20]. When $T(\text{K}) = T/k_B \leq 50 \text{ K}$ the Born approximation is inadequate for describing the Coulomb scattering in p-Ge [21] and hence curve B in figure 2 is associated with the present scattering model in this temperature region. The above analysis indicates that the influence of the explicit static field dependence of the collision integral is small for phonon scattering (in the range of the used approximations). The correction corresponding to ionised impurity scattering is essential in the

region of parameters, where $r_D \sim \lambda$, and it has a value of about 10–20%. In this region the static field influence on collisions modifies the temperature dependence of the semiconductor conductivity. For the materials considered, the region $r_D \sim \lambda$ corresponds to the situation when the ionised impurity scattering rate of electrons is dominant.

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