YU ISSN 0015-3206
FZKAAA 18 (3) 229 (1986)

ON THE MODIFICATION OF THE EINSTEIN RELATION IN DEGENERATE SEMICONDUCTORS IN THE PRESENCE OF CROSSED ELECTRIC AND MAGNETIC FIELDS

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Received 5 September 1984

Revised manuscript received 1 June 1986

UDC 538.9

Original scientific paper

An attempt is made to derive the modified form of the Einstein relation for the diffusivity-mobility ratio of the carriers in degenerate semiconductors in the presence of crossed electric and magnetic fields. It is found, taking *n*-GaAs as an example for the purpose of numerical computations, that such ratio shows an oscillatory magnetic field dependence as expected only under degenerate conditions and remains unaffected otherwise. Besides, the amplitude of oscillations is found to be significantly influenced by the electric field.

1. Introduction

It is well-known that the Einstein relation for the diffusivity-mobility ratio of the carriers in semiconductors (hereafter referred to as DMR) is a very useful one since one can determine the diffusivity from this relation by knowing the mobility and vice-versa. Besides, being a thermodynamic relation, this is independent of any scattering mechanism and is, therefore, more accurate than any of the individual relation for diffusivity or mobility which are considered to be the two most widely used parameter for carrier transport in semiconductors. Furthermore,

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in recent years, the connection of DMR with the velocity auto-correlation function[1], the modification due to non-linear charge transport[2], the relation of the ratio with the screening of the carriers in semiconductors[3,4] and its different modifications for degenerate semiconductors under various physical conditions[5–12] have been extensively investigated in the litearture. Nevertheless, the influence of crossed electric and magnetic fields on the Einstein relation in degenerate semiconductors has yet to be properly worked out. The more so since these semiconductors are being increasingly used for the fabrication of semiconductor devices for technical applications. In what follows, this is investigated theoretically by taking degenerate n-GaAs as an example for the purpose of numerical computations.

2. *Theoretical background*

The energy spectrum of the conduction electrons in degenerate semiconductors, forming band-tails, can be expressed[13] as

$$E = \frac{\hbar^2 k^2}{2m^*} - \frac{4\pi N_t A_s}{N \Omega a_0^2} - \frac{4\pi N_t m^* A_s^2}{N \Omega \hbar^2 a_0} (a^2 + 4k^2)^{-1} \tag{1}$$

where the energy E is measured from the edge of the unperturbed parabolic conduction band, $\hbar = h/2\pi$, h is the Planck's constant, m^* is the effective electron mass for unperturbed parabolic conduction band, N_t is the number of impurity atoms per N atoms of the crystal, Ω is the volume of the unit cell, $A_s \equiv [e^2/4\pi\varepsilon_s]$, e is the electron charge, ε_s is the semiconductor permittivity, $a_0 \equiv (\pi\varepsilon_s)^{1/2} (\pi/3)^{1/6} \cdot \cdot (N^{-1/3} d_0)^{1/2}$, $d_0 \equiv \hbar^2/me^2$ and m is the free electron mass. Eq. (1) can be written as

$$\frac{\hbar^2 k^2}{2m^*} = \gamma (E) \tag{2}$$

where

$$\gamma (E) \equiv \frac{1}{2} [P_0 + E + \{E^2 + 2QE + R_0\}^{1/2}],$$

$$P_0 \equiv b - AD,$$

$$b \equiv (4\pi N_t A_s / N\Omega a^2),$$

$$A \equiv \hbar^2/2m^*,$$

$$D \equiv a_0^2/4,$$

$$Q \equiv b + AD,$$

$$R_0 \equiv b^2 + A^2 D^2 + 2A (bD + 2C)$$

and

$$C \equiv (\pi N_t m^* A_s^2 / N\Omega a_0 \hbar^2).$$

Incidentally, following Zawadzki et al.[14], the modified electron energy spectrum under crossed electric and magnetic fields can be expressed as

$$\gamma(E) = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k^2}{2m^*} - \frac{E_0 \psi(E)}{B}\hbar k_y - \frac{m^* E_0^2 \psi^2(E)}{2B^2} \tag{3}$$

where n ($\equiv 0, 1, 2, \ldots$) is the Landau quantum number, $\omega_0 \equiv \frac{eB}{m^*}$, B is the quantizing magnetic field along z-direction, $\psi(E) \equiv \frac{1}{2}[1 + (E + Q) S^{-1}(E)]$, $S(E) \equiv$ $\equiv [E^2 + 2QE + R_0]^{1/2}$ and E_0 is the electric field along x-direction. For $N_t \to 0$, Eq. (3) takes the well-known form[15]

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} - \frac{E_0}{B}\hbar k_y - \frac{m^* E_0^2}{2B^2} \tag{4}$$

The use of Eq. (3) leads to the expression of the total density-of-states function as

$$\varrho(E) = \frac{B L_y L_z \sqrt{2m^*}}{E_0 \pi^2 \hbar^2} \sum_{n=0}^{n_{max}} [1 + (X(E)\, m^* E^2/B^2)] \times$$

$$\times [\sqrt{G(E) + eE_0 L_x \psi(E)} - \sqrt{G(E)}] \tag{5}$$

where

$$X(E) \equiv \frac{1}{2}[\{S(E)\}^{-1} - (Q + E)^2 \{S(E)\}^{-3}]$$

and

$$G(E) \equiv \left[\gamma(E) - \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{m^* E_0^2 \bar{\psi}^2(E)}{2B^2}\right].$$

For $E_0 \to 0$, Eq. (5) takes the form

$$\varrho(E) = L_x L_y L_z \cdot 2\pi\hbar\omega_0 \left(\frac{2m^*}{h^2}\right)^{3/2} \sum_{n=0}^{n_{max}} \frac{\psi(E)}{\sqrt{\gamma(E) - \left(n + \frac{1}{2}\right)\hbar\omega_0}}. \tag{6}$$

Furthermore, for $N_t \to 0$, Eq. (6) gets simplified into the well-known[16] form

$$\varrho(E) = L_x L_y L_z \cdot 2\pi\hbar\omega_0 \left(\frac{2m^*}{h^2}\right)^{3/2} \sum_{n=0}^{n_{max}} \left[E - \left(n + \frac{1}{2}\right)\hbar\omega_0\right]^{-1/2}. \tag{7}$$

Thus, combining Eq. (5) with the Fermi-Dirac occupation probability factor the electron concentration in degenerate semiconductors forming band-tails may be expressed, by using the generalized Sommerfeld's lemma[17] together with some tedious algebraic manipulations, under crossed electric and magnetic fields as

$$n_0 = \left[\frac{2B}{3\hbar E_0 \pi^2 L_x}\right] \sum_{n=0}^{n_{max}} [\beta(E_F) + \lambda(E_F)] \tag{8}$$

where the functions $\beta(E_F)$ and $\lambda(E_F)$ are defined in the Appendix. In the absence of electric field, the electron concentration can be written as

$$n_0 = \frac{eB}{\pi^2 \hbar} \sum_{n=0}^{n_{max}} [\xi(E_F) + \Delta(E_F)] \tag{9}$$

where the functions $\xi(E_F)$ and $\Delta(E_F)$ are defined in the Appendix. Besides, for $N_t \to 0$, Eq. (9) assumes the well-known[16] form

$$n_0 = N_c \sum_{n=0}^{n_{max}} F_{-\frac{1}{2}}(\eta) \tag{10}$$

where

$$\overline{N_c} \equiv N_c(\hbar\omega_0/k_B T),$$

$$N_c \equiv 2(2\pi m^* k_B T/h^2)^{3/2},$$

$$\eta \equiv (k_B T)^{-1}\left[E_F - \left(n + \frac{1}{2}\right)\hbar\omega_0\right]$$

and $F_j(\eta)$ is the Fermi-Dirac integral of order j as defined by Blakemore[16].

Thus, since the DMR of the electrons can, in general, be expressed[6] as

$$\frac{D}{\mu} = \frac{1}{e} n_0 \left| \frac{dn_0}{dE_F}\right. . \tag{11}$$

We can combine Eq. (8) and (11) to obtain an expression of the same ratio under crossed electric and magnetic fields as

$$\frac{D}{\mu} = \frac{1}{e}\left[\sum_{n=0}^{n_{max}} \{\beta(E_F) + \lambda(E_F)\}\right]\left[\sum_{n=0}^{n_{max}} \{p(E_F) + q(E_F)\}\right]^{-1} \tag{12}$$

where the functions $p(E_F)$ and $q(E_F)$ are defined in the Appendix. In the absence of electric field, the DMR can be expressed as

$$\frac{D}{\mu} = \frac{1}{e} \left[\sum_{n=0}^{n_{max}} \xi (E_F) + \Delta (E_F) \right] \left[\sum_{n=0}^{n_{max}} r(E_F) + s(E_F) \right]^{-1} \tag{13}$$

where the functions $r(E_F)$ and $s(E_F)$ are defined in the Appendix.

Incidentally, for $N_t \rightarrow 0$, the Eq. (13) assumes the form

$$\frac{D}{\mu} = \frac{k_B T}{e} \left[\sum_{n=0}^{n_{max}} F_{-\frac{1}{2}}(\eta) \right] \left[\sum_{n=0}^{n_{max}} F_{-\frac{3}{2}}(\eta) \right]^{-1} \tag{14}$$

as derived for the first time by Chakravarti et al.[7]. Under the condition of non-degeneracy, Eq. (14) converts into the conventional Einstein relation $D/\mu - k_B T/e$ as it should.

3. *Results and discussion*

For degenerate n-GaAs using Eqs. (5) and (8) and the parameters[6], $m^* = 0.067\, m_0$, $E_0 = 10^3$ V/m, $L_x = L_y = L_z = 1$ m and $\varepsilon_s = 11.8\, \varepsilon_0$, $n_0 \approx N_t \doteq 1 \times 10^{24}$ m^{-3}, $\Omega = \frac{1}{4}(.563)$ (nm)^3, $T = 4.2$ K, we have computed the DMR of the electrons under crossed electric and magnetic fields as a function of the inverse quantizing magnetic field, as shown in Fig. 1 in which the same dependence as computed from Eqs. (9) and (13), i. e. in the absence of electric field, is also shown for the purpose of comparison. It is seen from the figure that the DMR shows an oscillatory magnetic field dependence and the electric field significantly affects the amplitude of oscillations. The oscillatory dependence is due to the crossing over of the Fermi level by the sub-bands in steps resulting in a successive reduction in the number of the occupied Landau level with the Fermi level, there would be a discontinuity in the density-of-states function resulting in a peak of oscillations. Thus, the peaks should occur whenever the Fermi energy is a multiple of the energy separation between two successive Landau levels and it may be noted that the origin of the oscillations in diffusivity-mobility ratio is the same as that of the Shubnikov-de Hass (SdH) oscillations. Incidentally, the effects of electron spin and collision broadening have not been considered in obtaining the oscillatorry plot. The spin effects would simply increase the number of oscillatory spikes and the collision broadening effects, though small at low temperatures, may affect the amplitude. It may also be noted that the DMR, will, in general, be anisotropic in the presence of magnetic quantization. It appears then that, for investigating the DMR under crossed electric and magnetic field, we have to detemine DMR the element D_{zz}/μ_{zz} of the corresponding tensor under the above conditions. Thus, the DMR defined here refers to the direction z of the application of the magnetic field. Moreover, the effects of electron-electron interaction which increases with increasing electron concentration have not been considered in the analysis. Besides,

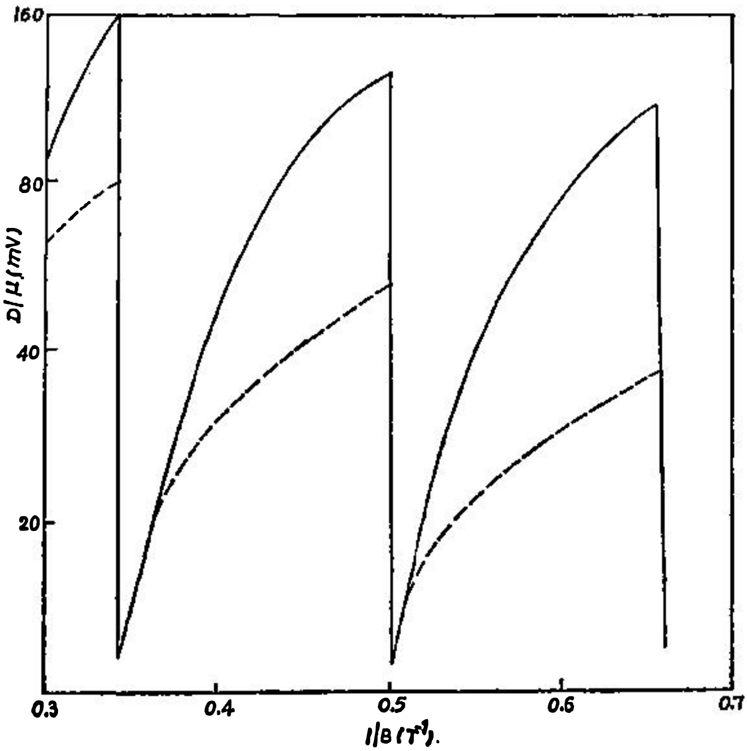

Fig. 1. Plot of the variation of DMR with magnetic field in degenerate n-GaAs at $T = 4.2K$ corresponding to an electron concentration of $1 \times 10^{24}\ m^{-3}$. The dotted plot corresponds to $E_0 = 0$.

the rigorous density-matrix approach should be properly considered, instead of this simplified analysis. However, the basic qualitative features will not be altered to a large extent even after the necessary modifications in view of the above discussion.

It may be stated that the above conclusions will be true only under the conditions of carrier degeneracy. However, the purpose of the present work is not solely to demonstrate the influence of the crossed fields on the DMR but also to formulate the simplified expression of the same ratio for the carriers in degenerate semiconductors placed in crossed electric and magnetic fields. Finally it may be noted that the conclusions made here would be of particular significance in view of the fact that the thermal noise, the switching speed, and the performance at the device terminals of the devices made of degenerate semiconductors can be related to the DMR[18-20].

Appendix

The functions $\beta (E_F)$, $\lambda (E_F)$, $\xi (E_F)$, $\Delta (E_F)$, $p (E_F)$, $q (E_F)$, $r (E_F)$ and $s (E_F)$ are defined as follows:

$$\beta (E_F) = [I (E_F) - J (E_F)] \tag{15}$$

$$\lambda(E_F) = \sum_{r=1}^{l} [\tau [I(E_F)] - \tau [J(E_F)]] \tag{16}$$

$$\xi(E_F) = \left[\gamma(E_F) - \left(n + \frac{1}{2}\right) \hbar \omega_0\right]^{1/2} \tag{17}$$

$$\Delta(E_F) = \tau [\xi(E_F)] \tag{18}$$

$$p(E_F) = \tau' [\beta(E_F)] \tag{19}$$

$$q(E_F) = \tau' [\lambda(E_F)] \tag{20}$$

$$r(E_F) = \tau' [\xi(E_F)] \tag{21}$$

$$s(E_F) = \tau' [\Delta(E_F)] \tag{22}$$

where

$$I(E_F) \equiv [\psi^{-1}(E) \{G(E) + e E_0 L_x \psi(E)\}^{3/2}]_{E=E_F},$$

$$J(E_F) \equiv [\psi^{-1}(E_F) \{G(E_F)\}^{3/2}], \quad \tau' \equiv \frac{\mathrm{d}}{\mathrm{d}E_F},$$

E_F is the Fermi energy in the presence of crossed electric and magnetic fields and is measured upwards from the edge of the unperturbed parabolic conduction band in the absence of any fields, $\tau \equiv 2(1 - 2^{1-2r})\,\delta(2r) \cdot (k_B T)^{2r}\, \mathrm{d}^{2r}/\mathrm{d}E_F^{2r}$, $\delta(2r)$ is the zeta function of order $2r$, k_B is the Boltzmann constant and T is the temperature.

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O MODIFICIRANOJ EINSTEINOVOJ RELACIJI ZA DEGENERIRANE POLUVODIČE U UKRŠTENOM ELEKTRIČNOM I MAGNETSKOM POLJU

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UDK 538.9

Originalni znanstveni rad

Izvedena je modificirana Einsteinova relacija za omjer difuznosti i mobilnosti nosioca naboja u degeneriranim poluvodičima koji se nalaze u ukrštenom električnom i magnetskom polju. Numerički račun proveden je za *n*-GaAs.