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B. R. Nag

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B. R. Nag

Center of Advanced Study in Radio Physics and Electronics, Calcutta University, India
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An iteration method is presented for the accurate calculation of the microwave magnetoconductivity of polar semiconductors. The method is an extension of Rode's iteration method for the evaluation of dc conductivity. The real and imaginary parts of the two perturbation components of the distribution function are obtained at each step of iteration by solving the four simultaneous equations relating the components. The iteration procedure is found to converge within 5–10 steps. The method has been applied to obtain the magnetoconductivity tensor of n-InSb at 10, 35, 85, and 135 GHz for magnetic induction up to 0.1 Wb/m^2. All the relevant scattering mechanisms and the effects of band nonparabolicity have been taken into account. The calculated values of conductivity differ significantly from those obtained by applying the Drude theory and do not agree with those deduced from a cavity perturbation experiment.

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INTRODUCTION

The magnetoconductivity of semiconductors are often studied[1,2] with microwave signals for the clarification of scattering processes. In a recent experiment, Eldumiati and Haddad[2] studied the magnetoresistance of n-InSb using a cavity perturbation technique and derived the mobility of the material from the analysis of the results, based on Drude's theory. It is, however, well known that Drude's theory grossly simplifies the scattering mechanism and we cannot expect that the results obtained from the simple theory would be valid. Accurately calculated theoretical values of microwave magnetoconductivity are needed for the understanding of the results of experiments of the kind mentioned above.

A difficulty encountered in the accurate evaluation of the conductivity tensor of materials like InSb, which are polar in nature, is that the relaxation time formalism cannot be applied. Electrons are scattered in these materials predominantly by polar optical phonons and since polar optical phonon scattering is neither elastic nor randomizing, the relaxation time formalism is inapplicable.[3] Accurate theoretical values of the conductivity of polar materials may be obtained only by solving the Boltzmann equation numerically. Such methods have been developed for the calculation of the conductivity.[4–8] The methods have been extended also for the calculation of Hall mobility[9–16] or ac conductivity.[15,17] In this paper we shall first present an iteration method, which may be employed for the evaluation of the ac magnetoconductivity tensor taking into account the full complexity of the scattering mechanisms. Results on the microwave magnetoconductivity tensor of n-InSb are then presented. These are also compared with those obtained from Drude's theory. The experimental results of Ref. 2 are examined finally in the light of the present calculations.

EQUATIONS TO BE SOLVED

The Boltzmann equation for the problem under consideration is

$$\frac{\partial f(\mathbf{k})}{\partial t} = -\frac{e}{\hbar}\left(\mathcal{E}_0 \exp(i\omega t) + \frac{1}{\hbar}\nabla_{\mathbf{k}} E \times \mathbf{B}\right)\nabla_{\mathbf{k}} f(\mathbf{k}) + \left.\frac{\partial f(\mathbf{k})}{\partial t}\right|_c , \quad (1)$$

where $f(\mathbf{k})$ is the distribution function, $\mathcal{E}_0 \exp(i\omega t)$ is the applied electric field of angular frequency ω, and $\mathbf{B}$ is the applied magnetic induction, e, $\mathbf{k}$, and E are, respectively, the charge, wave vector, and energy of an electron; $(\partial f(\mathbf{k})/\partial t)_c$ is the rate of change of $f(\mathbf{k})$ due to collisions.

We assume that the $E-\mathbf{k}$ relation[18] for the electrons is

$$\hbar^2 k^2/2m^* = \gamma(E), \quad (2)$$

where m^* is the band-edge effective mass, assumed to be isotropic. $\gamma(E)$ is, in general, a complex function of E, but in most of the cases may be simplified[19] to

$$\gamma(E) = E(1+\alpha E), \quad (3)$$

where

$$\alpha = \frac{1}{E_g}\left(1-\frac{2m^*}{m_0}\right)\left(1-\frac{E_g\Delta}{3(E_g+\Delta)(E_g+\frac{2}{3}\Delta)}\right).$$

E_g being the energy band gap and Δ the spin-orbit splitting energy.

Let the magnetic induction be in the z direction and let x direction be chosen in the direction of the electric field. The electric field is assumed to be small enough to prevent the occurrence of hot-electron effects. The distribution function $f(\mathbf{k})$ may then be expanded as

$$f(\mathbf{k}) = f_0(E) - \frac{e\hbar}{m^*}\mathcal{E}_0 \exp(i\omega t)[k_x\phi_x(E) + k_y\phi_y(E)]\frac{\partial f_0(E)}{\partial E}, \quad (4)$$

where $f_0(E)$ is the equilibrium distribution function in the absence of the fields.

Substituting expression (4) in Eq. (1) and equating the coefficients of k_x and k_y on the two sides we get

$$L_c\phi_x = \gamma_1(E) + \omega_B(E)\phi_y + i\omega\phi_x, \quad (5)$$

$$L_c\phi_y = -\omega_B(E)\phi_x + i\omega\phi_y, \quad (6)$$

where L_c is the collision operator, $\omega_B(E)$ is the cyclotron resonance frequency $(|e|B/m^*)\gamma_1(E)$, and $\gamma_1(E) = (\partial\gamma/\partial E)^{-1}$.

The collision operator L_c may be expressed as[4]

$$L_c\phi(E)=S_0(E)\phi(E)-S_e(E)\phi(E+k_B\theta_0)-S_a(E)\phi(E-k_B\theta_0) \quad (7)$$

where $k_B\theta_0$ is the optical phonon energy, k_B being the Boltzmann constant. S_e and S_a are related to the in-scattering due to emission and absorption processes involving polar optical phonons, S_0 is related to the out-scattering rate and includes the effects of all other collision processes, which are either elastic or randomizing. Detailed expressions for S_0, S_e, and S_a for nonparabolic bands (including the overlap integrals)[20] have been given by Rode[8] and also by Nag and Dutta[21] for the present formalism.

Equations (5) and (6) are thus the equations required to be solved for the evaluation of the ac magnetoconductivity tensor. We note that both ϕ_x and ϕ_y are complex and Eqs. (5) and (6) really give four difference equations involving four unknown functions.

The components of the conductivity tensor may be evaluated when ϕ_x and ϕ_y are known using the formula

$$\sigma_{ij}=-\frac{ne^2}{m^*}\frac{2}{3}\left(\int \phi_{ij}\frac{\partial f_0}{\partial E}\gamma^{3/2}\,dE\right)\left(\int f_0\gamma^{1/2}\frac{\partial\gamma}{\partial E}\,dE\right)^{-1}, \quad (8)$$

where σ_{ij} represents the real $(j=r)$ or imaginary $(j=i)$ parts of the x or y component of the conductivity tensor; n is the electron concentration.

METHOD OF SOLUTION

The collision operator for scattering mechanisms other than polar optical phonon scattering is such that $L_c\phi(E)$ may be written as $\phi(E)/\tau(E)$, where $\tau(E)$ is equal to $1/S_0(E)$ and is called the relaxation time constant. Solution of Eqs. (5) and (6) is then straightforward and we get

$$\phi_x=\phi_{xr}+i\phi_{xi}=\frac{\tau(E)[1+i\omega\tau(E)]\gamma_1(E)}{1+2i\omega\tau(E)+[\omega_B(E)^2-\omega^2]\tau(E)^2}, \quad (9)$$

$$\phi_y=\phi_{yr}+i\phi_{yi}=-\frac{\tau(E)\omega_B(E)\tau(E)\gamma_1(E)}{1+2i\omega\tau(E)+[\omega_B(E)^2-\omega^2]\tau(E)^2}. \quad (10)$$

In Drude's theory, Eq. (9) and (10) are simplified by neglecting the energy dependence of ϕ_x and ϕ_y and we get for the conductivity components

$$\sigma_x=\sigma_{xr}+i\sigma_{xi}=\frac{\sigma_0(1+i\omega\tau_0)}{1+2i\omega\tau_0+[\omega_B(0)^2-\omega^2]\tau_0^2}, \quad (11)$$

$$\sigma_y=\sigma_{yr}+i\sigma_{yi}=-\frac{\sigma_0\omega_B(0)\tau_0}{1+2i\omega\tau_0+[\omega_B(0)^2-\omega^2]\tau_0^2}, \quad (12)$$

where $\tau_0=m^*\sigma_0/ne^2$.

The analysis presented in Ref. 2 is based on the above equations. However, we find that in the presence of significant polar optical phonon scattering, an analytic solution of Eqs. (5) and (6) cannot be obtained. Numerical methods[4-8] were developed for obtaining the solution when ω_B and ω are both equal to zero, i.e., for dc fields in the absence of magnetic induction. Among the different methods available Rode's method[8] is the most convenient to work with. The method was extended earlier by the present author[5] to obtain solutions when either ω_B or ω is zero. In the present problem, however, neither ω_B nor ω is zero and this case has not been dealt with earlier. We may extend Rode's method of iteration also to the present problem as discussed below.

Let us consider the evaluation of ϕ for $E=E_i\pm lk_B\theta_0$, where l is a positive integer. Separating the real and imaginary parts we get from Eqs. (5) and (6),

$$S_0(E_i+lk_B\theta_0)\phi_{xr}(E_i+lk_B\theta_0)+\omega\phi_{xi}(E_i+lk_B\theta_0)-\omega_B(E_i+lk_B\theta_0)\phi_{yr}(E_i+lk_B\theta_0)$$
$$=\gamma_1(E_i+lk_B\theta_0)+S_e(E_i+lk_B\theta_0)\phi_{xr}[E_i+(l+1)k_B\theta_0]+S_a(E_i+lk_B\theta_0)\phi_{xr}[E_i+(l-1)k_B\theta_0] \quad (13)$$

$$S_0(E_i+lk_B\theta_0)\phi_{xi}(E_i+lk_B\theta_0)-\omega\phi_{xr}(E_i+lk_B\theta_0)-\omega_B(E_i+lk_B\theta_0)\phi_{yi}(E_i+lk_B\theta_0)$$
$$=S_e(E_i+lk_B\theta_0)\phi_{xi}[E_i+(l+1)k_B\theta_0]+S_a(E_i+lk_B\theta_0)\phi_{xi}[E_i+(l-1)k_B\theta_0], \quad (14)$$

$$S_0(E_i+lk_B\theta_0)\phi_{yr}(E_i+lk_B\theta_0)+\omega\phi_{yi}(E_i+lk_B\theta_0)+\omega_B(E_i+lk_B\theta_0)\phi_{xr}(E_i+lk_B\theta_0)$$
$$=S_e(E_i+lk_B\theta_0)\phi_{yr}[E_i+(l+1)k_B\theta_0]+S_a(E_i+lk_B\theta_0)\phi_{yr}[E_i+(l-1)k_B\theta_0], \quad (15)$$

$$S_0(E_i+lk_B\theta_0)\phi_{yi}(E_i+lk_B\theta_0)-\omega\phi_{yr}(E_i+lk_B\theta_0)+\omega_B(E_i+lk_B\theta_0)\phi_{xi}(E_i+lk_B\theta_0)$$
$$=S_e(E_i+lk_B\theta_0)\phi_{yi}[E_i+(l+1)k_B\theta_0]+S_a(E_i+lk_B\theta_0)\phi_{yi}[E_i+(l-1)k_B\theta_0]. \quad (16)$$

In the first step of iteration, $\phi_{xr}(E_i+lk_B\theta_0)$, $\phi_{xi}(E_i+lk_B\theta_0)$, $\phi_{yr}(E_i+lk_B\theta_0)$, and $\phi_{yi}(E_i+lk_B\theta_0)$ are obtained by solving Eqs. (13)–16 simultaneously, letting $\phi_{xr}[E_i+(l\pm 1)k_B\theta_0]$, $\phi_{xi}[E_i+(l\pm 1)k_B\theta_0]$, $\phi_{yr}[E_i+(l\pm 1)k_B\theta_0]$, and $\phi_{yi}[E_i+(l\pm 1)k_B\theta_0]$ equal zero. Such solutions are obtained for different integral values of l from 0 to n (to be chosen properly, as discussed later). In the second step of iteration, $\phi_{xr}[E_i+(l\pm 1)k_B\theta_0]$, etc., are replaced by their values obtained in the first step of iteration and new values of $\phi_{xr}(E_i+lk_B\theta_0)$, etc., are evaluated again solving the equations simultaneously. Note that $\phi_{xr}(E_i-k_B\theta_0)$, etc., occurring in the equations for $l=0$ are to be taken as zero. Also, note that in the second step of iteration we get values of ϕ up to $\phi[E_i+(n-1)k_B\theta_0]$; whereas in the first step we obtained values up to $\phi(E_i+nk_B\theta_0)$.

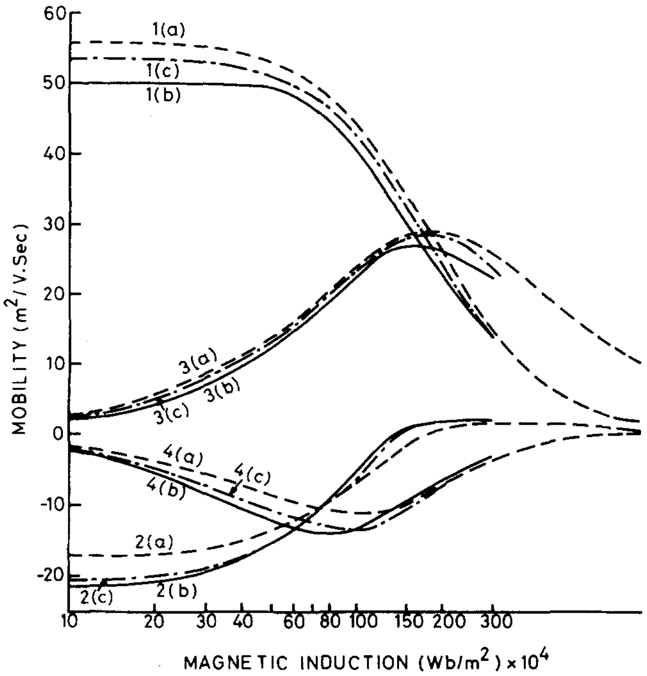

FIG. 1. Complex mobility of *n-InSb* at 77 °K at different magnetic fields for a frequency of 10 GHz. Curves numbered 1—4 represent, respectively, the components of the mobility tensor: μ_{xr}, μ_{xi}, μ_{yr}, and μ_{yi}. Letters in parenthesis indicate, respectively, the values obtained from the Drude theory, (a); and present calculations with $E_1 = 7.2$ eV, (b); and $E_1 = 30$ eV, (c).

The evaluation of ϕ is continued in successive steps of iteration in the same way as in the second step till the values of ϕ for two successive steps agree to within a specified accuracy. We note that if m iteration steps are necessary for the desired accuracy, we may evaluate ϕ up to $\phi[E_i + (n-m)k_B\theta_0]$, so that we should choose n in the first step as $q+m$, if values of ϕ for E up to $qk_B\theta_0$ are required for the evaluation of the integrals in Eq. (8) to a desired accuracy.

The procedure discussed above for a particular value of E_i is used to obtain ϕ for a number of values of E_i lying between 0 and $k_B\theta_0$ and chosen by the Gaussian quadrature method, so that values of $\phi(E)$ over the whole range of E between 0 and $qk_B\theta_0$ are obtained at the same time. These are then used to evaluate the integrals of Eq. (8) numerically.

The method outlined above was tested for its convergence taking some typical cases and was found to yield convergent values agreeing to within 0.01% in 7—10 iterations. In the following section we discuss the results obtained for n-InSb at 77 °K.

RESULTS FOR InSb

In order that we may calculate the conductivity tensor theoretically we need to know the physical parameters involved in the expressions for the scattering probabilities due to the various scattering mechanisms. In the case of InSb, values of most of the parameters are now well established. We have taken the values of the various parameters in accordance with Ref. 22 and the conductivity tensor was calculated for 77 °K and magnetic induction up to 0.5 Wb/m^2 (results up to 0.1 Wb/m^2 are only presented). All the scattering mechanisms, viz., deformation potential and piezoelectric acoustic phonon, polar optical phonon and ionized impurity scattering, were taken into account. Calculations were done for the two extreme values of the acoustic phonon deformation potential constant E_1, i.e., 7.2 and 30 eV, suggested in the literature. The concentration of ionized impurities N_I was chosen in each case so as to obtain the dc electron mobility of the sample, which was taken as 61 m^2/V sec. It may be pointed out that the above value of mobility is the same as that for the samples used in Ref. 2, and also that it is the most common value of the samples used by various other workers. The required value of N_I for obtaining an electron mobility of 61 m^2/V sec at 77 °K were $1.5\times10^{14}/cm^3$ and $4.5\times10^{14}/cm^2$, respectively, for the values of E_1 of 30 and 7.2 eV.

In the calculations, 16 values of E_i were chosen in the interval $0 < E_i < k_B\theta_0$ in accordance with the Gaussian quadrature method. The iteration procedure outlined in the previous section was found to yield a convergence of about 1 in 10^4 in 5 iterations, but the calculations were extended up to seven iterations in each case. Values of ϕ for E up to $6k_B\theta_0$ were used for the evaluation of the integrals.

The components of the magnetoconductivity tensor calculated as discussed above are presented for frequencies of 10, 35, 85, and 135 GHz in Figs. 1—4. The values obtained from Drude's theory, i.e., from Eqs. (11) and (12), are also plotted for comparison.

DISCUSSION

We find from Figs. (1)—(4) that the qualitative nature of the variation of the components of the conductivity tensor with magnetic field as obtained from the exact theory and from the Drude theory are the same. The magnitudes of the components are, however, different. The difference is larger for σ_x in comparison to that

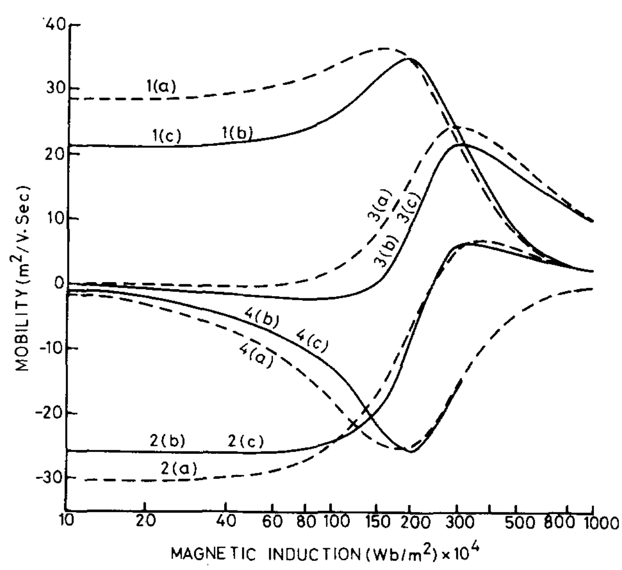

FIG. 2. Same as Fig. 1 except that the frequency is 35 GHz.

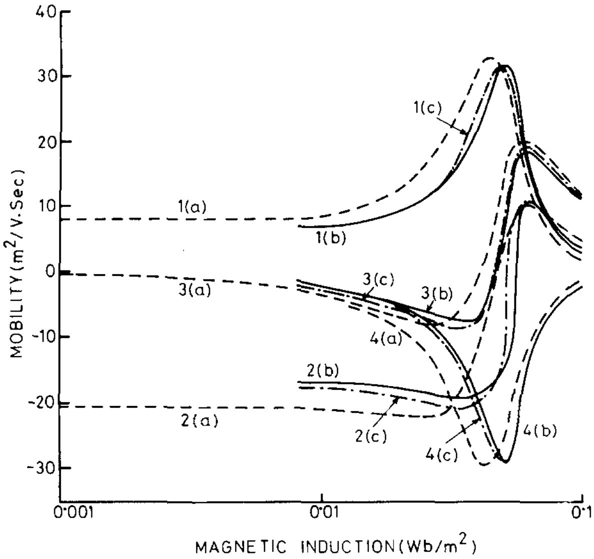

FIG. 3. Same as Fig. 1 except that the frequency is 85 GHz.

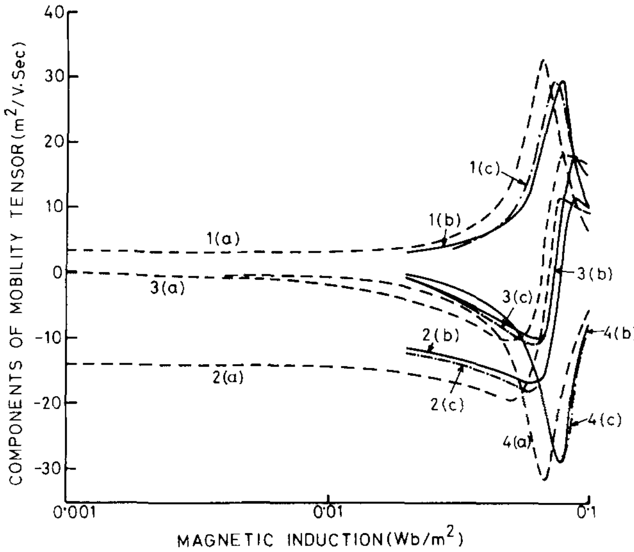

FIG. 4. Same as Fig. 1 except that the frequency is 135 GHz.

for σ_y, and it also varies with frequency, being greatest at 35 MHz. The positions of the critical points, i.e., where the components have a value of zero or where the values are extremum, given by the exact theory also do not agree with those obtained from the Drude theory. We may hence conclude that the Drude theory results are not accurate enough for a meaningful comparison with experiments.

We also find that the two values of E_1, with values of N_I adjusted to obtain the observed value of dc mobility, yield almost the same values of conductivity, particularly at high frequencies. The values differ by about 5% at 10 GHz, but at higher frequencies these are almost identical.

Last, we should point out that our calculations do not indicate any extremum in the value of σ_{xr}, as observed by Eldumiati and Haddad.[2] We find that the change in conductivity with increasing magnetic field should increase monotonically with magnetic field at 10 GHz and attain a limiting value for a magnetic induction of about 0.1 Wb/m^2. The experimental results of Ref. 2, in fact, cannot be explained as being due to electronic conduction if the electron mobility is 60 m^2/V sec or less. A curve with a peak may be obtained if the dc mobility is larger, but the peak then appears at magnetic fields much lower than that at which it has been observed experimentally. The interpretation of the experimental results of Ref. 2 cannot be made in terms of electronic conduction in a homogenous sample, and it is suspected that consideration would be required of the inhomogeneities and striations in the sample and perhaps also of mode mixing in the cavity. Contribution of holes could also be important as the peak in the curves occur near the hole cyclotron resonance field. However, if the experiment is carried out at higher frequencies or with high-mobility samples, the resonance behavior of the conductivity curves should be obtained, which may be analyzed to deduce or confirm the values of the mobility with the method of Ref. 2, but using the numerical method discussed in this paper for the theoretical calculations.

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