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Longitudinal magneto-Seebeck coefficient in a polar semiconductor in quantizing magnetic fields

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The magneto-Seebeck coefficient (Q_{zz}) in InSb is calculated in a quantizing magnetic field. The effect of polar–optical-phonon scattering is incorporated by an iterative solution of the Boltzmann equation abandoning the concept of the relaxation time. Results in the extreme quantum limit show that $|Q_{zz}|$ increases with magnetic field. Band nonparabolicity and elastic scattering mechanisms are found to enhance $|Q_{zz}|$ for a particular high magnetic field. The rise in the lattice temperature, however, reduces $|Q_{zz}|$ in conformity with experiments. The magnetophonon structure of $|Q_{zz}|$ when several Landau levels are occupied, is also studied in the no-broadening limit. The Pavlov and Firsov maxima are obtained at higher magnetic fields than those corresponding to the cyclotron resonance frequency (ω_c) equal to the integral multiple of polar–optical-phonon frequency (ω_0). A prominant pseudoresonance peak is observed at $\omega_c/\omega_0 = 0.5$ which is somewhat lower than for the nonpolar case.

I. INTRODUCTION

Any transport coefficient governed by inelastic optical-phonon scattering is expected to show an oscillatory structure in a quantizing magnetic field. Investigation of these oscillations in the longitudinal magneto-Seebeck coefficient for non-polar semiconductors has been reported by Arora and Peterson.[1] Similar studies for polar semiconductors were made by Pavlov and Firsov[2] on the basis of a relaxation-time formalism. However, the relaxation-time concept is, in general, not applicable for polar–optical-phonon scattering. Experiments on the magnetothermal emf in the longitudinal quantizing magnetic fields for polar semiconductors have been performed.[3,4] Hence it would be worthwhile to establish the magnetophonon effect in the longitudinal Seebeck coefficient for polar-mode scattering in an exact manner, abandoning the relaxation-time formalism. An attempt in this direction has been made in the present paper. The longitudinal magneto-Seebeck coefficient is calculated here by an iterative solution of the Boltzmann equation. The general theory is developed in the Sec. II. The computed results in the extreme quantum limit, when only the lowest Landau level is occupied, are presented in Sec. III. The effect of the scattering mechanisms other than the polar-optical mode, and the influence of the band nonparabolicity are also quantatively assessed in Sec. III. Finally, in Sec. IV the magnetophonon structure of the Seebeck coefficient for polar-mode scattering is given and discussed.

II. GENERAL THEORY

We assume an isotropic parabolic-band semiconductor subjected to a quantizing magnetic field $\vec{B}$ and an electric field $\vec{\mathcal{E}}$, applied along the z direction. The kinetic energy of the conduction electrons may then be written[5]

$$E_n(k_z)=\frac{\hbar^2k_z^2}{2m_g^*}+(n+\tfrac{1}{2})\hbar\omega_c\,, \tag{1}$$

where $\hbar$ is Plank's constant divided by 2π, m_g^* is the carrier effective mass, k_z is the component of the Bloch vector in the z direction, n is the Landau quantum number, and ω_c is the cyclotron frequency.

In the presence of a temperature gradient dT/dz along the z direction, the momentum-distribution function $f_n(k_z)$ for each level obeys the Boltzmann equation

$$v_z\frac{\partial f_n}{\partial E_n}\left\{e\mathcal{E}+\frac{dT}{dz}\left[\frac{E_n}{T}+T\frac{d}{dT}\left(\frac{E_F}{T}\right)\right]\right\}=\frac{\partial f_n}{\partial t}\bigg|_{\text{coll}}\,, \tag{2}$$

where v_z is velocity in the z direction, e is the electron charge, T is the lattice temperature. E_F is the Fermi energy, and $(\partial f_n/\partial t)|_{\text{coll}}$ is the rate of change of f_n due to collisions. We have[5]

$$\frac{\partial f_n}{\partial t}\bigg|_{\text{coll}}=L_nf_n(k_z)-f_n(k_z)/\tau_n(k_z)\,, \tag{3}$$

where

$$L_nf_n(k_z)=\sum_{\alpha'}w(\alpha,\alpha')f_{n'}(k_z') \tag{4}$$

and

$$1/\tau_n(k_z)=\sum_{\alpha'}w(\alpha,\alpha')\,. \tag{5}$$

In the above expressions $w(\alpha,\alpha')$ is the transition probability from state α to α'. Explicit expressions for $\tau_n(k_z)$ and $L_nf_n(k_z)$ for polar-mode scattering are given in Ref. 5. We expand the distribution function for the nth subband as

$$f_n(k_z)=g_n(k_z)+\phi_n(k_z)\,, \tag{6}$$

where $g_n(k_z)$ is the equilibrium distribution function in the nondegenerate limit given by[14]

$$g_n(k_z)=\left(\frac{\hbar^2}{2\pi m_g^* K_B T}\right)^{1/2}\left[1-\exp\left(-\frac{\hbar\omega_c}{K_B T}\right)\right] \times\exp\left(-n\frac{\hbar\omega_c}{K_B T}-\frac{\hbar^2 k_z^2}{2m_g^* K_B T}\right), \tag{7}$$

K_B denoting the Boltzmann constant. The function g_n is so normalized that

$$\sum_n \int g_n\, dk_z = 1\,.$$

Using Eqs. (3), (6), and (7), Eq. (2) reduces to

$$\frac{\phi_n(k_z)}{\tau_n(k_z)}=L_n\phi_n(k_z)-v_z\frac{\partial g_n}{\partial E_n}\left\{e\mathcal{E}+\frac{dT}{dz}\left[\frac{E_n}{T}+T\frac{d}{dT}\left(\frac{E_F}{T}\right)\right]\right\}. \tag{8}$$

When n number of Landau levels are considered, we obtain n number of coupled equations of the form Eq. (8), the coupling occurring through the term $L_n\phi_n$. Each of these equations is solved for ϕ_n by an iterative method similar to that suggested by Rode.[6] In a particular step of iteration, ϕ_n is calculated using the result of the last previous iteration in the term $L_n\phi_n$. In the first step of iteration $L_n\phi_n$ is taken to be zero. The convergence of the scheme is rapid and accurate results are obtained in four to five iterations. A similar method was used by Magnusson[5] in magnetoresistance calculations.

For an evaluation of the magnetothermal emf, we note that the heat and electric currents are given, respectively, by[1]

$$F_z=\gamma_{zz}E^*-\chi_{zz}\frac{dT}{dz} \tag{9}$$

and

$$J_z=\sigma_{zz}E^*-\beta_{zz}\frac{dT}{dz}\,, \tag{10}$$

where

$$E^*=\mathcal{E}+\frac{1}{e}\frac{\partial E_F}{\partial z}\,. \tag{11}$$

The thermo-emf is defined by the relation

$$E^*=Q_{zz}\frac{dT}{dz}\ \text{with}\ J_z=0\,. \tag{12}$$

Using the Onsagar relations we have[1]

$$Q_{zz}=\frac{\beta_{zz}}{\sigma_{zz}}=\frac{1}{T}\frac{\gamma_{zz}}{\sigma_{zz}}\,. \tag{13}$$

To evaluate γ_{zz} and σ_{zz}, one has to determine the heat current and the electric current. Denoting the electron concentration by n_e, and $\hbar k_z$ by p_z, these are expressed as

$$F_z=\frac{n_e}{m^*}\sum_n\langle p_z(H_e-E_F)\rangle \tag{14}$$

and

$$J_z=\frac{n_e e}{m^*}\sum_n\langle p_z\rangle\,, \tag{15}$$

where H_e is electron Hamiltonian and $\langle\ \rangle$ denote the average given by

$$\langle A\rangle=\int A\phi_n(k_z)\,dk_z\,. \tag{16}$$

Using Eq. (16) in Eqs. (14) and (15) and comparing these with Eqs. (9) and (10) we obtain for the coefficients σ_{zz} and γ_{zz}

$$\sigma_{zz}=-\frac{n_e e}{m^*}\sum\int p_z\phi_n^{(0)}(k_z)\,dk_z \tag{17}$$

and

$$\gamma_{zz}=\frac{n_e}{m^*}\sum\int E_n(k_z)p_z\phi_n^{(0)}(k_z)dk_z+\frac{1}{e}E_F\sigma_{zz}\,, \tag{18}$$

where $\phi_n^{(0)}$ is the coefficient of E^* in ϕ_n.

Finding the values of ϕ_n from the iterative solution discussed earlier, we can evaluate σ_{zz} and γ_{zz} from Eqs. (17) and (18), respectively, and hence Q_{zz} from Eq. (13).

III. EXTREME QUANTUM LIMIT CASE

We shall assume here the extreme quantum limit (EQL) case, i.e., the magnetic field is so large that the electrons occupy only the lowest Landau level. The Boltzmann equation for the problem becomes

$$v_z\frac{\partial g_0}{\partial E_0}\left\{e\mathcal{E}+\frac{dT}{dz}\left[\frac{E_0}{T}+T\frac{d}{dT}\left(\frac{E_F}{T}\right)\right]\right\}=L_0\phi_0-\frac{\phi_0}{\tau_0}\,. \tag{19}$$

We shall consider scattering by polar-optical phonons, the acoustical phonons via both deformation potential and piezoelectric coupling, and by ionized centers. All these scattering mechanisms other than the polar-mode scattering are elastic and do not contribute to $L_0\phi_0$. They only affect τ_0 in the manner

$$1/\tau_0=1/\tau_{0\,\mathrm{po}}+1/\tau_{0\,\mathrm{ac}}+1/\tau_{0\,\mathrm{pi}}+1/\tau_{0\,\mathrm{imp}}\,, \tag{20}$$

the abbreviations indicating the particular scattering processes. The expressions for $L_0\phi_0$ and $\tau_{0\,\mathrm{po}}$, $\tau_{0\,\mathrm{ac}}$, $\tau_{0\,\mathrm{pi}}$, and $\tau_{0\,\mathrm{imp}}$ are given in the Refs. 5 and 7. Equation (19) is solved for ϕ_0 by the iterative method described earlier.

We have computed the magneto-Seebeck coef-

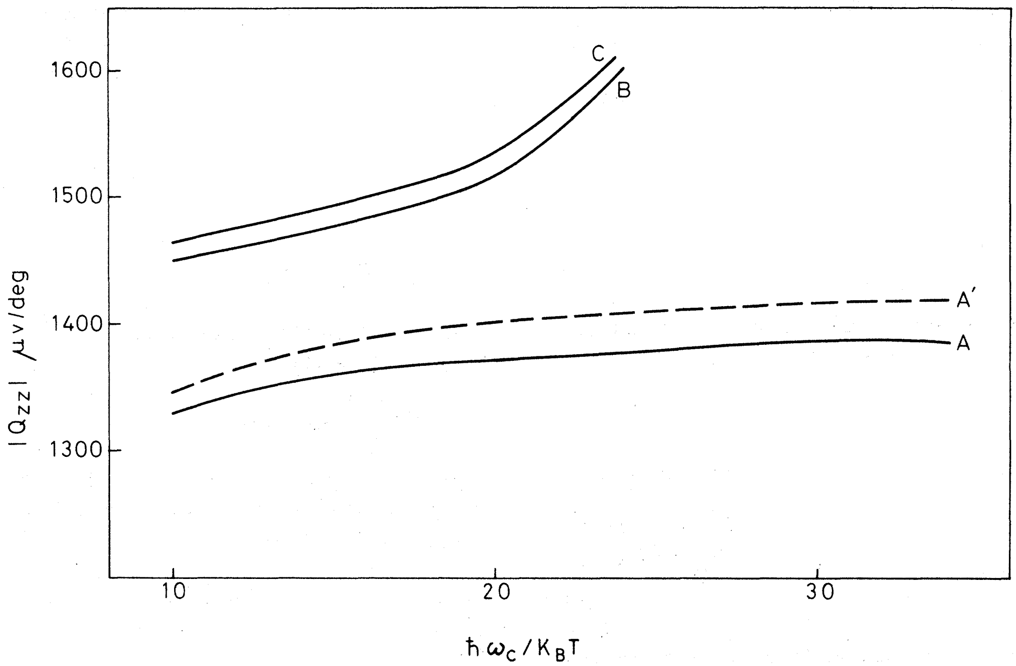

FIG. 1. Variation of the Seebeck coefficients with magnetic field in InSb in EQL. The solid curves are for a parabolic band and the broken curve is for a nonparabolic band. A and A′—polar optical scattering; B—polar optical, deformation-potential acoustic, and piezoelectric scattering; C—polar optical, deformation-potential acoustic, piezoelectric, and ionized-impurity scattering.

ficient from Eqs. (17) and (18), assuming the parameter values of InSb.[8] The effect of different scattering mechanisms on the Seebeck coefficient in the EQL is depicted in Fig. 1 for a lattice temperature of 77 K. It is found that the scattering mechanisms other than polar-mode scattering enhance the thermo-emf, the increase being significant at higher magnetic fields. In Fig. 2 the effect of the temperature on the thermo-emf is exhibited. It is found that with rise in temperature the magnitude of the thermo-emf decreases. This result is corrobrated by experimental results of Puri and Geballe.[4]

We shall now examine the effect of the band nonparabolicity on the magneto-Seebeck coefficient in EQL. The nonparabolic E-k relation[9] is given by

$$E_{0k} = -\tfrac{1}{2}E_g + \tfrac{1}{2}E_g a_0 + \hbar^2 k_z^2/2m_g^* a_0 \,, \quad (21)$$

where E_g is direct band gap and m_g^* is band-edge effective mass. The main contribution to transport parameters comes from small values of k_z. Hence we shall put $k_z = 0$ in the expression for a_0 given by Sharma and Phadke.[9] In this approximation a_0 becomes

$$a_0 = (1 + 2\hbar\omega_c/E_g)^{1/2} \,. \quad (22)$$

The effective mass for nonparabolic band is given by

$$m^* = \left(\frac{1}{\hbar^2 k_z}\frac{dE}{dk_z}\right)^{-1} = m_g^* a_0 \,. \quad (23)$$

It may be noted that as $E_g \to \infty$, $a_0 \to 1$, and we have the classical parabolic band. The expressions for

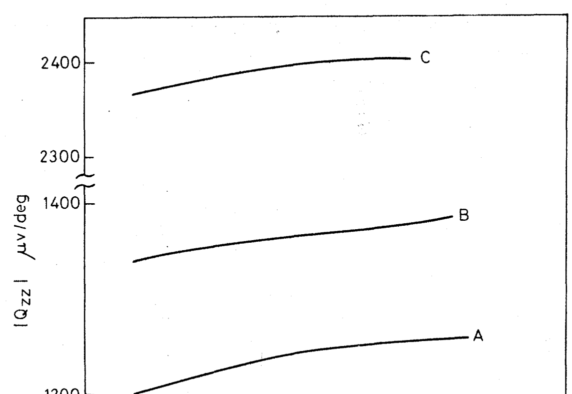

FIG. 2. Variation of the Seebeck coefficient with magnetic field for three different lattice temperature. Curves marked A, B, and C are for the ratios of 2.6, 3.6, and 9.2, respectively, between the polar-phonon Debye temperature and the lattice temperature.

the Fermi energies are different for parabolic and nonparabolic bands and are given in Refs. 1 and 10, respectively. Our results for the nonparabolic band are obtained by replacing m_z^* by m^* and using the appropriate expression for the Fermi energy in our previous calculations.

The Seebeck coefficient for the nonparabolic band and polar-mode scattering is shown in Fig. 1. It is found that band nonparabolicity enhances the magnitude of the thermopower particularly at very high magnetic fields.

IV. MAGNETOPHONON STRUCTURE

In this section we shall present the computed results for the longitudinal magneto-Seebeck coefficients for parabolic band when several Landau levels are occupied. The general theory and formula are given in Sec. II. Figure 3 shows the magnetophonon structure at 77 K for polar–optical-phonon scattering, assuming parameter values of InSb.[8] It is observed that the Pavlov and Firsov maxima dominate and they occur near $\omega_c = n\omega_0$, where n is an integer. However the peaks are somewhat shifted to higher-magnetic fields due to finite temperature. This feature of Pavlov-Firsov maxima is also observed for nonpolar scattering.[11,12] The shift is also revealed in the experiments of Shalyt *et al.*[3] on the longitudinal Seebeck coefficients in InSb.

There are some additional peaks in the magnetophonon structure. These may be identified with the pseudoresonance peaks discussed by Peterson[10,12] for nonpolar semiconductors. This effect arises when different electrons from different Landau levels are scattered with the same momentum k_z to infinite density of states. A prominent pseudoresonance peak in our case is observed at $\omega_c = 0.5\omega_0$. This corresponds to a somewhat lower-magnetic field than predicted for nonpolar case.[11,12] It may be mentioned here that the pseudoresonance structure is not revealed in the magnetothermopower calculations of Pavlov and Firsov.[2] These authors considered only two Landau levels, while the pseudoresonance structure originates from the consideration of a number of Landau levels, as revealed in the present investigation.

It should be further noted that Puri and Geballe[4] have experimentally observed in InSb some kinks in addition to the Pavlov and Firsov maxima. These kinks may be identified with the pseudoresonance structure theoretically demonstrated here.

We would point out that the effects of elastic scattering, level broadening, and nonparabolicity are not included in the present calculations. It is

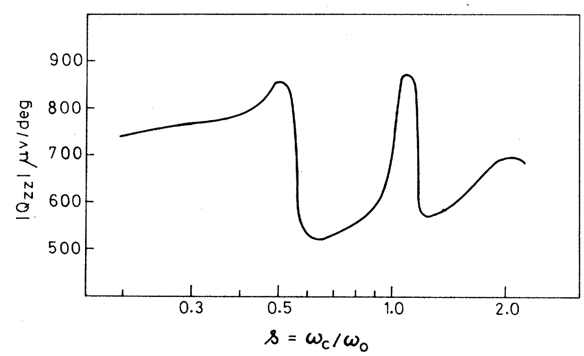

FIG. 3. Magnetophonon structure showing the variation of the Seebeck coefficient with $s(=\omega_c/\omega_0)$ in InSb at 77 K for polar-optical scattering.

found from the EQL results that the effects of nonparabolicity and elastic scattering would be significant only at very high magnetic fields. Since the magnetophonon structure is associated with lower-magnetic fields, the influences of nonparabolicity and elastic scattering are expected to be small. The effects caused by these factors will, however, be qualitatively discussed below.

As the effect of inelastic scattering is somewhat masked by elastic scattering, the inclusion of elastic scattering reduces the sharpness of the peaks and displaces them to higher fields.[1] The effect of the band nonparabolicity is to displace the main maxima and it will also split the pseudoresonance peaks due to unequal spacing of Landau levels.[1]

The effect of Landau-level broadening was examined by Barker.[13,14] It was found that this broadening also shifts the maxima to higher-magnetic fields. The present results in the limit of zero-level broadening coupled with Barker's results indicate that the shifts of peaks to the high-field side observed experimentally arises from the following factors: (i) finite lattice temperature, (ii) elastic scattering, and (iii) level broadening.

V. CONCLUSIONS

The longitudinal magneto-Seebeck coefficients are calculated for polar–optical-phonon scattering abandoning the concept of relaxation time. The effects of the band nonparabolicity and of the elastic-scattering processes on the coefficient in the EQL have been investigated. It is found that the band nonparabolicity and elastic scattering enhance the Seebeck coefficient particularly at high-magnetic fields. Increase of lattice temperature, on the contrary, decreases this coefficient for a given magnetic field.

The magnetophonon structure of the Seebeck coefficient for polar–optical-phonon-scattering shows that the Pavlov and Firsov maxima are somewhat shifted to higher fields. The pseudoresonance structure is also observed in addition to Pavlov and Firsov maxima. But these peaks are found to occur at somewhat lower-magnetic fields than those obtained in the nonpolar case.

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