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Effect of nonparabolicity on Ohmic magnetoresistance in semiconductors

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The effect of nonparabolicity of the conduction band of n-InSb type semiconductors is studied in the framework of the Arora-Peterson density-matrix formalism. To exhibit clearly the effect of nonparabolicity, only the case of elastic electron–acoustic-phonon scattering is considered. Numerical results are presented both for parabolic and nonparabolic models. The nonparabolicity enhances the magnetoresistance, the effect being larger for larger magnetic fields. The Hall coefficient decreases slightly with the increasing magnetic field.

I. INTRODUCTION

Magnetotransport properties are playing a vital role in our understanding of solids. In recent years, these studies have been used as a tool for the investigation of carrier scattering mechanisms as well as band structures. For a low magnetic field of the order of a few kilogauss, the semiclassical Boltzmann transport equation has been very successful. But under quantum conditions, $\hbar\omega_c \gtrsim k_B T$ (where $\omega_c = eB/m^*c$ is the cyclotron frequency of the electron with effective mass m^* in a magnetic field of strength B and T is the temperature of the solid), the quantization of the electron energy levels in a magnetic field becomes important. The semiclassical character of the Boltzmann transport equation then breaks down. A theory for magnetotransport under these conditions based on the solution of Liouville's equation for the density matrix has been worked out by Arora and Miller[1] and applied to the many-valley model of n germanium. This theory was further elaborated by Arora and Peterson[2,3] and was applied to reveal the magnetophonon structure[2] in a parabolic model of n-InSb, where the phonon distribution was assumed to be in equilibrium.

It has been recently shown[4-7] that the nonparabolicity of the conduction band may considerably affect the transport properties of semiconductors in the presence of a magnetic field. For example, Wu and Spector[4] have shown that the nonparabolicity will introduce a magnetic field dependence of ultrasound propagation in a longitudinal magnetic field. The effect of nonparabolicity is to introduce an energy and hence a magnetic-field dependent effective mass of the conduction electrons in the direction of the applied magnetic field. The effective mass increases with the magnetic field, therefore decreasing the conductivity or increasing the magnetoresistance. Sharma and Phadke[5] used the Boltzmann transport equation to show that this alone could lead to nonzero longitudinal magnetoresistance, even if the effect of the magnetic field on the relaxation time is neglected. In a later work,[6] they included the magnetic field dependence of the relaxation time and found that the effect of nonparabolicity is to give rise to a higher longitudinal magnetoresistance in the extreme quantum limit.

Pal and Sharma[7] found that in the extreme quantum limit, the nonparabolicity may give rise to a stronger damping of helicon waves in the transverse configuration. Their work was based on Kubo's formalism[8] which gives divergent results because of the large density of states at the bottom of the quantized Landau subband. Inelasticity of the acoustic phonons was used to offset this divergence. Arora and Peterson[2] by extending the scattering dynamics beyond the strict Born approximation have obtained finite results without use of any *ad hoc* cut-off procedure. The objective in their work was to display the appropriate transport expressions for the simplest case of the parabolic band model. They suggested that the refinements such as the anisotropy of the energy surfaces and nonparabolicity may be incorporated when needed. In this paper we use the Arora-Peterson scattering dynamics to study the effect of nonparabolicity on magnetoresistance for arbitrary values of magnetic field, assuming the phonon distribution to be undisturbed. We apply the results obtained to the nonparabolic model of n-InSb, where nondegenerate electrons are assumed to undergo elastic scattering by acoustic phonons.

In Sec. II, the density matrix based on the work of Arora and Peterson[2] is used to arrive at the expression for the components of the magnetoconductivity tensor. The numerical evaluation and discussion of magnetoresistivity is presented in Sec. III. In general, the nonparabolicity is found to give rise to higher values of magnetoresistance (both longitudinal and transverse) and lower values of the Hall coefficient.

II. MAGNETOCONDUCTIVITY COMPONENTS

The Hamiltonian for the coupled electron-phonon system having a nonparabolic conduction band characterized by an isotropic effective mass m^* and electron charge $-e$ in the presence of a magnetic field B with magnetic potential $\vec{A}=(0, Bx, 0)$ and electric field $\vec{\mathcal{E}}=(\mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z)$ is given by

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}', \tag{2.1}$$

with

$$\mathcal{H}_0=\mathcal{H}_e+\mathcal{H}_L, \tag{2.2}$$

$$\mathcal{H}_e=\tfrac{1}{2}E_g\{1+2[\vec{p}+(e/c)\vec{A}]^2/m^*E_g\}^{1/2}-\tfrac{1}{2}E_g, \tag{2.3}$$

$$\mathcal{H}_L=\sum_q (N_q+\tfrac{1}{2})\hbar\omega_q, \tag{2.4}$$

$$\mathcal{H}'=V+e\vec{\mathcal{E}}\cdot\vec{r}, \tag{2.5}$$

where N_q is the occupation-number operator and ω_q is the angular frequency for phonons of wave vector $\vec{q}$. V is the electron-phonon interaction and E_g is the band gap. The eigenvalues of $\mathcal{H}_e$ of Eq. (2.3) are given by[4]

$$E_{nk}=\tfrac{1}{2}E_g(1+4\epsilon_{nk}/E_g)^{1/2}-\tfrac{1}{2}E_g, \tag{2.6}$$

with

$$\epsilon_{nk}=(n+\tfrac{1}{2})\hbar\omega_c+\hbar^2k_z^2/2m^*, \quad n=0,1,2,\ldots . \tag{2.7}$$

The eigenfunctions $|\alpha\rangle$ of $\mathcal{H}_e$ in terms of harmonic oscillator functions $\phi(x)$ are[2] (normalized in a cube of unit length)

$$|\alpha\rangle=e^{i(k_y y+k_z z)}\phi_n(x+\lambda^2k_y), \tag{2.8}$$

where $\lambda=(\hbar c/eB)^{1/2}$ is the radius of the cyclotron orbit and k stands for (k_y, k_z).

The matrix elements of the density matrix ρ in the Landau representation of Eq. (2.8) are obtained by following the procedure outlined earlier[2,3]:

$$\langle n'k'|\rho|nk\rangle=f_{nk}\delta_{n'n}\delta_{k'k}+\frac{\langle n'k'|[\rho_0,F]|nk\rangle}{E_{n'k',nk}-i\hbar\tau^{-1}_{n'k',nk}}, \tag{2.9}$$

with

$$\langle n'k'|[\rho_0,F]|nk\rangle=\frac{f_{n'k',nk}}{E_{n'k',nk}}\frac{\hbar e}{2}\left[\left(1+\frac{2E_{n'k'}}{E_g}\right)^{-1}+\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}\right]\left[\mathcal{E}_x\left(\frac{\hbar\omega_c}{2m^*}\right)^{1/2}[(n+1)^{1/2}\delta_{n',n+1}-\sqrt{n}\,\delta_{n',n-1}]-\mathcal{E}_y i\left(\frac{\hbar\omega_c}{2m^*}\right)^{1/2}[(n+1)^{1/2}\delta_{n',n+1}+\sqrt{n}\,\delta_{n',n-1}]-\mathcal{E}_z i\frac{\hbar k_z}{m^*}\delta_{n'n}\right]\delta_{k'k}, \tag{2.10}$$

$$\tau^{-1}_{n'k',nk}=\tfrac{1}{2}(\tau^{-1}_{n'k'}+\tau^{-1}_{nk}), \tag{2.11}$$

$$f_{n'k',nk}=f_{n'k'}-f_{nk}, \tag{2.12}$$

$$E_{n'k',nk}=E_{n'k'}-E_{nk}. \tag{2.13}$$

Here f_{nk} is the equilibrium distribution function of nondegenerate electrons

$$f_{nk}\simeq e^{(\zeta-E_{nk})/k_BT}, \tag{2.14}$$

with Fermi energy ζ given by (see Appendix)

$$e^{\zeta/k_BT}\simeq\frac{n_e}{2a}\left(\frac{2\pi\hbar^2}{m^*k_BT}\right)^{3/2}\times\left\{\sum_{n=0}^{\infty}\left[\exp\left(\frac{-\frac{1}{2}E_g(a_n-1)}{k_BT}\right)\right]a_n^{1/2}\right\}^{-1}, \tag{2.15}$$

where n_e is the number of conduction electrons and

$$a_n=[1+4(n+\tfrac{1}{2})\hbar\omega_c/E_g]^{1/2}, \tag{2.16}$$

$$a=\hbar\omega_c/k_BT. \tag{2.17}$$

The relaxation time τ_{nk} of Eq. (2.11) for the electron–acoustic-phonon scattering is given by

$$\tau^{-1}_{nk}=A_{ac}\left(1+\frac{4\epsilon_{nk}}{E_g}\right)^{1/2}\times{\sum_{n'}}'[\epsilon_{nk}-(n'+\tfrac{1}{2})\hbar\omega_c]^{-1/2}, \tag{2.18}$$

with

$$A_{ac}=\frac{E_1^2k_BT(2m^*)^{1/2}}{2\pi\hbar^2\rho_d u^2\lambda^2}, \tag{2.19}$$

where E_1 is the deformation potential constant, ρ_d is the crystal density, and u is the average sound speed for longitudinal phonons. It may be noted that the energy shift term vanishes when elastic acoustic phonon scattering is considered.

The matrix elements of the one-electron current operator obtained from the Heisenberg equation of motion

$$\vec{j}=-e\vec{v}=-(ie/\hbar)[\mathcal{H},\vec{r}], \tag{2.20}$$

are given by

$$\langle n'k'|j_x|nk\rangle = -\frac{ie}{2}\left(\frac{\hbar\omega_c}{2m^*}\right)^{1/2} \times\left[\left(1+\frac{2E_{n'k'}}{E_g}\right)^{-1}+\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}\right] \times[(n+1)^{1/2}\delta_{n',n+1}-\sqrt{n}\,\delta_{n',n-1}]\delta_{k'k}, \quad (2.21)$$

$$\langle n'k'|j_y|nk\rangle = -\frac{e}{2}\left(\frac{\hbar\omega_c}{2m^*}\right)^{1/2} \times\left[\left(1+\frac{2E_{n'k'}}{E_g}\right)^{-1}+\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}\right] \times[(n+1)^{1/2}\delta_{n',n+1}+\sqrt{n}\,\delta_{n',n-1}]\delta_{k'k}, \quad (2.22)$$

$$\langle n'k'|j_z|nk\rangle = -e\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}\frac{\hbar k_z}{m^*}\delta_{n'n}\delta_{k'k}. \quad (2.23)$$

The components of the magnetoconductivity tensor $\vec{\sigma}$ are then obtained by

$$\langle\vec{j}\rangle = \mathrm{Tr}(\rho\hat{j}) \equiv \vec{\sigma}\cdot\vec{\mathcal{E}}. \quad (2.24)$$

Using the density matrix of Eq. (2.9) and Eqs. (2.21)–(2.24), we get for the magnetoconductivity tensor the results

$$\vec{\sigma} = \begin{pmatrix} \sigma_1 & -\sigma_2 & 0 \\ \sigma_2 & \sigma_1 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}, \quad (2.25)$$

with

$$\sigma_1 = -\left(\frac{\hbar^3 e^2\omega_c}{4m^*}\right) \times\sum_{nks}\left[\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}+\left(1+\frac{2E_{(n+1)k}}{E_g}\right)^{-1}\right]^2 \times(n+1)\frac{f_{nk,(n+1)k}}{E_{nk,(n+1)k}}\frac{\tau^{-1}_{nk,(n+1)k}}{E^2_{nk,(n+1)k}+\hbar^2\tau^{-2}_{nk,(n+1)k}}, \quad (2.26)$$

$$\sigma_2 = \frac{\hbar^2 e^2\omega_c}{4m^*} \times\sum_{nks}\left[\left(1+\frac{2E_{nk}}{E_g}\right)^{-1}+\left(1+\frac{2E_{(n+1)k}}{E_g}\right)^{-1}\right]^2 \times(n+1)f_{nk,(n+1)k}\frac{1}{E^2_{nk,(n+1)k}+\hbar^2\tau^{-2}_{nk,(n+1)k}}, \quad (2.27)$$

$$\sigma_3 = \frac{e^2}{k_BT}\sum_{nks}f_{nk}\left(1+\frac{2E_{nk}}{E_g}\right)^{-2}\left(\frac{\hbar k_z}{m^*}\right)^2\tau_{nk}, \quad (2.28)$$

where s stands for two spin states.

These components reduce to those obtained for the parabolic case[2] when limit $E_g\to\infty$ is made. Obviously, the transverse components are nondivergent for $\tau_{nk}\to 0$, when electrons make transition to the bottom of a Landau subband ($k_z\to 0$). When limit $B\to 0$ is made, the conductivity tensor of Eq. (2.25) becomes diagonal with all diagonal components equal to[6]

$$\sigma(0) = \frac{2n_e e^2}{3m^*k_BT}\left(\int_0^\infty \gamma^{3/2}\gamma'^{-2}\tau(0)e^{-E/k_BT}dE\right)\Big/\left(\int_0^\infty \gamma^{1/2}\gamma' e^{-E/k_BT}dE\right), \quad (2.29)$$

where the zero-field relaxation time $\tau(0)$ for electron-acoustic-phonon scattering is given by

$$\tau(0)^{-1} = \sqrt{2}\,E_1^2 m^{*3/2}k_BT\gamma^{1/2}\gamma'/\pi\rho_d u^2\hbar^4, \quad (2.30)$$

with

$$\gamma = E(1+E/E_g), \quad (2.31)$$

$$\gamma' = 1+2E/E_g. \quad (2.32)$$

Following the transformation and resummation technique used earlier,[3,9,10] we have the expressions for σ_1, σ_2, and σ_3:

$$\sigma_1 = c_1\int_0^1 dy\sum_{N=0}^\infty\left(e^{-B_N(y)a\epsilon_g/2}-e^{-B_{N+1}(y)a\epsilon_g/2}\right)\left[\tfrac{1}{2}B_N^{-1}(y)+\tfrac{1}{2}B_{N+1}^{-1}(y)\right]^2\left(N+1+\sqrt{y}\sum_{m=1}^N\frac{N-m+1}{(m+y)^{1/2}}\right)T_N(y)\Big/F_N(y)D_N(y), \quad (2.33)$$

$$\sigma_2 = c_2\int_0^1 dy\,\sqrt{y}\sum_{N=0}^\infty\left(e^{-B_N(y)a\epsilon_g/2}-e^{-B_{N+1}(y)a\epsilon_g/2}\right)\left[\tfrac{1}{2}B_N^{-1}(y)+\tfrac{1}{2}B_{N+1}^{-1}(y)\right]^2\left(N+1+\sqrt{y}\sum_{m=1}^N\frac{N-m+1}{(m+y)^{1/2}}\right)\Big/D_N(y), \quad (2.34)$$

$$\sigma_3 = c_3\int_0^1 dy\,\sqrt{y}\sum_{N=0}^\infty e^{-B_N(y)a\epsilon_g/2}\sum_{m=0}^N(m+y)^{1/2}B_N^{-3}(y), \quad (2.35)$$

with

$$\epsilon_g = E_g/\hbar\omega_c\,, \tag{2.36}$$

$$B_N(y) = [1 + 4(N + \tfrac{1}{2} + y)/\epsilon_g]^{1/2}\,, \tag{2.37}$$

$$F_N(y) = B_N(y) - B_{N+1}(y)\,, \tag{2.38}$$

$$T_N(y) = B_N(y)\left(1 + \sqrt{y}\sum_{m=1}^{N}(m+y)^{-1/2}\right) + B_{N+1}(y)\left(1 + \sqrt{y}\sum_{m=1}^{N+1}(m+y)^{-1/2}\right), \tag{2.39}$$

$$D_N(y) = \tfrac{1}{4}y\epsilon_g^2 F_N^2(y) + A_{ac}^2 T_N^2(y)/4\hbar\omega_c^3\,, \tag{2.40}$$

$$c_1 = cA_{ac}(\hbar\omega_c)^{1/2}/\epsilon_g\,, \tag{2.41}$$

$$c_2 = c\hbar\omega_c^2 \tag{2.42}$$

$$c_3 = \frac{4\sqrt{2}\, e^2 e^{(\zeta + E_g/2)/k_BT} a(\hbar\omega_c)^{1/2}}{m^*\lambda^3 A_{ac} 4\pi^2}\,, \tag{2.43}$$

$$c = \frac{2\sqrt{2}\, e^2 e^{(\zeta + E_g/2)/k_BT}}{m^*\lambda^3\omega_c^3\hbar\, 4\pi^2}\,. \tag{2.44}$$

III. RESULTS AND DISCUSSION

The experimentally measurable physical quantities are $\Delta R_{xx}/R(0)$ (transverse magnetoresistance), $\Delta R_{zz}/R(0)$ (longitudinal magnetoresistance), and normalized Hall coefficient R_H/R_H^0, where $R(0) = [\sigma(0)]^{-1}$ is the zero-field resistivity of the sample and $R_H^0 = -1/n_e ec$ is the high-field Hall coefficient for parabolic semiconductors. In terms of σ_1, σ_2, and σ_3, these can be written

$$\Delta R_{xx}/R(0) = \sigma_1\sigma(0)/(\sigma_1^2 + \sigma_2^2)\,, \tag{3.1}$$

$$\Delta R_{zz}/R(0) = \sigma(0)/\sigma_3\,, \tag{3.2}$$

$$R_H/R_H^0 = n_e ec\sigma_2/B(\sigma_1^2 + \sigma_2^2)\,. \tag{3.3}$$

The numerical results for these physically observable quantities are shown in Fig. 1. The parameters used in these calculations are essentially those used earlier[3]: $E_1 = 30$ eV, $m^* = 0.016$, $\rho_d = 5.77$ g/cm^3, $u = 3.7\times10^5$ cm/sec, $T = 77°$K, and $E_g = 0.265$ eV. The numerical value of E_1 is not very well established in literature. The values ranging from 7 to 30 eV are usually quoted.[11] Tsidilkovskii and Demchuk[12] conclude strongly that $E_1 = 30$ eV. We will, therefore, use this value in our calculations.

The expression for longitudinal magnetoresistance when reduced to the extreme quantum limit are quite similar to those obtained by Phadke and Sharma[6] by using the Boltzmann transport equation. The detailed comparison with these works was not possible as they analyze their results in the extreme quantum limit only. But, we arrive at the same qualitative conclusion that nonparabolicity enhances the longitudinal magnetoresistance. In the extreme quantum limit the approximate dependence of the effective mass in a direction parallel to the magnetic field is given by[4,6]

$$m^*(B) = m^*(0)(1 + 2\hbar\omega_c/E_g)^{1/2}\,. \tag{3.4}$$

This increase in effective mass with the magnetic field reduces the conductivity and hence increases the magnetoresistance.

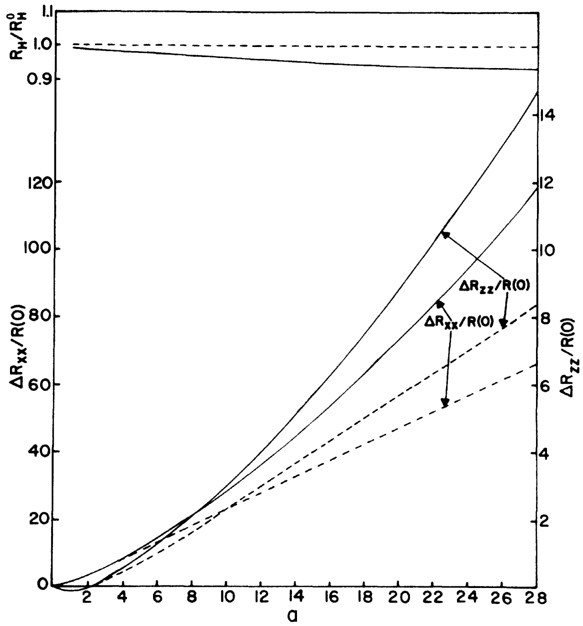

FIG. 1. Magnetoresistance ratio and normalized Hall coefficient vs $a = \hbar\omega_c/k_BT$ for the nonparabolic band model (solid curves) and parabolic band model (dashed curves) of n-type InSb at temperature $T = 77$ K, assuming electron-acoustic phonon scattering to be the dominant mechanism of scattering.

The expressions for transverse magnetoresistance were not expected to agree with those obtained earlier.[7] As stated earlier, these works are based on Kubo's formalism[8] which gives divergent results, the divergence difficulty becoming more apparent when electrons tend to move slowly in the direction of strong magnetic field. The reasons for this divergence difficulty and disagreements with older theories were carefully explained by Arora and Peterson,[2] where the results obtained were shown to reduce to those obtained from the Boltzmann transport equation in the low-field limit. The numerical results for the transverse magnetoresistance also show an enhancement due to nonparabolicity, the enhancement increasing with increasing values of the applied magnetic field. The results for Hall coefficient are quite interesting. Earlier theoretical works[7] show that the normalized Hall coefficient R_H/R_H^0 is close to unity independent of scattering. But, our results indicate that nonparabolicity will decrease this

Hall coefficient. This is in agreement with the low field work of Nag and Dutta,[11] where the Hall effect is found to decrease with magnetic field.

For low magnetic fields ($\hbar\omega_c \ll E_g$), the effect of nonparabolicity is quite small. When $\hbar\omega_c \sim E_g$, there is a marked increase in magnetoresistance, both transverse and longitudinal. In summary, we have shown for a very simple case of elastic acoustic phonon scattering that nonparabolicity may have a pronounced effect on magnetotransport properties, the effect increasing with the increasing values of magnetic field.

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APPENDIX

In this appendix, we calculate the Fermi energy expression of Eq. (2.15) from the normalization condition

$$\sum_{nk_yk_zs} f_{nk} = n_e , \tag{A1}$$

where f_{nk} is given by Eq. (2.14).

The electron energy E_{nk} of Eq. (2.6) can be approximated[4] by the expression

$$E_{nk} \simeq -\tfrac{1}{2}E_g + \tfrac{1}{2}E_g a_n + \hbar^2 k_z^2/2m^* a_n , \tag{A2}$$

since

$$(\hbar k_{z\,\max})^2/2m^* \simeq k_B T \ll E_g \tag{A3}$$

for InSb at temperature $T = 77$ K. [In Eq. (A2), a_n is given by Eq. (2.16).]

The summation over spin states gives a factor of 2, and the summations over k_y and k_z can be replaced by integrations

$$\sum_{k_yk_z} \to \frac{1}{(2\pi)^2}\int_{-\infty}^{+\infty} dk_z \int_{-1/2\lambda^2}^{+1/2\lambda^2} dk_y . \tag{A4}$$

The limits over k_y result from the fact that the center of the cyclotron orbit, $x_k = -\lambda^2 k_y$, must reside within the crystal ($-\frac{1}{2} \leq \lambda^2 k_y \leq +\frac{1}{2}$), assumed to be a unit cube. Since f_{nk} is independent of k_y, and is an even function of k_z, we can write Eq. (A1) as

$$e^{\zeta/k_BT}\sum_n e^{-E_g(a_n-1)/2k_BT}\frac{4}{(2\pi\lambda)^2} \times \int_0^\infty dk_z\, e^{-\hbar^2k_z^2/2m^*a_nk_BT} = n_e . \tag{A5}$$

Evaluating the integral over k_z and writing $\lambda = (\hbar/m\omega_c)^{1/2}$ leads us to Eq. (2.15).

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