Ohmic magnetoresistance for inelastic acoustic phonon scattering in semiconductors

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The effect on both the longitudinal and the transverse magnetoresistance of a parabolic semiconductor with isotropic effective mass of the inelasticity of the acoustic phonons is studied in the framework of the Arora-Peterson density-matrix formalism. To exhibit clearly the effect of inelasticity, the numerical computations are done for a model where electrons are assumed to interact strongly with phonons of wave vector $q \sim 1/\lambda$, where λ is the radius of the cyclotron orbit. It is found that inelasticity changes the transverse magnetoresistance dramatically, while the Hall coefficient and the longitudinal magnetoresistance remain essentially unchanged.

I. INTRODUCTION

The study of the effect of a magnetic field on transport properties yields useful information about the role various scattering interactions are expected to play in solids. The transverse and longitudinal magnetoresistance are the two most investigated properties in which the effect of a magnetic field is exhibited. Although the Boltzmann transport equation has been quite successful in interpreting longitudinal magnetoresistance, the case of transverse magnetoresistance has not been easy to analyze,¹ especially for strong magnetic fields. Reviews of earlier theoretical works are given by Kubo $et a {l_{\circ}}^2$ and Roth and Argyres.³ Although consistent in their results, these works had the unpleasant drawback of divergent results for the transverse case. To offset this divergence, various cutoff mechanisms have been suggested.^{2,3}

One of the cutoff mechanisms which has been considered to be important among others is the inelasticity of the acoustic phonons. Kubo et al.² considered in detail the effect of inelasticity of the acoustic phonons in the quantum limit. The cutoff corresponds to the energy of a phonon whose wavelength is comparable to that of the radius of the cyclotron orbit. Their approximation was based on the assumption that $q^2/q_z^2 \gg 1$, so that $q \sim q_1 \sim 1/\lambda$, where $\lambda = (\hbar c/eB)^{1/2}$ is the radius of the cyclotron orbit in a magnetic field of strength B, q is the wave number of the phonon, and $q_{\perp} = (q_x^2 + q_y^2)^{1/2}$ is the transverse component of the wave number. They also analyzed the results when q_1 was not assumed to be constant. Pal and Sharma⁴ used the cutoff corresponding to $q_{\perp}\!\sim\!1/\lambda$ to study the damping of helicon waves in the framework of Kubo's formalism. Cassiday and Spector⁵ incorporated the inelasticity of the acoustic phonons in the magnetoconductivity expression obtained by other workers.^{2,3} They also included in their work the assumption $q_1^2/q_z^2 > 1$ in the high-temperature approximation, but did not replace q_{\perp} by $1/\lambda_{\circ}$. The expression for the transverse magnetoresistivity was

obtained in terms of integrals of Bessel functions. In the development of a numerical computation, they assumed that the maximum values of the wave vector for phonons that interact with the electrons are of order $q_T = (2m^*k_BT/\hbar^2)^{1/2}$ when $\hbar\omega_c/k_BT < <1$ and of order $1/\lambda$ when $\hbar\omega_c/k_BT > 1$, where $\omega_c = eB/m^*c$ is the frequency of the cyclotron motion of an electron with isotropic effective mass m^* . The primary purpose of all the above works has been to obtain a finite expression for the magneto-conductivity by including inelasticity.

It has been demonstrated by Arora and Peterson¹ that divergence could be eliminated by extending the scattering dynamics beyond the strict Born approximation. Their conclusion was that no artificial cutoff mechanism was necessary for removal of divergence. Other details like phonon drag, inelasticity, etc., could be incorporated when deemed important. In the present work to exhibit clearly the effect of inelasticity of the acoustic phonons, we use the magnetoconductivity expressions arrived at by Arora and Peterson.¹ To make the theory simple and comparison with other works possible, we will make the same simplifying assumption that $1/\lambda$ is the wave number of phonons which interact most strongly with electrons, and thus $\hbar u/\lambda$ is the typical energy of an acoustic phonon, as has been considered by others.^{2,4}

In Sec. II, the magnetoconductivity expressions of Arora and Peterson are given for the case of acoustic-phonon scattering and then modified to include the inelasticity of the acoustic phonons. Numerical results are presented in Sec. III with the conclusion that although the longitudinal magnetoresistance and the Hall coefficient remain essentially unaffected by inelasticity, this may dramatically change the value of the transverse magnetoresistance.

II. THEORETICAL DEVELOPMENT

The Hamiltonian describing an electron system interacting with the lattice is⁶

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$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_L + e \,\mathcal{E} \cdot \vec{\mathbf{r}} + V, \qquad (2.1)$$

where $\vec{\mathbf{r}}$ is the carrier position, $\vec{\mathcal{S}}$ is the applied electric field, \mathcal{H}_L is the lattice Hamiltonian, and *V* is the electron-lattice interaction, assuming electron-acoustic-phonon to be the dominant mechanism of scattering:

$$V = \sum_{\mathbf{q}} C(q) b_{\mathbf{q}} e^{i \mathbf{q} \cdot \mathbf{r}} + \text{Hermitian conjugate, (2.2)}$$

with

$$|C(q)|^{2} = E_{1}^{2} \hbar q^{2}/2\rho \Omega \omega_{q}$$
, (2.3)

where E_1 is deformation potential energy, and ω_q is the frequency of a phonon of wave vector \vec{q} , customarily taken to be uq with u the directionally averaged longitudinal sound velocity, C(q) is the coupling coefficient, b_q is a phonon destruction operator, Ω is the volume of the sample, and ρ its mass density. The electronic Hamiltonian \mathcal{K}_0 for an electron of momentum \vec{p} , isotropic mass m^* , charge -e (e > 0) in a magnetic field \vec{B} in the z direction is given by

$$\mathcal{H}_{0} = \left[p_{\mathbf{x}}^{2} + (p_{\mathbf{y}} + m^{*}\omega_{c}x)^{2} + p_{\mathbf{z}}^{2} \right] / 2m^{*} , \qquad (2.4)$$

where ω_{σ} is the cyclotron frequency of an electron. The energy eigenvalues of \mathcal{H}_0 are

$$\epsilon_{nk} = (n + \frac{1}{2})\hbar \omega_c + \hbar^2 k_z^2 / 2m^*$$
, $n = 0, 1, 2, ..., (2.5)$

corresponding to eigenfunctions

$$\psi_n(k_y, k_z, \dot{\mathbf{r}}) = \varphi_n(x - x_k) \exp[i(k_y y + k_z z)] / (L_y L_z)^{1/2},$$
(2.6)

where $\varphi_{\mathbf{n}}$ are harmonic-oscillator functions centered at

$$x_k = -\lambda^2 k_y , \qquad (2.7)$$

 $\lambda = (\hbar c/eB)^{1/2}$ being the length of the cyclotron orbit. L_{y} and L_{z} are sample dimensions.

The magnetoconductivity tensor σ for a parabolic semiconductor for the simple case of acoustic phonon scattering is given by¹

$$\underline{\sigma} = \begin{pmatrix} \sigma_1 & -\sigma_2 & 0 \\ \sigma_2 & \sigma_1 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix} , \qquad (2.8)$$

where

$$\sigma_{1} = \frac{e^{2}}{m^{*}} \left(1 - e^{-s}\right) \sum_{nk \neq s} (n+1) f_{n}^{0}(k) \frac{\tau_{n,n+1}^{-1}(k)}{\omega_{c}^{2} + \tau_{n,n+1}^{-2}(k)} , \quad (2.9)$$

$$\sigma_2 = \frac{e^2}{m^*} (1 - e^{-s}) \sum_{nk*} (n+1) f_n^0(k) \frac{\omega_c}{\omega_c^2 + \tau_{n,n*1}^{-2}(k)} , \qquad (2.10)$$

$$\sigma_{3} = \frac{e^{2}\hbar^{2}}{m^{*2}k_{B}T} \sum_{nk\pm} k_{z}^{2}\tau_{nn}(k)f_{n}^{0}(k) , \qquad (2.11)$$

with

$$f_n^0(k) = n_e \left(\frac{2\pi\hbar^2}{m^* k_B T}\right)^{3/2} \frac{\sinh(s/2)}{s} e^{-\epsilon_{nk}/k_B T} , \qquad (2.12)$$

$$s = \hbar \omega_c / k_B T , \qquad (2.13)$$

$$1/\tau_{n,n+1}(k) = \frac{1}{2}1/\tau_n(k) + \frac{1}{2}1/\tau_{n+1}(k) . \qquad (2.14)$$

All notations are same as those used in Ref. 1. The relaxation time $\tau_n(k)$ can be obtained from the equation

$$\frac{1}{\tau_{n}(k)} = \frac{2\pi}{\hbar} \sum_{n'k' \pm} |\langle nk | V | n'k' \rangle|^{2} \\ \times \delta(\epsilon_{n'k'} - \epsilon_{nk} \pm \hbar \omega_{q}) , \qquad (2.15)$$

where $\pm \hbar \omega_q$ is the energy of a phonon involved in emission and absorption of an acoustic phonon. With the use of potential V of Eq. (2.2), we obtain

$$\frac{1}{\tau_{n}(k)} = \frac{2\pi}{\hbar} \sum_{n'k'_{q}} |C(q)|^{2} \delta_{k'_{y},k_{y}+q_{y}} \delta_{k'_{g},k_{g}+q_{g}} |J_{n'n}|^{2} \times [\overline{n}_{q} \delta(\epsilon_{n'k'} - \epsilon_{nk} + \hbar\omega_{q}) + (\overline{n}_{q} + 1) \delta(\epsilon_{n'k'} - \epsilon_{nk} - \hbar\omega_{q})], \qquad (2.16)$$

with

$$J_{n'n} = \int_{-\infty}^{+\infty} dx \exp(iq_x x) \varphi_n^* (x + \lambda^2 k_y + \lambda^2 q_y) \varphi_n (x + \lambda^2 k_y)$$
(2.17)

 \overline{n}_q is the equilibrium phonon number given by Bose-Einstein distribution, which in the high-temperature approximation ($\hbar\omega_q \ll k_B T$) can be approximated as

$$\overline{n}_{g} \approx \overline{n}_{g} + 1 \approx k_{B} T / \hbar \omega_{g} . \qquad (2.18)$$

Summing over k'_y and q_z , and converting summations into integrations, we get

$$\frac{1}{\tau_{n}(k)} = \sum_{n'} \frac{E_{1k_{B}}^{2}T}{2\pi\hbar\rho u^{2}} \int_{0}^{\infty} dk'_{z} \int_{0}^{\infty} dq_{\perp} q_{\perp} |J_{n'n}|^{2} \times \left[\delta(\epsilon_{n'k'} - \epsilon_{nk} + \hbar\omega_{q}) + \delta(\epsilon_{n'k'} - \epsilon_{nk} - \hbar\omega_{q})\right].$$
(2.19)

The presence of $\hbar \omega_q \approx \hbar u [q_1^2 + (k_z' - k_z)^2]^{1/2}$ in the δ function makes it quite difficult for us to integrate. Some simplification is therefore necessary. As discussed in the Introduction, we follow Kubo *et al.* to make an approximation

$$q_{\perp}^2/q_{z}^2 \gg 1$$
, (2.20)

which will make $\hbar \omega_q = \hbar u q_\perp$. Now, we make the simplifying assumption that the phonons which interact strongly with electrons have wave numbers of the order of $1/\lambda$. This assumption is justifiable on the ground that for $n' \neq n$, ω_q can be neglected on the ground that $\omega_q \ll \omega_c$, but when n = n' (intralevel scattering), the integrand of integral involving q_\perp has a maximum at $q_\perp \sim 1/\lambda$ (for n = n' = 0, $|J_{n'n}|^2 \sim e^{-q_\perp^2/2\lambda^2}$). Therefore, it does not look like too crude an approximation if we use for $\hbar \omega_o$, the aver-

age phonon energy:

$$\langle \hbar \omega_{q} \rangle = \gamma \hbar u / \lambda ,$$
 (2.21)

where γ is a parameter which is zero for elastic scattering and describes the extent of inelasticity of the collision. This approximation will further allow us to use the property⁷ of $J_{n'n}$:

$$\int_{0}^{\infty} d\zeta \left| J_{n'n}(\zeta) \right|^{2} = 1 , \qquad (2.22)$$

to get a simplified expression for $1/\tau_n(k)$:

$$\frac{1}{\tau_n(k)} = \frac{1}{2} A_{ac} \sum_{n'} \left\{ \left[\epsilon_{nk} - (n' + \frac{1}{2}) \hbar \omega_c - \gamma \hbar u / \lambda \right]^{-1/2} + \left[\epsilon_{nk} - (n' + \frac{1}{2}) \hbar \omega_c + \gamma \hbar u / \lambda \right]^{-1/2} \right\}, \quad (2.23)$$

with

$$A_{\rm ac} = E_1^2 k_B T (2m^*)^{1/2} / 2\pi \rho \hbar^2 u^2 \lambda^2 , \qquad (2.24)$$

where prime on the summation means that all terms of the form $x^{-1/2}$, where x < 0 are excluded.

III. RESULTS AND DISCUSSION

The experimentally observable properties are $\Delta \rho_{xx} / \rho(0)$ (transverse magnetoresistance), $\Delta \rho_{zz} / \rho(0)$ (longitudinal magnetoresistance) and the Hall coefficient $R_H = R_{yx} / B$, which in terms of σ_1 , σ_2 , and $\sigma_3 \text{ are}^8$

 $\Delta \rho_{\rm xx} / \rho(0) = \sigma_1 / (\sigma_1^2 + \sigma_2^2) \rho(0) - 1 , \qquad (3.1)$

$$\Delta \rho_{ss} / \rho(0) = 1 / \sigma_3 \rho(0) - 1 , \qquad (3.2)$$

$$R_{H} = -\sigma_{2} / (\sigma_{1}^{2} + \sigma_{2}^{2})B , \qquad (3.3)$$

where $\rho(0)$, the zero-field resistivity, is given by⁸

$$\rho(0) = 3(2\pi m * k_B T)^{1/2} m *^2 E_1^2 k_B T / 4 n_e e^2 \pi \hbar^4 \rho u^2.$$

(3.4)

To facilitate numerical computation, we use the transformation and resummation technique used earlier⁸:

$$\sigma_{1} = C_{1} \int_{0}^{1} dy \ e^{-sy} \sum_{N=0}^{\infty} e^{-Ns} \left(\sum_{m=0}^{N} \frac{N-m+1}{(m+y)^{1/2}} \right) \\ \times \frac{G_{N}(y)}{\hbar \omega_{c}^{2} + A_{ac}^{2} G_{N}^{2}(y)} , \qquad (3.5)$$

$$\sigma_{2} = C_{2} \int_{0}^{1} dy \ e^{-sy} \sum_{n=0}^{\infty} e^{-Ns} \left(\sum_{m=0}^{N} \frac{N-m+1}{(m-y)^{1/2}} \right)$$

$$\times \frac{1}{\hbar\omega_{o}^{3} + A_{2o}^{2}G_{N}^{2}(y)}, \qquad (3.6)$$

$$\sigma_3 = C_3 \int_0^1 dy \ e^{-sy} \sum_{N=0}^\infty \ e^{-Ns} \sum_{m=0}^N (m+y)^{1/2} \xi_N^{-1}(y) \ , \quad (3.7)$$

with

$$\xi_{N}(y) = \frac{1}{2} \sum_{N'=-\infty}^{N} \left[(N' + y + P)^{-1/2} + (N' + y - P)^{-1/2} \right],$$
(3.8)

$$G_N(y) = \xi_N(y) + \frac{1}{4} \left[(N+1+y+P)^{-1/2} + (N+1+y+P)^{-1/2} \right]$$

$$P = \gamma u / \lambda \omega_{c} , \qquad (3.10)$$

$$C_1 = CA_{\rm ac} (\hbar\omega_c)^{1/2} , \qquad (3.11)$$

$$C_0 = C\hbar\omega_{\rm e}^2 \,. \tag{3.12}$$

$$C_{3} = 2^{5/2} e^{2} m^{*1/2} s \omega_{c}^{2} e^{-s/2} e^{\xi/k_{B}T} / 4A_{ac} \pi^{2} \hbar , \qquad (3.13)$$

$$C = 2^{3/2} e^2 e^{-s/2} (1 - e^{-s}) e^{\zeta/k_B T} / 4\pi^2 m^* \lambda^3, \qquad (3.14)$$

$$e^{\zeta/k_BT} = n_e (2\pi\hbar^2/m^*k_BT)^{3/2}\sinh(\frac{1}{2}s)/s. \qquad (3.15)$$

The parameters used are those appropriate to a parabolic model of *n*-InSb.⁸ The numerical results are shown in Fig. 1. The longitudinal magnetoresistance $\Delta \rho_{xx} / \rho(0)$ remains essentially unaffected by the inelasticity of the acoustic phonons, whereas the transverse magnetoresistance changes dramatically with inelasticity, decreasing with increasing value of the inelasticity parameter γ . The high-field Hall coefficient (not shown on figure) retains its value of $1/n_ec$ indpendent of scattering or inelasticity. As discussed in Sec. II, the main contribution of inelasticity comes from intralevel scattering (n = n'), which for slowly moving electrons $(k_x \approx 0)$ in the direction of the magnetic field is given by

$$[1/\tau_n(k_z=0)]$$
 (intralevel) = $\frac{1}{2}A_{ac}(\gamma \hbar u/\lambda)^{-1/2}$. (3.16)

For elastic scattering ($\gamma = 0$), this diverges, as has been noted earlier.⁸ But this divergence of the relaxation rate makes a zero contribution to the conductivity tensor of Eq. (2.8). For the longitudinal case, these slowly moving electrons will not contribute to the longitudinal conductivity, no matter whether $\gamma = 0$ or not, as is obvious from Eq. (2.11). For the transverse case, $k_z \approx 0$ electrons do not make a contribution if the elastic scattering assumption is made, but they do contribute if inelasticity is included. This is the reason why transverse magnetoresistance is so sensitive to inelasticity of the acoustic phonons, whereas longitudinal magnetoresistance is not.

An excellent analysis of these slowly moving electrons in terms of wave-packet description is given by Kubo $et al.^2$ The stronger the magnetic field is, the more slowly the electrons move in the direction of the magnetic field. This causes inelasticity to play an even larger role in high magnetic fields. In the extreme quantum limit, when only the n = 0 level is appreciably occupied, the resultant wave packet will look like a cigar, which is greatly elongated in the direction of the magnetic field and has a small cross section $\pi \lambda^2 \sim 1/B_{\circ}$ When the elongation becomes of the order of the mean distance of scatterers, the wave packet can be simultaneously scattered by two scatterers, making the scattering process even more complicated. Assuming that the magnetic field is not ultrastrong,

(3 0)



FIG. 1. Magnetoresistance ratio vs magnetic field for the parabolic model of *n*-type InSb at temperature T = 77 K. Solid curves are for elastic scattering and dashed curves for inelastic scattering. The values of the inelasticity parameter γ are shown on each curve.

these slowly moving electrons will interact with phonons of $q_z \ll q_\perp \sim 1/\lambda$, making the assumption made in the above theory valid to reasonable extent.

To conclude, inelasticity may be expected to play an active role and hence should be included for electronic transport in the transverse configuration.

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