Quantum and classical-limit longitudinal magnetoresistance for anisotropic energy surfaces

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A theory developed earlier is analyzed in the strong-field quantum as well as the weak-field classical limit for the longitudinal magnetoresistance for an anisotropic model of a multivalley semiconductor band structure. The simple analytical expressions so obtained show a change in the power law of the magnetoresistance as a function of magnetic field from the classical limit (quadratic behavior) to the quantum limit (linear behavior), in agreement with the experimental observations. The anisotropic effect which is quite important in the classical limit becomes negligible in the quantum limit.

It is well known that at intermediate temperatures, the acoustic-phonon scattering is the predominant mechanism of scattering in semiconductors.[1] The theories[2–4] for the longitudinal magnetoresistance (LMR) for the acoustic-phonon scattering in isotropic parabolic semiconductors based on the solution of the Boltzmann transport equation give no LMR in the weak-field classical limit, but a linearly increasing LMR is obtained in the strong-field quantum limit. But, the experimental results for *n*-type germanium, which has anisotropic ellipsoidal energy surface, indicate a quadratic rise in the classical limit[5] and an approximately linear rise in the quantum limit[6] of LMR. It is interesting to observe from the experimental results that the classical-limit LMR is not only nonzero, but is bigger than the transverse effect.

A quantum theory based on the solution of Liouville's equation for the density matrix for arbitrary values of the magnetic field was developed earlier.[7] The numerical computations of the complicated expressions so obtained show that the LMR is larger than the transverse magnetoresistance in the classical limit. In the theoretical development, it was found that the longitudinal velocity operator v_z is given by[7]

$$v_z=(\alpha_{13}p_x+\alpha_{33}p_z)/m_0\ , \tag{1}$$

where p_x and p_z are the x and z components of the momentum of an electron, $\alpha_{ij}=(m_0/m^*)_{ij}$ are the components of the normalized inverse effective mass tensor (m_0/m^*), and m_0 is the free-electron mass. Here, (x,y,z) and $(1,2,3)$ are used interchangeably for the coordinate axes in the laboratory frame in which the applied magnetic field B is along the z axis $(\vec{B}\parallel\hat{z})$. Equation (1) indicates that the longitudinal velocity operator v_z is not only dependent on the momentum component p_z, but also is dependent on p_x through effective-mass anisotropy $(\alpha_{13}\neq 0)$. These transverse components cannot be averaged by the solution of the Boltzmann transport equation[8] as these are off diagonal in the basis representation in a magnetic field. If this anisotropic term is neglected, as in the approach following the Boltzmann transport equation, a difficulty arises in the correct approach to the zero-field limit. In this Brief Report, we derive analytical expressions for LMR in the weak-field classical as well as the strong-field quantum limit to study the importance of this effective mass anisotropy.

In the cubic-axis coordinate system, the longitudinal magnetoconductivity σ_L (σ_{zz}) in a many-valley model of a semiconductor with ellipsoidal energy surface is given by the expression[7]

$$\sigma_L(B)=\sum_{i=1}^{g_v}\left[\sigma_3(i)+\left(\frac{\alpha_{13}^2(i)}{\alpha_{11}(i)}\right)\sigma_1(i)\right]\ , \tag{2}$$

with

$$\sigma_1(i)=(e^2/m_0)[1-\exp(-a_i)]\times\sum_{nks}f(\epsilon_{nk}^i)(n+1)\tau_{nk,(n+1)k}^{-1}(i)\times[\omega_i^2+\tau_{nk,(n+1)k}^{-2}(i)]^{-1}\ , \tag{3}$$

$$\sigma_3(i)=-e^2\sum_{nks}\tau_{nk}(i)\left(\frac{\hbar k_z}{m_i^*}\right)^2\frac{df}{d\epsilon_{nk}^i}\ , \tag{4}$$

$$\alpha_{11}(i)=\alpha_t\cos^2\theta_i+\alpha_l\sin^2\theta_i\ , \tag{5}$$

$$\alpha_{13}(i)=(\alpha_t-\alpha_l)\sin\theta_i\cos\theta_i\ , \tag{6}$$

$$a_i^*=\hbar\omega_i^*/k_BT\ , \tag{7}$$

$$\omega_i^*=[\alpha_t\alpha_{11}(i)]^{1/2}\omega\ ,\quad \omega=eB/m_0c\ , \tag{8}$$

$$\epsilon_{nk}^i=(n+\tfrac{1}{2})\hbar\omega_i^*+\hbar^2k_z^2/2m_i^*\ , \tag{9}$$

$$m_i^*=m_0[\alpha_{11}(i)/\alpha_l\alpha_t]\ , \tag{10}$$

$$f(\epsilon_{nk}^i)=(2\pi\lambda^2)n_e\exp(-\epsilon_{nk}^i/k_BT)\times\left[\sum_i\frac{(2\pi m_i^*k_BT/\hbar^2)^{1/2}}{\sinh(a_i/2)}\right]^{-1}\ , \tag{11}$$

$$\tau_{nk}^{-1}(i) = [E_1^2 k_B T(2m_i^*)^{1/2}/2\pi\hbar\rho_d u^2\lambda^2] \times \sum_{n'}{}' [\epsilon_{nk}^i - (n'+\tfrac{1}{2})\hbar\omega_i^*]^{-1/2} , \quad (12)$$

$$\tau_{nk,(n+1)k}^{-1}(i) = \tfrac{1}{2}[\tau_{nk}^{-1}(i) + \tau_{(n+1)k}^{-1}(i)] , \quad (13)$$

and

$$\lambda = (\hbar c/eB)^{1/2} . \quad (14)$$

Here i stands for the valley index, g_v being the number of valleys ($g_v = 4$ in Germanium). θ_i is the angle between the principal (longitudinal) axis of the ith ellipsoid and the direction of the magnetic field $\vec{B}$. α_t and α_l are the principal components of the reciprocal effective-mass tensor in the ellipsoidal frame ($\alpha_t = 12.3$, $\alpha_l = 0.63$ for n-Ge). $(nk) = (n, k_y, k_z)$ stands for the set of quantum numbers of eigenfunctions in a magnetic field ($n = 0, 1, 2, \ldots$ is the Landau quantum number, and k_y, k_z are the components of quasicontinuous momentum wave vector $\vec{k} = \vec{p}/\hbar$). s is for the two spin states of an electron. n_e is the electronic concentration, E_1 is the deformation potential constant for electron-acoustic-phonon scattering, ρ_d is the crystal density, u is the sound velocity, and the prime on the summation indicates that $x^{-1/2} = 0$ when $x < 0$.

In the limit of zero magnetic field ($\vec{B} \to 0$), $\sigma_L(B)$ of Eq. (2) approaches $\sigma(0)$ given by

$$\sigma(0) = n_e e^2 \tau_0 / m_c^* , \quad (15)$$

with

$$\tau_0 = \frac{8\hbar\rho_d u^2}{3\pi E_1^2}(\alpha_t^2\alpha_l)^{1/2}\left(\frac{\pi\hbar^2}{2m_0 k_B T}\right)^{3/2} , \quad (16)$$

and

$$m_c^* = 3m_0/(2\alpha_1 + \alpha_3) \quad (17)$$

is the conductivity effective mass.

In the classical weak-field limit ($\hbar\omega_i^* << k_B T$, $\omega_i^* << \tau_0^{-1}$) for a magnetic field applied in any of the equivalent crystallographic $\langle 100\rangle$ directions ($\cos\theta_i = 1/\sqrt{3}$ for all four $\langle 111\rangle$-oriented valleys in n-Germanium), $\sigma_L(B)$ of Eq. (2) reduces to

$$\sigma_L^c(B) = \sigma(0)[(2\alpha_t + \alpha_l)(\alpha_t + 2\alpha_l)]^{-1} \times \{9\alpha_l\alpha_t + 2(\alpha_t - \alpha_l)^2[1 - (9\pi/16)(\omega^*\tau_0)^2]\} \quad (18)$$

which is consistent with Eq. (15) in the limit $B \to 0$. Here index i on ω_i^* is suppressed since all four valleys are equivalent in the $\langle 100\rangle$-configuration considered. The relative change in LMR $\Delta\rho^c/\rho_0$ is then given by

$$\Delta\rho^c/\rho_0 = (\sigma_0 - \sigma)/\sigma_0 = 9\pi(\alpha_t - \alpha_l)^2 \times [8(2\alpha_t + \alpha_l)(\alpha_t + 2\alpha_l)]^{-1}(\omega^*\tau_0)^2 . \quad (19)$$

This equation is an agreement with that obtained by Abeles and Meiboom[9] by the classical treatment. Equation (19) gives a quadratic rise of LMR with increasing magnetic field. The ratio $\Delta\rho^c/[\rho_0(\omega^*\tau_0)^2] = 1.4$ for n-type Germanium and gives $\Delta\rho^c/\rho_0 B^2 = 8.7 \times 10^{-8}$ G^{-2} at 77 K, where $\tau_0 = 1.9 \times 10^{-12}$ s is obtained from the zero-field mobility data. This is consistent with the experimental results of Pearson and Suhl.[5] In terms of $a = \hbar\omega^*/k_B T$, the Eq. (19) can be written as

$$\Delta\rho^c/\rho_0 = 1.4(k_B T\tau_0/\hbar)^2 a^2 = 512a^2 . \quad (20)$$

The value of the magnetic field at which $\omega^*\tau_0 \sim 1$ is $B \sim 4$ kG which corresponds to $a = 0.05$ at 77 K. Equation (20) is, therefore, expected to be valid for magnetic fields lower than 4 kG. This is indeed apparent from the experimental data. In Fig. 1, we show, on a log-log plot, the relationship between $\Delta\rho^c/\rho_0$ vs a. The straight line (dashed) so obtained has a slope of value 2.

The other extreme ($\hbar\omega^* >> k_B T$, $\omega^* >> \tau_0^{-1}$) defines the quantum limit, and most of the electrons occupy the lowest quantized level ($n = 0$). The onset of the strong-field quantum limit ($a = \hbar\omega^*/k_B T \sim 1$) for the $\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$ directions, respectively, occurs at $B = 1.01$, 2.7, and 1.54 times the temperature T, where B is in kG. At 77 K, $B = 77.8$, 208, 118 kG, respectively, for the three orientations given above. Obviously, the quantum limit in $\langle 100\rangle$ configuration sets in at much lower values of the magnetic field. In this limit, only $n = 0$ level is appreciably populated, and Eq. (2) can be approxi-

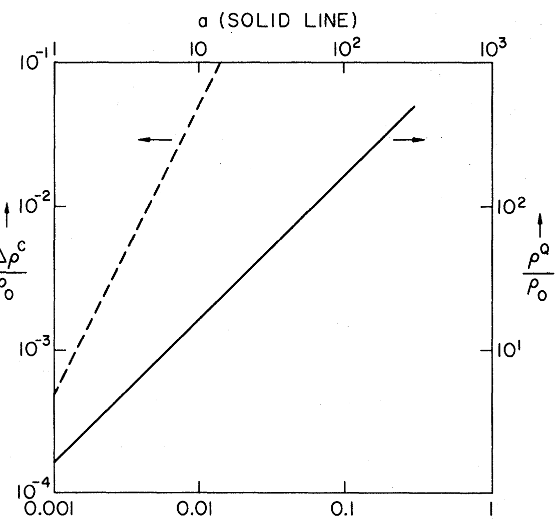

FIG. 1. Log-log plot of the relative change in the classical magnetoresistance $\Delta\rho^c/\rho_0$ vs $a = \hbar\omega^*/k_B T$ (dashed line which has a slope of value 2) and the relative quantum magnetoresistance ρ^Q/ρ_0 vs a (solid line which has a unity slope).

mated[10] to give the analytical expression

$$\sigma_L(B) = 27\sigma_0 a^{-1}[(2\alpha_t+\alpha_l)(\alpha_t+2\alpha_l)]^{-1} \times [\alpha_l\alpha_t + (4/81\pi)(\alpha_t-\alpha_l)^2 \times (\hbar/\tau_0 k_B T)^2 \exp(\alpha_c) E_1(\alpha_c)] , \quad (21)$$

with

$$\alpha_c = \{2\alpha_t[\alpha_t\alpha_l(\alpha_t+2\alpha_l)/3]^{1/2}/3\pi^{1/2}\}^2 \times (\hbar/\tau_0 k_B T)^2 , \quad (22)$$

and

$$E_1(\alpha_c) = \int_{\alpha_c}^{\infty} dy \exp(-y)/y . \quad (23)$$

In semiconductors, for acoustic-phonon scattering, the collision broadening $\hbar\tau_0^{-1}$ is usually much smaller than the thermal broadening ($\hbar/\tau_0 k_B T \ll 1$). In *n*-Ge, at 77 K, $\hbar/\tau_0 k_B T = 0.052$. In this case, the anisotropic effect becomes negligible, and the relative LMR ρ^Q/ρ_0 is given by the simple formula

$$\rho^Q(B)/\rho(0) = \sigma(0)/\sigma_L(B) = a[(2\alpha_t+\alpha_l)(\alpha_t+2\alpha_l)/27\alpha_t\alpha_l] = 1.64a . \quad (24)$$

Equation (24) shows a linear rise in the LMR with the magnetic field. Equations (21) and (24) are valid for all temperatures and magnetic fields in any orientation provided the quantum limit is satisfied and $\alpha_{11}(i)$ used in the evaluation of ω_i^*, and m_i^* is that corresponding to a valley with least ω^*. This is because the valleys with greater ω^* have been depleted of their carrier concentration in the quantum limit (quantum transfer effect).[8] Numerical factor in Eq. (24) will then be different for different orientations. In an isotropic parabolic semiconductor ($\alpha_l = \alpha_t = 1$), the coefficient of a in Eq. (24) is $\frac{1}{3}$. Equation (24) is an agreement with the expression obtained by Miller and Omar,[8] where the anisotropic effect was absent because of the use of the Boltzmann transport equation. The value of $\rho^Q/\rho_0 a = 1.64$, is in agreement with the high-field experimental data.[6] When plotted on a log-log scale, ρ^Q/ρ_0 versus a relationship is represented by a straight line which has a unity slope (solid line in Fig. 1).

A point regarding the correct use of the Boltzmann transport equation for high-field transport needs a little clarification. For an isotropic parabolic band model, the anisotropic term is absent ($\alpha_{13}=0$). The matrix elements of v_z of Eq. (1) are then diagonal and can be properly averaged by the distribution function obtained from the Boltzmann transport equation. This distribution function is the diagonal matrix element of the more complete density matrix. When $\alpha_{13} \neq 0$, the matrix elements of v_z contain matrix elements $\langle n'k'|p_x|nk\rangle$, in addition to diagonal matrix elements of p_z. $\langle n'k'/p_x|nk\rangle$ is nondiagonal in the basis representation (nk),[7] and gives zero for the expectation value of p_x if the Boltzmann transport function is used. But, if the density matrix is used, which is also nondiagonal in the basis representation, a nonzero expectation value of p_x is obtained. This is precisely what we have for the anisotropic term above. In the classical limit, this term is quite important as this makes $\sigma_L(B)/\sigma(0)=1$ in the limit $B \to 0$. If this anisotropic term is absent,[8] $\sigma_L(B)/\sigma(0) = 0.2$. But, for high fields, this anisotropic term is negligible, confirming the correctness of the theory of Miller and Omar[8] in analyzing the high-field LMR experiments.

We have thus shown that the general theory developed earlier extrapolates very well to the weak-field classical and the high-field quantum limit behavior of the LMR in a many-valley semiconductor. The anisotropic part of the magnetoconductivity which gives the nonzero LMR in the classical limit is found to be negligible in the quantum limit.

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