

EFFECT OF BAND STRUCTURES ON LONGITUDINAL MAGNETORESISTANCE IN SEMIMETALS AND SEMICONDUCTORS

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Abstract—*The effect of the Cohen nonellipsoidal nonparabolic (NENP) band structure on the propagation of ultrasound in a semimetal such as bismuth in the presence of a dc magnetic field is investigated by using a quantum-mechanical treatment which is valid at high frequencies and in strong magnetic fields. It is found that the longitudinal magnetoresistance oscillates with the dc magnetic field. This dependence on the dc magnetic field arises from the nonlinear effect of the energy bands owing to the NENP model for the energy band structure of bismuth. We compare these results with those of the ellipsoidal parabolic (EP) band structure of bismuth. We also present numerical results for the nondegenerate and degenerate semiconductors like n-type InSb. It is found that the longitudinal magnetoresistance in the nondegenerate case changes with the dc magnetic field only for the nonparabolic band structure. In the degenerate case, however, the longitudinal magnetoresistance for the parabolic and nonparabolic band structures will oscillate with the dc magnetic field. These oscillations are interpreted as the so-called "giant quantum oscillations" which occur in a degenerate electron gas.*

1. INTRODUCTION

The electrical resistivity in materials is usually affected somewhat by the presence in materials of a dc magnetic field. This magnetoresistance may be large or small, and it depends on the nature of the materials, the strength of the magnetic field, and the temperature.¹ It has been shown that the nonparabolicity of the energy bands in semiconductors can lead to a nonzero longitudinal magnetoresistance even if the energy and magnetic-field dependence of the relaxation time is ignored in strong magnetic fields.² This is contrary to the zero magnetoresistance predicted by the usual Boltzmann theory which assumes the collisions unaffected by the magnetic field. In the case of a semimetal like bismuth, it was found that the strong magnetic field dependence of some phenomena in this material can be explained using a two-band model for the energy band structure.^{3,4} However, from theoretical calculations⁵ and

experimental results,^{4,6} it was pointed out that the energy band in bismuth structure is the Cohen nonellipsoidal nonparabolic (NENP) model. In this paper we present theoretical calculations of the longitudinal magnetoresistance for a semimetal like bismuth by using a quantum-mechanical treatment which is valid at high frequencies and in strong magnetic fields. Since this kind of treatment is valid for high frequencies such that $|\vec{q}|l \gg 1$, where \vec{q} is the wavevector of the ultrasound and l is the electron mean free path, therefore the effect of collisions on electrons can be assumed to be insignificant in our present works. We also limit ourselves to the case where the ultrasound propagates parallel to the dc magnetic field.

In Section II, the energy eigenvalue equation for an electron gas in a dc magnetic field \vec{B} is solved by using time-independent perturbation theory. Using the eigenfunctions and eigenvalues obtained, we calculate the longitudinal conductivity tensor. In Section III, we present the numerical results for the variation of the longitudinal magnetoresistance for the NENP and EP models as the energy band structures of bismuth.^{5,7} The numerical results for the parabolic and nonparabolic band structures as the energy bands of a semiconductor like n -type InSb are also presented. Finally, a brief discussion is given.

2. THEORETICAL DEVELOPMENT

In the NENP model, the relation between the energy and momentum of an electron gas in the absence of the dc magnetic field is⁵

$$E\left(1 + \frac{E}{E_g}\right) = -\frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} \left[1 + \frac{E}{E_g} \left(1 - \frac{m_2}{m'_2}\right)\right] + \frac{p_z^2}{2m_3} + \frac{p_y^4}{4m_2 m'_2 E_g} \quad (1)$$

From experimental results,^{4,8} it has been indicated that the difference between m_2 and m'_2 is very small, *i. e.*, $m_2 \approx m'_2$. Thus the term in the square brackets of Eq. (1) can be considered constant. For the sake of convenience, some parameters are defined as follows:

$$\begin{aligned} \alpha_1 &= \frac{m}{m_1}, \\ \alpha_2 &= \frac{m}{m_2} \left[1 + \frac{E}{E_g} \left(1 - \frac{m_2}{m'_2}\right)\right] \approx \frac{m}{m_2}, \\ \alpha_3 &= \frac{m}{m_3}, \end{aligned} \quad (2)$$

and

$$\alpha_4 = \frac{m}{2m_2 m'_2 E_g},$$

where m is the mass of the free electron.

We introduce a dc uniform magnetic field of induction \vec{B} directed parallel to the z direction, then the vector potential in the Landau gauge can be expressed in the form $\vec{A}_0 = (0, Bx, 0)$. The energy eigenvalue equation in the magnetic field \vec{B} directed along the z direction can thus be written as

$$\begin{aligned}
 H_0(1+H_0/E_g)\psi_{\vec{k}n} = & \left(\frac{1}{2m}\right) [\alpha_1 p_x^2 + \alpha_2 (p_y - eBx/c)^2 + \alpha_3 p_z^2 \\
 & + \alpha_4 (p_y - eBx/c)^4] \psi_{\vec{k}n} \\
 = & E_{\vec{k}n}^{\pm}(1+E_{\vec{k}n}^{\pm}/E_g)\psi_{\vec{k}n},
 \end{aligned} \tag{3}$$

where $E_{\vec{k}n}$ is the true energy of the system defined by $H_0\psi_{\vec{k}n} = E_{\vec{k}n}\psi_{\vec{k}n}$, and E_g is the energy gap between the conduction and valence bands. By using time-independent perturbation theory, the eigenfunctions and eigenvalues up to first order for Eq. (3) are given by

$$\begin{aligned}
 \psi_{\vec{k}n}^{\pm} = & \exp(ik_y y + ik_z z) \{ \phi_n(x-x_0) + (\delta/16\hbar\omega_0) [n(n-1)(n-2) \\
 & \times (n-3)]^{1/2} \phi_{n-4}(x-x_0) + (\delta/4\hbar\omega_0) [n(n-1)]^{1/2} (2n-1) \phi_{n-2}(x-x_0) \\
 & - (\delta/4\hbar\omega_0) [(n+1)(n+2)]^{1/2} (2n+3) \phi_{n+2}(x-x_0) - (\delta/16\hbar\omega_0) \\
 & \times [(n+1)(n+2)(n+3)(n+4)]^{1/2} \phi_{n+4}(x-x_0) \},
 \end{aligned} \tag{4}$$

and

$$\begin{aligned}
 E_{\vec{k}n}^{\pm} = & -\frac{1}{2} E_g \left(1 - \left\{ 1 + (4/E_g) \left[\left(n + \frac{1}{2} \right) \hbar\omega_0 + (\hbar^2 k_z^2)/2m^* + (3\delta/2) \right. \right. \right. \\
 & \left. \left. \left. \times \left(n^2 + n + \frac{1}{2} \right) \right] \right\}^{1/2} \right),
 \end{aligned} \tag{5}$$

where $\omega_0 = (|e|B/mc) (\alpha_1 \alpha_2)^{1/2}$, $\delta = (\alpha_1 \alpha_4 / \alpha_2) (e^2 B^2 \hbar^2 / 2mc^2)$, $x_0 = ck_y \hbar / eB$, $m^* = m / \alpha_3$, and $\phi_n(x)$ is the harmonic-oscillator wave function. If the electron spin splitting is considered, then the eigenfunctions and eigenvalues of the system can be expressed by

$$\psi_{\vec{k}n s}(\vec{r}) = \begin{pmatrix} \frac{1+s}{2} \\ \frac{1-s}{2} \end{pmatrix} \psi_{\vec{k}n}(\vec{r}), \tag{6}$$

and

$$\begin{aligned}
 E_{\vec{k}n s}^{\pm} = & -\frac{1}{2} E_g \left(1 - \left\{ 1 + (4/E_g) \left[\left(n + \frac{1}{2} \right) \hbar\omega_0 + (s/2) \hbar\omega_s + (\hbar^2 k_z^2)/2m^* \right. \right. \right. \\
 & \left. \left. \left. + (3\delta/2) \left(n^2 + n + \frac{1}{2} \right) \right] \right\}^{1/2} \right),
 \end{aligned} \tag{7}$$

where $s = \pm 1$, ω_s is defined by $\omega_s = |e|B/m_s c$, and m_s is the spin effective mass which has a relation with the spin splitting factor g such that $m_s/m = 2/g$. For bismuth, the spin effective mass is equal to the cyclotron mass,^{3,9,10} i. e., $m_s = m / (\alpha_1 \alpha_2)^{1/2}$. Consequently, $\omega_s = \omega_0$ for the pure bismuth. Equations (6) and (7) are the eigenfunctions and eigenvalues for a two-band model. When $(n + \frac{1}{2})\hbar\omega_0 + (s/2)\hbar\omega_s + (\hbar^2 k_z^2)/2m^* \ll E_g$ and $\delta = 0$, Eqs. (6) and (7) are reduced to the results obtained using the EP band structure for a one-band model,⁷ and their results will be

$$\psi_{\vec{k}n s}(\vec{r}) = \begin{pmatrix} \frac{1+s}{2} \\ \frac{1-s}{2} \end{pmatrix} \exp(ik_y y + ik_z z) \phi_n(x-x_0) \tag{8}$$

and

$$E_{\vec{k}n s}^{\pm} = \hbar\omega_0 \left(n + \frac{1}{2} \right) + (s/2) \hbar\omega_s + (\hbar^2 k_z^2)/2m^*. \tag{9}$$

The interaction of the conduction electrons with the ultrasound can be taken into account via the vector potential $\vec{A}_1 = \vec{A}_0 \exp(i\vec{q} \cdot \vec{r} - i\omega t)$ which arises from the self-consistent field accompanying the ultrasonic wave. To first order in \vec{A}_1 , the Hamiltonian for an electron in the presence of the dc magnetic field and self-consistent field is

$$H = H_0 + H_1, \tag{10}$$

where H_0 is defined as shown in Eq. (3). The second term in Eq. (10),

$$H_1 = -(e/2c) (\vec{v} \cdot \vec{A}_1 + \vec{A}_1 \cdot \vec{v}), \tag{11}$$

is the interaction Hamiltonian. Here \vec{v} is the velocity operator for the unperturbed Hamiltonian $\vec{v} = -(i/\hbar) [\vec{r}, H_0]$. The effective Hamiltonian for the NENP model is defined by

$$\begin{aligned} F(p_x, p_y, p_z) &\equiv H_0(1 + H_0/E_g) \\ &= \left(-\frac{1}{2m}\right) [\alpha_1 p_x^2 + \alpha_2 (p_y - eBx/c)^2 + \alpha_3 p_z^2 \\ &\quad + \alpha_4 (p_y - eBx/c)^4]. \end{aligned} \tag{12}$$

Then the components of the velocity operator are given by

$$v_i = (1 + 2H_0/E_g)^{-1} \frac{\partial F}{\partial p_i}. \tag{13}$$

To obtain the longitudinal magnetoresistance we first calculate the longitudinal component of the electrical conductivity tensor. The equation of motion for the density operator $\hat{\rho}$ is¹¹

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [H, \hat{\rho}]. \tag{14}$$

The density operator can be expanded into the unperturbed density operator $\hat{\rho}_0$ plus a term which is the change in $\hat{\rho}$ due to the self-consistent field thereby linearizing the equation of motion (14), i. e., $\hat{\rho} = \hat{\rho}_0 + \hat{\rho}_1$. Taking the matrix elements of the linearized equation of motion in the representation of Eqs. (6) and (7) for the NENP model, or (8) and (9) for the EP model, we find that

$$\langle \vec{k}'n' | \hat{\rho}_1 | \vec{k}n \rangle = \frac{(f_{\vec{k}'n'} - f_{\vec{k}n}) \langle \vec{k}'n' | H_1 | \vec{k}n \rangle}{E_{\vec{k}'n'} - E_{\vec{k}n} - \hbar\omega}, \tag{15}$$

where $f_{\vec{k}n} = \langle \vec{k}n | \hat{\rho} | \vec{k}n \rangle$ is the Fermi-Dirac distribution for electrons in semimetals and degenerate semiconductors, or the Maxwell-Boltzmann distribution for electrons in nondegenerate semiconductors. The induced current density is

$$\vec{J} = \text{Tr}(\hat{\rho} \cdot \vec{J}_{op}) = \sum_{\vec{k}, \vec{k}', m, m'} \langle \vec{k}'n' | \hat{\rho} | \vec{k}n \rangle \langle \vec{k}n | \vec{J}_{op} | \vec{k}'n' \rangle, \tag{16}$$

where the current density operator to first order in \vec{A}_1 at a point \vec{r}_0 is

$$\vec{J}_{op} = -(e/2) [(\vec{v} + \vec{v}'), \delta(\vec{r} - \vec{r}_0)]_+ \tag{17}$$

Here $[\]_+$ denotes the anticommulator. The velocity operator \vec{v} is defined by Eq.

(13), and the velocity operator $\vec{v} = -(i/\hbar) [r, H_1]$. From Eq. (12), we obtain

$$v'_i = -(e/c) (1+2H_0/E_g)^{-1} \frac{\partial^2 F}{\partial p_i \partial p_j} A_{1j} + (e/c E_g) (1+2H_0/E_g)^{-3} \times \frac{\partial F}{\partial p_i} \left(A_{1j} \frac{\partial F}{\partial p_j} + \frac{\partial F}{\partial p_j} A_{1j} \right). \tag{18}$$

Using the gauge where the scalar potential is zero, we find the relation between the self-consistent field \vec{E} and the vector potential \vec{A}_1 ,

$$\vec{E} = (i\omega/c) \vec{A}_1. \tag{19}$$

In our present case we are interested in an ultrasound propagating parallel to the dc magnetic field, so that the only component of the conductivity tensor of interest is σ_{zz} . Using Eqs. (6), (7), (10)-(19), we find that

$$\begin{aligned} \sigma_{zz}(q, \omega) = & i(\omega_p^*)^2 \left(8 \sqrt{2} \pi \omega \sum_{n,s} (\Delta E_{ns})^{1/2} \right)^{-1} \left(- (E_g)^{1/2} \right. \\ & \times \sum_{n,s} \tan^{-1} \left(\frac{2\sqrt{2} a_{ns} (E_g \Delta E_{ns})^{1/2}}{a_{ns}^2 E_g - 2\Delta E_{ns}} \right) + \frac{(m^*)^{3/2} E_g^2}{4q\hbar^3} \\ & \times \sum_{n,s} a_{ns}^3 \left[\left(\frac{q^2}{4} + \frac{\omega^2 (m^*)^2 a_{ns}^2}{q^2 \hbar^2} + \frac{m^* a_{ns}^2 E_g}{\hbar^2} \right)^2 - \frac{\omega^2 (m^*)^2 a_{ns}^2}{\hbar^2} \right]^{-1} \\ & \times \left\{ \frac{4\omega^2 (m^*)^2 a_{ns}^2}{q^2 \hbar^2} \left[\ln \left(\frac{(\Delta E_{ns})^{1/2} + q\hbar/2\sqrt{2} (m^*)^{1/2} - \omega(m^*)^{1/2} a_{ns}/\sqrt{2} q}{-(\Delta E_{ns})^{1/2} + q\hbar/2\sqrt{2} (m^*)^{1/2} - \omega(m^*)^{1/2} a_{ns}/\sqrt{2} q} \right) \right. \right. \\ & - \ln \left(\frac{(\Delta E_{ns})^{1/2} - q\hbar/2\sqrt{2} (m^*)^{1/2} - \omega(m^*)^{1/2} a_{ns}/\sqrt{2} q}{-(\Delta E_{ns})^{1/2} - q\hbar/2\sqrt{2} (m^*)^{1/2} - \omega(m^*)^{1/2} a_{ns}/\sqrt{2} q} \right) \\ & - \frac{1}{2} \ln \left(\frac{[(\Delta E_{ns})^{1/2} + q\hbar/\sqrt{2} (m^*)^{1/2}]^2 + \frac{1}{2} a_{ns}^2 E_g}{[-(\Delta E_{ns})^{1/2} + q\hbar/\sqrt{2} (m^*)^{1/2}]^2 + \frac{1}{2} a_{ns}^2 E_g} \right) \\ & + \frac{\hbar}{(m^* E_g)^{1/2} a_{ns}} \left[\frac{q^3}{4} + \frac{2m^* a_{ns}^2 q E_g}{\hbar^2} - \frac{\omega^2 (m^*)^2 a_{ns}^2}{q\hbar^2} \right. \\ & + \frac{4(m^*)^2 a_{ns}^4 E_g^2}{q\hbar^4} + \frac{4\omega^2 (m^*)^3 a_{ns}^4 E_g}{q\hbar^4} \left. \right] \left[\tan^{-1} \left(\frac{2\sqrt{2} a_{ns} (E_g \Delta E_{ns})^{1/2}}{a_{ns}^2 E_g - 2\Delta E_{ns}} \right) \right. \\ & \left. \left. - \tan^{-1} \left(\frac{2\sqrt{2} a_{ns} (E_g \Delta E_{ns})^{1/2}}{a_{ns}^2 E_g - 2\Delta E_{ns} + q^2 \hbar^2 / m^*} \right) \right] \right\}, \tag{20} \end{aligned}$$

where $\omega_p^* = (4\pi n_0 e^2 / m^*)^{1/2}$ is the plasma frequency, $E_{ns} = E_F (1 + E_F / E_g) - (n + \frac{1}{2}) \hbar \omega_c - (s/2) \times \hbar \omega_s - (3\delta/2)(n^2 + n + \frac{1}{2})$, and $a_{ns} = \{1 + (4/E_g)[(n + \frac{1}{2}) \hbar \omega_c + (s/2) \hbar \omega_s + (3\delta/2)(n^2 + n + \frac{1}{2})]\}^{1/2}$. In obtaining the above result, we have used the expansion of Eq. (7),

$$E_{k_{ns}} = -\frac{1}{2} E_g + \frac{1}{2} E_g a_{ns} + (\hbar^2 k_{ns}^2) / 2m^* a_{ns} \tag{21}$$

for energy levels of the conduction electrons, since $(\hbar^2 k_{ns}^2) / 2m^* \ll E_g$ for the case in a very low temperature limit. From Eq. (20), it can be seen that the longitudinal conductivity tensor σ_{zz} depends on the dc magnetic field due to the parameters ω_c , ω_s , and δ . In the absence of the dc magnetic field, the longitudinal conductivity $\sigma_{zz}(0) = \sigma_0$ can be obtained by putting $\omega_c = \omega_s = 0$, $\delta = 0$, and $a_{ns} = 1$ in Eq. (20).

For, since $\sigma_{xx} = \sigma_{yy} = 0$,¹² we have the longitudinal magnetoresistance $\rho_{zz}(B) = 1/\sigma_{zz}(B)$, and thus the variation of the longitudinal magnetoresistance $\Delta\rho/\rho_0$ can be calculated as

$$\frac{\Delta\rho}{\rho_0} = \frac{\rho_{ss}(B) - \rho_{ss}(0)}{\rho_{ss}(0)} = \frac{\sigma_{ss}(0)}{\sigma_{ss}(B)} - 1. \tag{22}$$

3. NUMERICAL RESULTS AND DISCUSSIONS

As a numerical example for bismuth, the relevant parameters are¹³ $n_0 = 2.75 \times 10^{17} \text{ cm}^{-3}$, $\alpha_1 = 172$, $\alpha_2 = 0.8$, $\alpha_3 = 88.5$, $E_g = 0.0153 \text{ eV}$, $E_F = 0.0276 \text{ eV}$, and the sound velocity v_s is assumed to be 10^5 cm/sec . The results for the variation of the longitudinal magnetoresistance $\Delta\rho/\rho_0$ are shown in Fig. 1 without including the spin splitting and Fig. 2 including the spin splitting for the NENP band structure. It can be seen that the longitudinal magnetoresistance oscillates with the dc magnetic field in the region of high sound frequencies and strong magnetic fields. When the spin-splitting energy is comparable to the Landau level, the oscillations in $\Delta\rho/\rho_0$ will be shifted to the high magnetic field region. Therefore, the spin-splitting effect will appear much more significant in the region of strong magnetic fields. However, these oscillations will be diminished with increasing the sound frequency ω , and the screening effect will thus be broken down at very high frequencies. The oscillations in $\Delta\rho/\rho_0$ with the dc magnetic field can be explained by the fact that the longitudinal conductivity tensor has the logarithmic singularities of a purely quantum origin related to the electron gas.^{14,15} Since we are interested in the frequencies in the microwave region, these oscillations can be interpreted as the so-called "giant quantum oscillations".^{16,17} These giant quantum oscillations occur in a degenerate electron gas in the case when the electron level is near the Fermi surface and the sound wave-vector \vec{q} has a component along the dc magnetic field. Moreover, the dependence on the dc magnetic field arises from the nonlinear effect of the energy bands owing to the NENP model

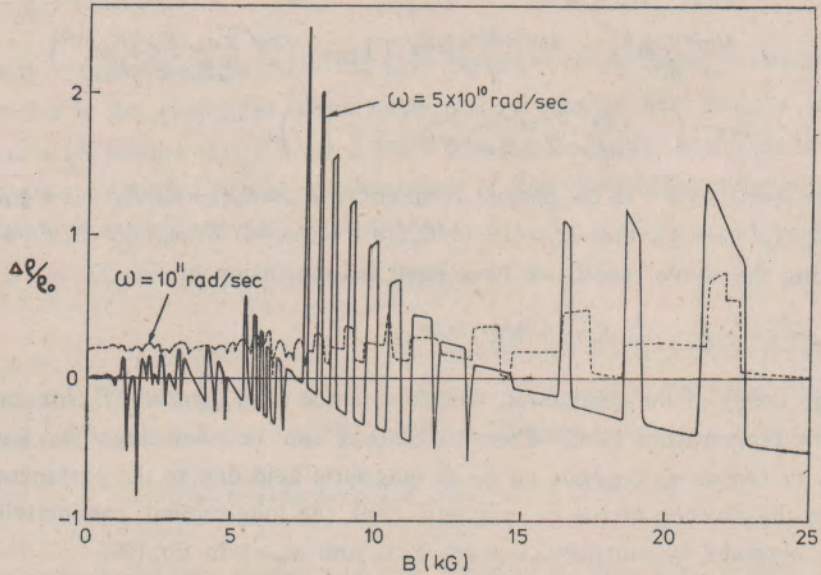


Fig. 1. Variation of longitudinal magnetoresistance (without including the spin splitting) with the dc magnetic field B for the NENP model as the energy band structure of bismuth.

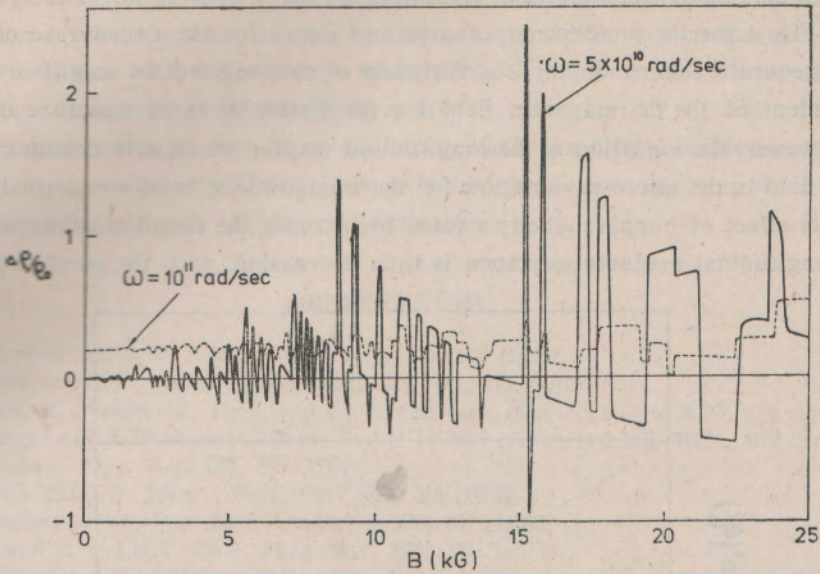


Fig. 2. Variation of longitudinal magnetoresistance (including the spin splitting) with the dc magnetic field B for the NENP model as the energy band structure of bismuth.

for bismuth. This effect of NENP model in the band structure of bismuth is to introduce an energy, and therefore, a magnetic-field-dependent effective mass for the electrons. This effective mass for electrons in an energy level of quantum number n and spin quantum number s is m^*a_{ns} . The factor a_{ns} depends on the dc magnetic field owing to the parameters ω_e , ω_s , and δ . Consequently, the effective mass of electrons defined by m^*a_{ns} depends strongly upon the dc magnetic field.

We plot the variation of the longitudinal magnetoresistance $\Delta\rho/\rho_0$ for the EP model as the energy band structure of bismuth as shown in Fig. 3. It can be seen that the oscillation in EP model are diminished much more than those in NENP

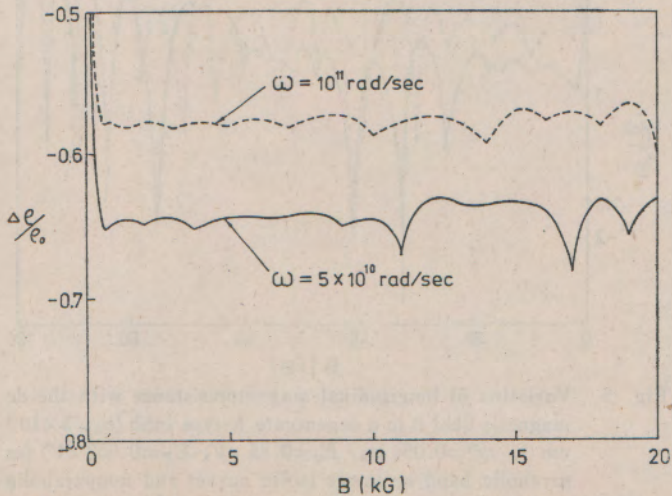


Fig. 3. Variation of longitudinal magnetoresistance with the dc magnetic field B for the EP model as the energy band structure of bismuth.

model. We also apply our quantum treatment to the *n*-type InSb. The results are shown in Fig. 4 for the nondegenerate case and Fig. 5 for the degenerate case. For the nondegenerate semiconductor, the variation of the longitudinal magnetoresistance is independent of the dc magnetic field for the parabolic band structure in *n*-type InSb. However, the variation of the longitudinal magnetoresistance changes with the magnetic field in the microwave region for the nonparabolic band structure in *n*-type InSb. This effect of nonparabolicity causes to increase the longitudinal conductivity, and the longitudinal magnetoresistance is thus decreasing with the magnetic field in

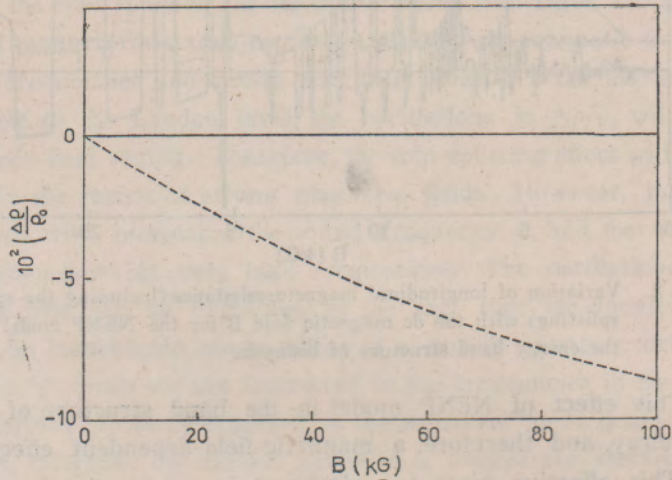


Fig. 4. Variation of longitudinal magnetoresistance with the dc magnetic field B in a nondegenerate n-type InSb ($n_0=1.75 \times 10^{14} \text{ cm}^{-3}$, $m^*=0.013 m_0$, $E_g=0.2 \text{ eV}$) for parabolic band structure (solid curve) and nonparabolic band structure (dashed curve) at $\omega=10^{11} \text{ rad/sec}$, $T=10^\circ \text{K}$, and $v_s=4 \times 10^4 \text{ cm/sec}$.

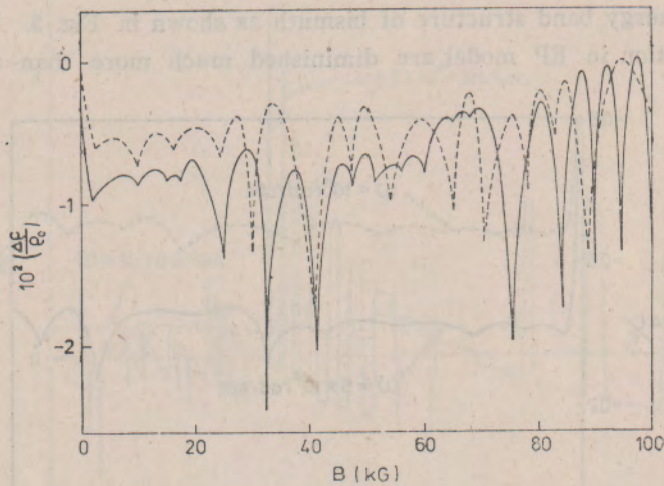


Fig. 5. Variation of longitudinal magnetoresistance with the dc magnetic field B in a degenerate n-type InSb ($n_0=3 \times 10^{19} \text{ cm}^{-3}$, $m^*=0.054 m_0$, $E_g=0.85 \text{ eV}$, $E_F=0.652 \text{ eV}$) for parabolic band structure (solid curve) and nonparabolic band structure (dashed curve) at $\omega=5 \times 10^{12} \text{ rad/sec}$, and $v_s=4 \times 10^5 \text{ cm/sec}$.

the low-temperature region.¹⁸ For the degenerate semiconductor, it can be seen that the variation of the magnetoresistance for both parabolic and nonparabolic band structures oscillates with the magnetic field. This is due to the resonant interaction between the ultrasound and conduction electrons in material.¹⁹ These oscillations can also be interpreted as the giant quantum oscillations. Therefore, we conclude that the giant quantum oscillations can only be observed in degenerate materials like semimetals and heavily doped semiconductors.

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