High-Field Magnetoresistance of Nonparabolic-Band and Bismuth-Type Metals

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A quantum-mechanical study has been made of the galvanomagnetic effect including intraband elastic scattering for electrons in bismuth-type metals with ellipsoidal-nonparabolic dispersion relation. The analysis is based on the Kubo formulas for static electrical conductivity. The magnetoconductivity tensor in the strong-magnetic-field region has been worked out in the general case where the magnetic field is in an arbitrary direction with respect to the Fermi ellipsoid. The relative- and center-coordinate operators for the electron cyclotron motion are properly redefined in order to accommodate the nonzero off-diagonal effective masses resulting from the arbitrariness in direction of the applied magnetic field. The difficulty arising from the nonparabolicity in the dispersion relation is also overcome, thus all of the magnetoconductivity tensor elements can be obtained in compact forms when the magnetic field is sufficiently strong. An explicit curve for the transverse magnetoresistance of bismuth in crossed electric and magnetic fields has been computed. We find that, by using $\tau_{\text{electron}} = 2.3 \times 10^{-10}$ sec and $\tau_{\text{hole}} = 1.2 \times 10^{-10}$ sec, our computed result is in reasonable agreement with some experimental data taken at $T = 4.2\,^{\circ}\text{K}$.

I. INTRODUCTION

When the magnetic field applied to an electron gas is so strong that there are only a few Landau levels below the Fermi energy, the quantization of energy levels plays an important role. In this case, the classical Boltzmann kinetic equation is no longer applicable for the treatment of the galvanomagnetic effects; a quantum-mechanical formulation is required.

For electrons with spherical-parabolic (SP) dispersion relation, theoretical discussions of galvanomagnetic effects in the quantum regime can be found in the papers by Titeica,[1] Argyres and Adams,[2] Kubo and his co-workers,[3,4] Argyres,[5] Adams and Holstein,[6] Kahn and Frederikse,[7] Skobov,[8] Zyryanov and Kuleyev,[9] etc. Some of these authors have limited their work to either the transverse or longitudinal magnetoresistance effect only.

For electrons with ellipsoidal-parabolic (EP) dispersion relation, a quantum theory of the transverse magnetoconductivity was developed by Davydov and Pomeranchuk (DP) early in 1940.[10] In their paper, a transverse magnetoresistance curve (up to 25 kG) for bismuth was computed by assuming that the hole Fermi surface consists of three ellipsoids,[11] and that electrons and holes are spinless. This paper marked an important advance in the theoretical study of magnetoconductivity. The sound logical basis of the authors's interpretation of the electrical conduction in terms of migrating centers in a magnetic field has later been justified.[4]

For electrons with ellipsoidal-nonparabolic (ENP) dispersion relation, theoretical investigation of the magnetoconductivity in the quantum regime does not seem to have appeared in the literature.[12] The study of this model of electrons lends its usefulness to the investigation of electronic properties of bismuth-type metals as theoretical and experimental results have both indicated that conduction electrons in these metals obey the ENP model.[13-16] In bismuth, for example, the electron Fermi surface consists of three Fermi ellipsoids. One of them (ellipsoid I) can, in the absence of a magnetic field, be described by the ENP model energy-momentum relation[16]

$$E\left(1+\frac{E}{E_G}\right)=\frac{1}{2}\vec{p}\cdot\overleftrightarrow{\mu}\cdot\vec{p}=\tfrac{1}{2}(p_x,p_y,p_z)\begin{pmatrix}\mu_{xx}&\mu_{xy}&\mu_{xz}\\ \mu_{xy}&\mu_{yy}&\mu_{yz}\\ \mu_{xz}&\mu_{yz}&\mu_{zz}\end{pmatrix}\begin{pmatrix}p_x\\ p_y\\ p_z\end{pmatrix}, \tag{1}$$

where E_G is the energy gap in the two-band model, E the energy measured from the bottom of the conduction band, and $\overleftrightarrow{\mu}$ the inverse-effective-mass tensor at the bottom of the band, which, in the crystallographic axes system (with the x, y, and z axes respectively parallel to the binary, bisectrix, and

trigonal axes), is of the form

$$\vec{\vec{\mu}}(I)=\begin{pmatrix}\alpha_{xx}^{(e)} & 0 & 0\\ 0 & \alpha_{yy}^{(e)} & \alpha_{yz}^{(e)}\\ 0 & \alpha_{yz}^{(e)} & \alpha_{zz}^{(e)}\end{pmatrix}. \tag{2}$$

The other two electron Fermi ellipsoids (ellipsoid II and III) are generated by rotating the coordinate axes used in Eq. (1) through $\pm 120^\circ$ about the trigonal (z) axis. The hole Fermi surface of bismuth, however, contains only one Fermi ellipsoid, which in the above-mentioned axes system can be characterized by[16]

$$E^h = E_0 - E_h = \tfrac{1}{2}(\alpha_x^{(h)} p_x^2 + \alpha_y^{(h)} p_y^2 + \alpha_z^{(h)} p_z^2), \tag{3}$$

where E_0 is the band overlap, E^h and E_h are the hole energies measured, respectively, from the top of the hole band and from the bottom of the electron band, and $\alpha_x^{(h)}$, $\alpha_y^{(h)}(=\alpha_x^{(h)})$, and $\alpha_z^{(h)}$ are the inverse effective masses of holes.

In the present paper, we shall first present the quantum-mechanical formulation for the magnetoconductivity of ENP electrons closely following the calculation by Kubo *et al.*[3,4] The magnetic field region in which we are interested is essentially governed by the relation $\Omega\tau \gg 1$, where $\Omega(=eH/m_c c)$ is the cyclotron angular frequency and τ the average time between successive collisions. This condition assures that the "center-migration" picture can be appropriately used[3] for the cyclotron motion, thus simplifying the calculation problem.

II. KUBO CONDUCTIVITY FORMULAS APPLIED TO ENP ELECTRONS

It is well established that the *one-particle* Hamiltonian of the ENP electrons in a uniform magnetic field $\vec{H}$ can be expressed in the form, due to Lax,[13]

$$\hat{H}^{(L)}=\left(\frac{1}{2}\,\vec{\pi}\cdot\vec{\vec{\mu}}\cdot\vec{\pi}+\frac{e\hbar}{2m_{sH}c}\,\vec{\vec{\sigma}}\cdot\vec{H}\right)\Big/\left(1+\frac{E^{(L)}}{E_G}\right), \tag{4}$$

where $\vec{\vec{\sigma}}$ is the Pauli spin matrix, $\vec{\pi}$ the canonical momentum defined by the quasimomentum $\vec{p}$ and the vector potential $\vec{A}$ through the relation

$$\vec{\pi}=\vec{p}+e\vec{A}/c, \tag{5}$$

m_{sH} the spin-precession effective mass with respect to the magnetic field direction, $E^{(L)}$ the eigenvalue of $\hat{H}^{(L)}$ measured from the bottom of the conduction band, and e, c, $\hbar$ assume their usual meanings. When investigating the galvanomagnetic effect, we should take into consideration the perturbations due to the electric field and to impurity scattering, and some other collision processes. Following the equivalent-Hamiltonian theorem of Luttinger,[17] and the perturbation method used by Baraff,[18] we now assert that the total Hamiltonian $\hat{H}_T$ can be written as

$$\hat{H}_T=\hat{H}_K+\hat{H}_P+\hat{H}_I+\hat{H}_F\equiv\hat{H}_{KPI}+\hat{H}_F, \tag{6}$$

where $\hat{H}_{\vec{F}}$ is the perturbation energy due to the weak electric field $\vec{F}$, $\hat{H}_I$ that due to impurity scattering, $\hat{H}_P$ the over-all perturbation energy due to all other sources, and $\hat{H}_K$ the Hamiltonian for an ENP electron in the absence of perturbation. It is defined by

$$\hat{H}_K\equiv-\tfrac{1}{2}E_G+(\tfrac{1}{4}E_G^2+E_G\hat{\mathcal{H}})^{1/2}, \tag{7}$$

in which

$$\hat{\mathcal{H}}=\tfrac{1}{2}\vec{\pi}\cdot\vec{\vec{\mu}}\cdot\vec{\pi}+\frac{e\hbar}{2m_{sH}c}\,\vec{\vec{\sigma}}\cdot\vec{H}\equiv\hat{H}_K\left(1+\frac{\hat{H}_K}{E_G}\right). \tag{8}$$

As a first trial to solve the galvanomagnetic problem of the ENP electrons systematically, we shall restrict ourselves to the lowest-order perturbation expressions for the magnetoconductivity. Thus, we shall only use the unperturbed wave functions to calculate the scattering matrices. In the unperturbed case, since both $\hat{H}^{(L)}$ and H_K represent the same physical quantity (the total Hamiltonian for one ENP electron), they will have the same complete set of eigenfunctions. Therefore, we need not bother with the relativistic resemblance[14] of Eq. (7); in Secs. III–VIII, we shall not distinguish $\hat{H}^{(L)}$ from $\hat{H}_K$ and use a single symbol $\hat{H}$ to denote either one of them.

According to Eq. (6), we may write the *many-electron* Hamiltonian $\hat{\mathcal{H}}_T^N$ for a system of N ENP electrons in a weak electric field as

$$\hat{\mathcal{H}}_T^N=\hat{\mathcal{H}}_K^N+\hat{\mathcal{H}}_P^N+\hat{\mathcal{H}}_I^N+\hat{\mathcal{H}}_F^N=\hat{\mathcal{H}}_{KPI}^N+\hat{\mathcal{H}}_F^N, \tag{9}$$

where $\hat{\mathcal{H}}_i^N$ ($i=K,\ P,\ I,\ F$) are partial many-electron Hamiltonians corresponding, respectively, to $\hat{H}_i$ ($i=K,\ P,\ I,\ F$). So long as $\hat{\mathcal{H}}_F^N$ is an additive term in $\hat{\mathcal{H}}_T^N$, we may readily apply Kubo's static conductivity formulas[3,4,19] to the ENP electron system:

$$\sigma_{\mu\nu}(\vec{H})=(1/V)\int_0^\infty dt\int_0^\beta d\lambda\ \mathrm{Tr}\left[\hat{\rho}_{KPI}\hat{J}_\nu(i\hbar\lambda)\hat{J}_\mu(t)\right],\quad(\mu,\ \nu=x,\ y,\ z), \tag{10}$$

where V is the volume of the system, $\hat{\rho}_{KPI}$ the density operator defined by the many-electron Hamiltonian $\hat{\mathcal{H}}_{KPI}^N$, $\beta=1/kT$ (k is the Boltzmann constant, T is the absolute temperature), Tr denotes taking trace in the many-electron space, and $\hat{J}_\mu(t)$ is a Heisenberg operator defined by

$$\hat{J}_\mu(t)=e^{i\hat{\mathcal{H}}_{KPI}^N t/\hbar}\hat{J}_\mu e^{-i\hat{\mathcal{H}}_{KPI}^N t/\hbar}, \tag{11}$$

with

$$J_\mu\equiv\sum_{i=1}^N j_\mu^{(i)}=-e\sum_{i=1}^N \dot{r}_\mu^{(i)}\quad(\mu=x,\ y,\ z). \tag{12}$$

III. CENTER AND RELATIVE-COORDINATE OPERATORS FOR CYCLOTRON MOTION OF ENP ELECTRONS

If the applied magnetic field is along the z direction in a Cartesian coordinate system oriented

arbitrarily with respect to the electron Fermi ellipsoid, i.e., $\vec{H}=(0, 0, H_z)$, and the vector potential given by

$$\vec{A}=(0, xH_z, 0), \tag{13}$$

the completely unperturbed state $\psi(\vec{r}, S)$ of an ENP electron satisfies the Schrödinger equation

$$\left\{\frac{\mu_{xx}}{2}\hat{p}_x^2+\frac{\mu_{yy}}{2}\left(\hat{p}_y+\frac{eH_z}{c}x\right)^2+\frac{\mu_{zz}}{2}\hat{p}_z^2 + \frac{\mu_{xy}}{2}\left[\hat{p}_x\left(\hat{p}_y+\frac{eH_z}{c}x\right)+\left(\hat{p}_y+\frac{eH_z}{c}x\right)\hat{p}_x\right] + \mu_{yz}\left(\hat{p}_y+\frac{eH_z}{c}x\right)\hat{p}_z+\mu_{xz}\hat{p}_x\hat{p}_z + \frac{\hbar\omega_z}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\}\psi(\vec{r}, S)=E\left(1+\frac{E}{E_G}\right)\psi(\vec{r}, S), \tag{14}$$

where

$$\omega_z=eH_z/m_{sz}c \tag{15}$$

is the spin precession angular frequency with respect to the magnetic field (z) direction.

It is found that the left-hand side of Eq. (14) can be diagonalized by two successive unitary transformations defined, respectively, by the unitary operators[20]

$$\hat{\mathfrak{A}}=\exp\left(-\frac{i\mu_{xy}(x\hat{p}_y+eH_z x^2/2c)}{\hbar\mu_{xx}}\right) \tag{16}$$

and

$$\hat{\mathfrak{B}}=\exp\left(-\frac{i\mu_{xz}x\hat{p}_z}{\hbar\mu_{xx}}\right). \tag{17}$$

Therefore, Eq. (14) can be easily solved. The eigenfunctions and the corresponding eigenvalues are[21]

$$\psi_{nSk_yk_z}(\vec{r}, S)=e^{i\Theta(x,k_y,k_z)}\phi_n(\kappa(x-x_0)) \times(L_yL_z)^{-1/2}e^{i(k_yy+k_zz)}\chi_S \tag{18}$$

and

$$E_{nSk_yk_z}=-\tfrac{1}{2}E_G+\{\tfrac{1}{4}E_G^2+E_G[(n+\tfrac{1}{2})\hbar\Omega_z+S\tfrac{1}{2}\hbar\omega_z +\hbar^2k_z^2/2m_{zz}]\}^{1/2}, \tag{19}$$

respectively, where

$$\Omega_z=\frac{eH_z}{(\Delta m/m_{zz})^{1/2}c} \tag{20}$$

is the cyclotron angular frequency, $\Delta m\equiv\det|m_{ij}|$, $m_{ij}(i, j=x, y, z)$ are the effective-mass tensor elements ($\overleftrightarrow{m}=\overleftrightarrow{\mu}^{-1}$);

$$x_0=-\frac{(\hbar k_y-m_{yz}\hbar k_z/m_{zz})c}{eH_z} \tag{21}$$

is the center coordinate of the wave function,

$$\Theta(x, k_y, k_z)=\frac{-\mu_{xy}eH_zx^2}{2\mu_{xx}\hbar c}-\frac{(\mu_{xy}k_y-\mu_{xz}k_z)x}{\mu_{xx}} \tag{22}$$

is the phase factor,

$$\phi_n(\kappa(x-x_0))=N_n\,e^{-\kappa^2(x-x_0)^2/2}H_n(\kappa(x-x_0)), \quad[\kappa=(\Omega_z/\hbar\mu_{xx})^{1/2},\quad N_n=(\kappa/\sqrt{\pi}\;2^n n!)^{1/2}] \tag{23}$$

is the nth order linear harmonic-oscillator wave function, χ_S the spin-wave function, $S=\pm1$, $n=0, 1, 2\ldots$, and $k_{y,z}=(2\pi/L_{y,z})N_{y,z}$ ($N_{y,z}=0, \pm1, \pm2, \ldots$; L_x, L_y, L_z being the dimensions of the system).

With the aid of Eq. (21), we may define the center- and relative-coordinate operators (with reference to the center of migration) for the ENP electron's cyclotron motion in a magnetic field along the z direction (but for arbitrary vector potential $\vec{A}$) as

$$\hat{x}_c=\frac{-(\hat{p}_y-m_{yz}\hat{p}_z/m_{zz})c}{eH_z}, \quad \hat{y}_c=\frac{(\hat{p}_x-m_{xz}\hat{p}_z/m_{zz})c}{eH_z} \tag{24}$$

and

$$\hat{x}_r=\frac{(\hat{\pi}_y-m_{yz}\hat{p}_z/m_{zz})c}{eH_z}, \quad \hat{y}_r=\frac{-(\hat{\pi}_x-m_{xz}\hat{p}_z/m_{zz})c}{eH_z}, \tag{25}$$

respectively, where

$$\hat{\pi}_x=\hat{p}_x+eA_x/c, \quad \hat{\pi}_y=\hat{p}_y+eA_y/c, \quad (\hat{\pi}_z=\hat{p}_z). \tag{26}$$

[For SP electrons, or for a magnetic field along one of the principal axes of the Fermi ellipsoid, Eqs. (24) and (25) reduce to the simple forms given by Kubo *et al.*[3,4]]

IV. MAGNETOCONDUCTIVITY TENSOR ELEMENTS OF ENP ELECTRONS EXPRESSED IN TERMS OF MIGRATION-CENTER COORDINATES

With the one-particle center- and relative-coordinate operators of the electron's cyclotron motion defined above, we can follow the method of Kubo *et al.*[3,4] to calculate the magnetoconductivity tensor for a system of N ENP electrons using Eq. (10). In the case where the magnetic field $\vec{H}$ is along the z axis, the results are[20]

$$\sigma_{xx}(H_z)=\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{X}}_c(-i\hbar\lambda)\dot{\hat{X}}_c(t)\rangle, \tag{27}$$

$$\sigma_{yy}(H_z)=\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{Y}}_c(-i\hbar\lambda)\dot{\hat{Y}}_c(t)\rangle, \tag{28}$$

$$\sigma_{zz}(H_z)=\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{Z}}(-i\hbar\lambda)\dot{\hat{Z}}(t)\rangle, \tag{29}$$

$$\sigma_{xy}(H_z)=\frac{-nec}{H_z}+\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{Y}}_c(-i\hbar\lambda)\dot{\hat{X}}_c(t)\rangle, \tag{30}$$

$$\sigma_{yx}(H_z)=\frac{nec}{H_z}+\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{X}}_c(-i\hbar\lambda)\dot{\hat{Y}}_c(t)\rangle, \tag{31}$$

$$\sigma_{xz}(H_z)=\frac{m_{yz}}{m_{zz}}\frac{nec}{H_z}+\frac{e^2}{V}\int_0^\infty dt\int_0^\beta d\lambda\,\langle\dot{\hat{Z}}(-i\hbar\lambda)\dot{\hat{X}}_c(t)\rangle, \tag{32}$$

$$\sigma_{zx}(H_z) = -\frac{m_{yz}}{m_{zz}}\frac{nec}{H_z} + \frac{e^2}{V}\int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\hat{X}}_c(-i\hbar\lambda)\dot{\hat{Z}}(t)\rangle, \tag{33}$$

$$\sigma_{yz}(H_z) = -\frac{m_{xz}}{m_{zz}}\frac{nec}{H_z} + \frac{e^2}{V}\int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\hat{Z}}(-i\hbar\lambda)\dot{\hat{Y}}_c(t)\rangle, \tag{34}$$

$$\sigma_{zy}(H_z) = \frac{m_{xz}}{m_{zz}}\frac{nec}{H_z} + \frac{e^2}{V}\int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\hat{Y}}_c(-i\hbar\lambda)\dot{\hat{Z}}(t)\rangle, \tag{35}$$

where

$$n = \frac{N}{V}, \quad X_c = \sum_{i=1}^{N} x_c^{(i)}, \quad Y_c = \sum_{i=1}^{N} y_c^{(i)}, \quad Z = \sum_{c=1}^{N} z^{(i)}.$$

It is worth noting that two essential conditions must be satisfied for the validity of these equations.[3] One is $\Omega_z\tau \gg 1$; under this condition, the correlation between successive jumps of the centers of electronic cyclotron motion due to collisional processes can be neglected, convenient for the use of center-migration picture. The other is that the relative coordinates of the electronic cyclotron motion are bounded; therefore, the statistical averages of the relative velocities in this motion are zero. We thus can get rid of the relative-relative and center-relative terms in the derivation of these equations. The latter condition is satisfied for a system of ENP electrons as long as they are moving on closed Fermi surfaces.

In the following discussions we shall assume that the applied magnetic field is sufficiently strong so that the second terms in Eqs. (30)–(35) can be neglected[22] when compared with their respective first terms. Therefore, we have

$$\begin{aligned}
&\sigma_{xy}(H_z) = -\sigma_{yx}(H_z) = -nec/H_z,\\
&\sigma_{xz}(H_z) = -\sigma_{zx}(H_z) = (m_{yz}/m_{zz})(nec/H_z),\\
&\sigma_{yz}(H_z) = -\sigma_{zy}(H_z) = -(m_{xz}/m_{zz})(nec/H_z).
\end{aligned} \tag{36}$$

As for the diagonal magnetoconductivity tensor elements shown in Eqs. (27)–(29), they can be further reduced from the many-electron description to the one-electron description with the aid of similar manipulations as have been used by Kubo *et al.* for the SP electrons.[3,4] If we omit all the perturbations other than those due to the weak applied electric field and the impurity scattering, and further assume that the impurity scattering centers are distributed randomly in the sample, we have, in the lowest-order of perturbation,[20]

$$\sigma_{xx}(H_z) = \frac{\pi\hbar e^2}{V}\int_{E_{\min}}^\infty dE\left(-\frac{\partial f_0}{\partial E}\right) \times [\mathrm{tr}(\delta(E-\hat{H})\dot{\hat{x}}_c\,\delta(E-\hat{H})\dot{\hat{x}}_c)]_{sc}, \tag{37}$$

$$\sigma_{yy}(H_z) = \frac{\pi\hbar e^2}{V}\int_{E_{\min}}^\infty dE\left(-\frac{\partial f_0}{\partial E}\right) \times [\mathrm{tr}(\delta(E-\hat{H})\dot{\hat{y}}_c\,\delta(E-\hat{H})\dot{\hat{y}}_c)]_{sc}, \tag{38}$$

$$\sigma_{zz}(H_z) = \frac{\pi\hbar e^2}{V}\int_{E_{\min}}^\infty dE\left(-\frac{\partial f_0}{\partial E}\right) \times [\mathrm{tr}(\delta(E-\hat{H})\hat{v}_z\,\delta(E-\hat{H})\hat{v}_z)]_{sc}, \tag{39}$$

where $f_0 \equiv f_0(E) = 1/[1+e^{\beta(E-\zeta)}]$, ζ is the chemical potential, tr denotes taking the trace in the one-electron space, $\delta(x)$ is the Dirac δ function, $E_{\min} = -\frac{1}{2}E_G$ measured from the bottom of the conduction band as can be easily seen from Eq. (19), subscript sc means averaging over variables of the scatters contained in the scattering potential, and $\hat{v}_z$ is the one-electron velocity (z component) operator, which in this magnetic field (parallel to the z axis) configuration can be expressed as

$$\hat{v}_z = i[\hat{H}+\hat{H}_I(\hat{\mathbf{r}}), z]/\hbar = \frac{\mu_{zz}\hat{p}_z + \mu_{yz}(\hat{p}_y + eH_z x/c) + \mu_{xz}\hat{p}_x}{1+2\hat{H}/E_G}, \tag{40}$$

$\dot{\hat{x}}_c$ and $\dot{\hat{y}}_c$ are related to the impurity scattering potential $\hat{H}_I(\hat{\mathbf{r}})$ [henceforth denoted by $U(\hat{\mathbf{r}})$], respectively, by the relations

$$\dot{\hat{x}}_c = i[U(\hat{\mathbf{r}}), \hat{x}_c]/\hbar \quad \text{and} \quad \dot{\hat{y}}_c = i[U(\hat{\mathbf{r}}), \hat{y}_c]/\hbar \tag{41}$$

because $\hat{x}_c$ and $\hat{y}_c$ as defined in Eq. (24) both commute with $\hat{H}$. Equations (37)–(39) are correct only for elastic scattering process. The two Dirac δ functions appearing in these equations indicate that the energies of the electrons in the initial and final states are equal as required by the conservation of energy in this scattering process.

To account for the nonparabolicity explicitly in the magnetoconductivity formulas, we now introduce a variable ϵ, which is defined by

$$\epsilon = E(1+E/E_G) \quad \text{or} \quad E = -\tfrac{1}{2}E_G + (\tfrac{1}{4}E_G^2 + E_G\epsilon)^{1/2}, \tag{42}$$

consistent with $\hat{\mathcal{H}} = \hat{H}(1+\hat{H}/E_G)$ as defined in Eq. (8). As[23]

$$\delta(\epsilon - \hat{\mathcal{H}}) = \frac{\delta(E-\hat{H}) + \delta(E+E_G+\hat{H})}{1+2\hat{H}/E_G}, \tag{43}$$

and according to the work of Smith, Baraff, and Rowell[16] (SBR) the energy of the ENP electrons can not be so small as to fall below $-\frac{1}{2}E_G$ measured from the bottom of the conduction band [see Eq. (19)], we have, when these operators are acting on the eigenfunction of $\hat{H}$,

$$\delta(E-\hat{H}) = (1+2E/E_G)\,\delta(\epsilon - \hat{\mathcal{H}}). \tag{44}$$

We have now reached the point for detailed calculation of the diagonal magnetoconductivity tensor elements for the ENP electrons. Let us start with the transverse magnetoconductivity. Substituting Eq. (44) into Eq. (37), making use of Eq. (41) and

the basis functions shown in Eq. (18), and noting that these functions are also the eigenfunctions of $\hat{x}_c$ with eigenvalues x_0 defined in Eq. (21), we can thus obtain

$$\sigma_{xx}(H_z) = \frac{\pi e^2}{\hbar V} \int_{-E_G/2}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\left(1+\frac{2E}{E_G}\right)^2 \times \sum_{\nu,\nu'} [\,|\langle \nu | U(\vec{r}) | \nu' \rangle|^2]_{sc}(x_0 - x_0')^2 \times \delta(\epsilon - \epsilon_\nu)\,\delta(\epsilon - \epsilon_{\nu'}), \quad (45)$$

where $\nu \equiv nSk_y k_z$, $\nu' \equiv n'S'k_y'k_z'$, $|\nu\rangle$ is just $\psi_{nSk_yk_z}(\vec{r}, S)$ as defined in Eq. (18), $\epsilon_\nu = \epsilon_{nSk_yk_z}$, and x_0' is defined by $-(\hbar k_y' - m_{yz}\hbar k_z'/m_{zz})c/eH_z$ [Eq. (21)].

To simplify the problem, we may assume that the ENP electrons are elastically scattered by N_I randomly distributed centers with δ-function-like impurity scattering potential, i.e.,

$$U(\vec{r}) = \sum_{j=1}^{N_I} U\delta(\vec{r} - \vec{R}_j), \quad (46)$$

where U is the strength of the potential, $\vec{r}$ the electron coordinate, and $\vec{R}_j$ the position of the jth impurity scattering center. Further calculation starting directly from Eq. (45) can be easily made, the final result is[20]

$$\sigma_{xx}(H_z) = \frac{e^2 W \Delta m}{(2\pi)^3 \hbar^5}\,\mu_{xx}\hbar\,\Omega_z \int_{-E_G/2}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\left(1+\frac{2E}{E_G}\right)^2 \times \sum_{nn'S} \frac{n+n'+1}{[\epsilon - (n+\frac{1}{2})\hbar\Omega_z - S\frac{1}{2}\hbar\omega_z]^{1/2}[\epsilon - (n'+\frac{1}{2})\hbar\Omega_z - S\frac{1}{2}\hbar\omega_z]^{1/2}}, \quad (47)$$

where the quantum numbers n, n', and S run over those values such that the quantities in the radicands are non-negative[16] (this restriction shall be maintained whenever such radicands appear in the following discussions), and

$$W \equiv N_I U^2/V. \quad (48)$$

It is obvious that Eq. (47) goes over to DP's result for EP electrons when $E_G \to \infty$, and to that of Kubo *et al.*[4] for SP electrons when appropriate limit is taken.

Equation (47), as it shows, is a consequence of ideally sharp energy levels. It might be a good approximate (lowest-order-perturbation) expression if its value remains finite. As was first pointed out by DP, and later carefully investigated by Kubo *et al.*,[4] the corresponding sharp-level result for SP (or EP) electrons leads to logarithmic divergence. The presence of this same feature in the ENP electron case can be easily seen as follows: Since $\epsilon = E(1+E/E_G)$, and $E(n,S)$, the lower limit of integration (on E) of the term $n=n'$ ($S=+$ or $-$) in $\sigma_{xx}(H_z)$ of Eq. (47), is determined by the relation

$$E(n,S)[1+E(n,S)/E_G] \equiv \epsilon(n,S) = (n+\tfrac{1}{2})\hbar\Omega + \tfrac{1}{2}S\hbar\omega,$$

we have, when integrating this single term,

$$\int_{E(n,S)}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\frac{(1+2E/E_G)^2\,dE}{\epsilon - \epsilon(n,S)} \geq \int_{E(n,S)}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\frac{\{1+[E+E(n,S)]/E_G\}^2}{E(1+E/E_G) - E(n,S)[1+E(n,S)/E_G]} \geq \left(1+\frac{2E(n,S)}{E_G}\right)\int_{E(n,S)}^{\infty}\left(-\frac{\partial f_0}{\partial E}\right)\frac{dE}{E - E(n,S)}. \quad (49)$$

The last integral on the right-hand side of this equation is approximately equal[4] to $(kT)^{-1}\{\ln[kT/(E - E(n,S))]\}_{E=E(n,S)}$. Thus, $\sigma_{xx}(H_z)$ as given in Eq. (47) also shows logarithmic divergence.

To avoid this divergence, we employed the theoretical damping formulation developed by van Hove.[24] In doing this, we first replace $\delta(E-\hat{H})$ in Eq. (37) by $(1+2E/E_G)\,\delta(\epsilon - \hat{\mathcal{H}})$ [see Eq. (44)], and then make use of the substitution

$$\delta(\epsilon - \hat{\mathcal{H}}) \to \hat{S}(\epsilon) = \hat{\Gamma}(\epsilon)/\pi\,\{[\hat{\mathcal{H}} + \hat{\Delta}(\epsilon) - \epsilon]^2 + \hat{\Gamma}^2(\epsilon)\}, \quad (50)$$

where $\hat{\Gamma}(\epsilon)$ is the effective level-width operator and $\hat{\Delta}(\epsilon)$ the effective level-shift operator. To first-order-perturbation approximation in the ENP electron case, $\hat{\Gamma}(\epsilon)$ and $\hat{\Delta}(\epsilon)$ are defined by the relations

$$\hat{\Delta}(\epsilon) \mp i\hat{\Gamma}(\epsilon) = \lim_{\eta \to 0^+} \hat{G}(\epsilon \pm i\eta), \quad (51)$$

$$\hat{G}(\epsilon) = -U_{eff}(\vec{r})[\hat{\mathcal{H}} + \hat{G}(\epsilon) - \epsilon]^{-1} U_{eff}(\vec{r}), \quad (52)$$

and

$$U_{eff}(\vec{r}) = U(\vec{r}) + [\hat{H}U(\vec{r}) + U(\vec{r})\hat{H}]/E_G. \quad (53)$$

The last equation is due to the fact that

$$\delta(\epsilon - [\hat{H} + U(\vec{r})]\{1 + [\hat{H} + U(\vec{r})]/E_G\}) \cong \delta(\epsilon - \hat{\mathcal{H}} - U(\vec{r}) - [\hat{H}U(\vec{r}) + U(\vec{r})\hat{H}]/E_G) \quad (54)$$

when we retain only the first-order terms of $U(\vec{r})$. Exact solutions for the average values of $\hat{\Gamma}(\epsilon)$ and $\hat{\Delta}(\epsilon)$ are rather difficult to find as the value of $\langle G_\nu(\epsilon)\rangle_{sc} \equiv [\langle \nu | \hat{G}(\epsilon) | \nu \rangle]_{sc}$ is determined by the following complicated equation:

$$\langle G_\nu(\epsilon)\rangle_{sc} = -\sum_{\nu'} \frac{\langle |\langle \nu | U_{eff}(\vec{r}) | \nu' \rangle|^2 \rangle_{sc}}{\epsilon_{\nu'} + \langle G_{\nu'}(\epsilon)\rangle_{sc} - \epsilon} = -\sum_{\nu'} \frac{[1 + (E + E_{\nu'})/E_G]\langle |\langle \nu | U(\vec{r}) | \nu' \rangle|^2 \rangle_{sc}}{\epsilon_{\nu'} + \langle G_{\nu'}(\epsilon)\rangle_{sc} - \epsilon}. \quad (55)$$

In practical problems, $\langle \Gamma_\nu(\epsilon)\rangle_{sc}$ as well as $\langle \Delta_\nu(\epsilon)\rangle_{sc}$ is not too large. We may then put $E_{\nu'} \approx E$ in (55). This approximation does not lead to serious error because $\langle G_\nu(\epsilon)\rangle_{sc}$ has a dominant value only at $\epsilon = \epsilon_{\nu'}$ (or $E = E_{\nu'}$). With this preparation and after Kubo *et al.*[4] and Miyake's[25] treatment of the SP electrons, we can easily find the transverse magnetoconductivity of ENP electrons in the broadened-level case as

$$\sigma_{xx}(H_z) = \frac{e^2 W \Delta m}{2(2\pi)^3 \hbar^5} \mu_{xx} \hbar\Omega_z \int_{-E_G/2}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\left(1 + \frac{2E}{E_G}\right)^2 \sum_{nn'S} (n + n' + 1) \times \prod_{i=n,n'} \left(\frac{[\epsilon - (i + \tfrac{1}{2})\hbar\Omega_z - S\tfrac{1}{2}\hbar\omega_z - \Delta] + \{[\epsilon - (i + \tfrac{1}{2})\hbar\Omega_z - S\tfrac{1}{2}\hbar\omega_z - \Delta]^2 + \Gamma^2\}^{1/2}}{[\epsilon - (i + \tfrac{1}{2})\hbar\Omega_z - S\tfrac{1}{2}\hbar\omega_z - \Delta]^2 + \Gamma^2} \right)^{1/2}, \quad (56)$$

where

$$\Gamma = \frac{\sqrt{3}}{2}\left[\frac{W}{4\pi}\frac{eH_z}{\hbar c}\left(1 + \frac{2E}{E_G}\right)^2 \left(\frac{2m_{zz}}{\hbar^2}\right)^{1/2}\right]^{2/3}, \quad \Delta = -\frac{\Gamma}{\sqrt{3}} \quad (57)$$

when the magnetic field is so strong that the Landau level separation is large and the transitions between different Landau levels can be neglected. As both Γ and Δ approach zero, Eq. (56) obviously goes over to Eq. (47).

The expressions for $\sigma_{yy}(H_z)$ can be obtained in a similar way, or simply by replacing all the subscripts x by y in Eq. (47) for the sharp-level result and in Eq. (56) for the broadened-level result.

V. LONGITUDINAL MAGNETOCONDUCTIVITY TENSOR ELEMENTS

From Eq. (40) we see that the longitudinal component velocity operator $\hat{v}_z$ does not depend on the perturbation potential $U(\vec{r})$; thus the longitudinal magnetoconductivity tensor element $\sigma_{zz}(H_z)$ as given in Eq. (39) is much easier for further calculation. By making use of Eqs. (18), (22), and (40), we arrive at

$$\langle \nu' | \hat{v}_z | \nu \rangle = \left(1 + \frac{2E}{E_G}\right)^{-1} \left[\langle \nu' | \mu_{zz}\hbar k_z + \mu_{yz}\left(\hbar k_y + \frac{eH_z x}{c}\right) + \mu_{xz}\hbar\frac{\partial\Theta}{\partial x} | \nu \rangle + \frac{\hbar}{i}\mu_{xz}\int \phi^*_{n'}(\kappa(x - x_0))\frac{\partial}{\partial x}\phi_n(\kappa(x - x_0))dx \right] \delta_{k_y', k_y}\delta_{k_z', k_z}\delta_{S',S}, \quad (58)$$

where δ_{k_y', k_y}, etc, are the Kronecker δ symbols. It follows that

$$|\langle \nu | \hat{v}_z | \nu' \rangle^2| = \left(1 + \frac{2E_\nu}{E_G}\right)^{-2}\left(\frac{\hbar k_z}{m_{zz}}\right)^2 \delta_{\nu',\nu} + \left(1 + \frac{2E_\nu}{E_G}\right)^{-1}\left(1 + \frac{2E_{\nu'}}{E_G}\right)^{-1} \times \frac{1}{2}\left(\mu_{zz} - \frac{1}{m_{zz}}\right)[n\delta_{n',n-1} + (n+1)\delta_{n',n+1}]\delta_{k_y', k_y}\delta_{k_z', k_z}\delta_{S',S}, \quad (59)$$

and Eq. (39) reduces to the form

$$\sigma_{zz}(H_z) = \frac{\pi\hbar e^2}{V}\int_{-E_G/2}^{\infty} dE \left(-\frac{\partial f_0}{\partial E}\right)\left(1 + \frac{2E}{E_G}\right)^{-2}\left[\sum_\nu \left(\frac{\hbar k_z}{m_{zz}}\right)^2 \delta(E - E_\nu)\,\delta(E - E_\nu)\right]_{sc} \quad (60)$$

as the off-diagonal terms in $|\langle \nu | \hat{v}_z | \nu' \rangle|^2$ have all been dropped out in the case of elastic scattering. The two identical δ functions appearing in this equation indicate that the longitudinal current will be infinitely large if the collision with crystalline imperfections is absent. This can be compared with the transverse case; without collision, the transverse magnetoconductivity will be zero [see Eq.

(56)]. Thus, both of these results are in agreement with the classical picture of electronic motion in constant and uniform electric and magnetic fields.

Since $\delta(E-E_\nu)\,\delta(E-E_{\nu'})=\delta(0)\,\delta(E-E_\nu)$, if we consider transitions in a given time interval $(-\tau,\tau)$, the δ function will be smeared out and $\delta(0)$ can be related to the relaxation time τ by[26]

$$\delta(0)=\tau/\pi\hbar\,. \tag{61}$$

We may, with the aid of Eq. (44), obtain

$$\sigma_{zz}(H_z)=\frac{e^2}{V}\int_{-E_G/2}^{\infty}dE\left(-\frac{\partial f_0}{\partial E}\right)\left(1+\frac{2E}{E_G}\right)^{-1}\times\sum_{nSk_yk_z}\left(\frac{\hbar k_z}{m_{zz}}\right)^2\tau(E,S)\,\delta(\epsilon-\epsilon_\nu), \tag{62}$$

or, after some mathematical manipulation,[20]

$$\sigma_{zz}(H_z)=\frac{e^2}{4\pi^2}\,\frac{(2\Delta m)^{1/2}}{\hbar^3}\,\frac{\hbar\Omega_z}{m_{zz}}\int_{-E_G/2}^{\infty}dE\left(-\frac{\partial f_0}{\partial E}\right)\left(1+\frac{2E}{E_G}\right)^{1}\times\sum_{n,S}\tau(E,S)\left[\epsilon-(n+\tfrac{1}{2})\hbar\Omega_z-S\tfrac{1}{2}\hbar\omega_z\right]^{1/2}, \tag{63}$$

where we have, for the reason to be made clear in the following paragraph, assumed τ to be energy and spin dependent. This equation is in agreement with that of Argyres[5] for the spinless SP electrons when we take the appropriate limits.

The relaxation time $\tau(E,S)$ appearing in the above equations can be computed from the definition[27]

$$1/\tau(E_\nu,S)=\sum_{\nu'}W_{\nu\nu'}(k_z-k_z')/k_z,$$
$$W_{\nu\nu'}=(2\pi/\hbar)\left[\,|\langle\nu|\,U(\vec{\mathbf{r}})\,|\nu'\rangle|^2\right]_{sc}\delta(E_\nu-E_{\nu'}). \tag{64}$$

Simple calculations making use of the δ-function-like potential defined in Eq. (46) lead to the expression

$$\frac{1}{\tau(E,S)}=\frac{2\pi}{\hbar}\,W\,\frac{(2\Delta m)^{1/2}}{4\pi^2\hbar^3}\,\hbar\Omega_z\left(1+\frac{2E}{E_G}\right)\times\sum_{n'}\left[E\left(1+\frac{E}{E_G}\right)-\left(n'+\frac{1}{2}\right)\hbar\Omega_z-S\tfrac{1}{2}\hbar\omega_z\right]^{-1/2}. \tag{65}$$

This result, when appropriate limit is taken, is also in agreement with that of Argyres[5] for spinless SP electrons.

On substituting Eq. (65) into Eq. (63), we obtain a longitudinal magnetoconductivity formula, which, like the transverse magnetoconductivity [Eq. (47) or (56)], can be evaluated if the strength of the δ-function-like scattering potential U (and thus $W=N_IU/V$) is known. Equations (65) and (63) are indeed "sharp-level" expressions. However, since they give, respectively, only finite values of τ and $\sigma_{zz}(H_z)$, these equations can be considered as reasonable lowest-order-perturbation results. Thus we shall not discuss the broadened-level case for these quantities.

Up to now we have worked out all the magnetoconductivity tensor elements for the ENP electrons in a magnetic field arbitrarily oriented with respect to the Fermi ellipsoid. Further calculation for the magnetoresistance and Hall effect in a sufficiently strong magnetic field (such that there are only a few Landau levels below the Fermi energy and $\Omega_z\tau\gg1$) can be easily carried out starting from these explicit expressions. In the above discussion, we have restricted ourselves to the case of a magnetic field along the z direction. However, as we have mentioned before, this direction is arbitrarily oriented with respect to the Fermi ellipsoid. Thus, for a magnetic field along the other directions (x,y), similar expressions can be easily obtained from these results simply by cyclic permutation over the subscripts x, y, and z. It is to be remarked that, for short-range (other than the δ-function-like) scattering potential, the above-mentioned results are still valid if W is appropriately redefined.[4,20] In this connection, the usefulness of these expressions can be extended somewhat.

VI. MODERATELY STRONG-FIELD LIMIT

If the magnetic field is so strong that Eq. (36) is approximately valid, and sufficiently weak that $\hbar\Omega_z\ll\zeta$ but the condition $\Omega_z\tau\gg1$ still holds, we can neglect the electron spin and replace the summations in Eqs. (47) [or (56)], (63), and (65) by integrations. The result is

$$\vec{\sigma}(H_z)=\begin{bmatrix}\mu_{xx}I_T & -nec/H_z & (m_{yz}/m_{zz})\,nec/H_z\\ nec/H_z & \mu_{yy}I_T & -(m_{xz}/m_{zz})\,nec/H_z\\ -(m_{yz}/m_{zz})\,nec/H_z & (m_{xz}/m_{zz})\,nec/H_z & I_L/m_{zz}\end{bmatrix}, \tag{66}$$

where

$$[I_T,I_L]\equiv\frac{e^2}{3\pi^2\Delta m}\,\frac{(2\Delta m)^{3/2}}{\hbar^2}\int_0^{\infty}dE\left(-\frac{\partial f_0}{\partial E}\right)\epsilon^{3/2}\left(\frac{1+2E/E_G}{\Omega_z^2\tau(E)},\ \frac{\tau(E)}{1+2E/E_G}\right), \tag{67}$$

and $\tau(E)$ the zero-field relaxation time, which is related to W by the expression

$$\frac{1}{\tau(E)} = \frac{W}{\pi\hbar^4}\left(1+\frac{2E}{E_G}\right)(2\Delta m\epsilon)^{1/2} \tag{68}$$

as can be easily figured out with the aid of Eq. (64).

These results are the same as those derived in a separate paper[20,28] where we discussed the galvanomagnetic properties of the ENP electrons in weak magnetic fields by means of a "drift-momentum" approach, and, after taking the limit $E_G \to \infty$, agree with that obtained by Mase *et al.*[21]

VII. TRANSVERSE MAGNETORESISTANCE OF BISMUTH

Let us calculate the transverse magnetoresistance of bismuth as an application of the above results derived for the magnetoconductivity of ENP electrons. In order to compare our calculated result with some published experimental data[29] and other computations,[10] we assume that $T = 4.2\ ^\circ\mathrm{K}$, the applied electric field is along the trigonal (z) axis, and the strong magnetic field along the bisectrix (y) axis of single-crystal bismuth. Summing up all the contributions due to the holes and the ENP electrons residing on the three Fermi ellipsoids, we have the total magnetoconductivity tensor as [see Eqs. (36), (56), and (63)]

$$\vec{\sigma}^{(t)}(H_y,T) = \sum_{i=i}^{4}\begin{bmatrix} \sigma_{xx}^{(i)}(H_y) & n_i q_i m_{yz}^{(i)}/m_{yy}^{(i)}H_y & -n_i q_i c/H_y \\ -n_i q_i c m_{yz}^{(i)}/m_{yy}^{(i)}H_y & \sigma_{yy}^{(i)}(H_y) & n_i q_i c m_{xy}^{(i)}/m_{yy}^{(i)}H_y \\ n_i q_i c/H_y & -n_i q_i c m_{xy}^{(i)}/m_{yy}^{(i)}H_y & \sigma_{zz}^{(i)}(H_y) \end{bmatrix}, \tag{69}$$

where $q_i = -e$ ($i = 1, 2, 3$, for electrons), $q_i = +e$ ($i = 4$ for holes), n_i is the electron ($i = 1, 2, 3$) or the hole ($i = 4$) concentration, and $m_{jk}^{(i)}$ ($i = 1, 2, 3$; $j, k = x, y, z$) are related by C_3 symmetry. The explicit expressions of $\sigma_{zz}^{(i)}(H_y)$ [as well as $\sigma_{xx}^{(i)}(H_y)$] and $\sigma_{yy}^{(i)}(H_y)$ can be obtained, respectively, from Eqs. (56) and (63) by cyclic permutation in the subscripts x, y, z, and the corresponding expression for $i = 4$ assumes a simpler form as the holes follow EP model dispersion relation.

Values of the chemical potential at the specified constant temperature, implicitly contained in the magnetoconductivity formulas through the Fermi distribution function for electrons and holes, can be determined with the aid of the charge neutrality condition

$$\sum_{i=1}^{4} q_i n_i = -e(n_1+n_2+n_3-n_4) = 0. \tag{70}$$

The explicit forms of the n_i's of ENP electron are

$$n_i = \frac{(2\Delta m^{(i)})^{1/2}}{2\pi^2\hbar^3}\hbar\Omega_y^{(i)}\int_{-E_G/2}^{\infty} dE\left(-\frac{\partial f_0}{\partial E}\right)\sum_{n,S}\left[E(1+E/E_G)-(n+\tfrac{1}{2})\hbar\Omega_y^{(i)}-S\tfrac{1}{2}\hbar\omega_y^{(i)}\right]^{1/2} \quad \text{(electrons, } i=1,2,3\text{)},$$
$$n_i = \frac{(2\Delta m^{(i)})^{1/2}}{2\pi^2\hbar^3}\hbar\Omega_y^{(i)}\int_{E_{4\,\min}}^{\infty} dE\left(-\frac{\partial f_0^{(h)}(E-E_0)}{\partial E}\right)\sum_{n,S}\left[E-(n+\tfrac{1}{2})\hbar\Omega_y^{(i)}-S\tfrac{1}{2}\hbar\omega_y^{(i)}\right] \quad \text{(holes, } i=4\text{)}, \tag{71}$$

where $E_{4\,\min} = \frac{1}{2}\hbar(\Omega_y^{(4)} - \omega_y^{(4)})$. Numerical calculation has been performed using SBR's data. The results[30] are illustrated in Figs. 1 and 2. From Fig. 1, in which n_i is denoted by $n_i^{(e)}$ for $i = 1, 2, 3$, and n_4 by $n^{(h)}$, we see that n_1 is approximately equal to n_2 ($= n_3$ by symmetry) for a magnetic field roughly up to 26 kG.

By making use of this approximation as well as Eq. (70), we can simplify Eq. (69) to the form

$$\vec{\sigma}^{(t)}(H_y,T) = \sum_{i=1}^{4}\begin{bmatrix} \sigma_{xx}^{(i)}(H_y) & n_i q_i c m_{yz}^{(i)}/m_{yy}^{(i)}H_y & 0 \\ -n_i q_i c m_{yz}^{(i)}/m_{yy}^{(i)}H_y & \sigma_{yy}^{(i)}(H_y) & 0 \\ 0 & 0 & \sigma_{zz}^{(i)}(H_y) \end{bmatrix} \tag{72}$$

since $m_{xy}^{(1)} = 0$, $m_{xy}^{(2)} = -m_{xy}^{(3)}$, and $m_{xy}^{(4)} = 0$. Therefore, when the applied electric field is along the trigonal (z) direction and the applied magnetic field along the bisectrix (y) direction, the total transverse magnetoresistivity $\rho_{zz}(H_y, T)$ of single-crystal bismuth is approximately of the simple form

$$\rho_{zz}(H_y,T) = 1\Big/\sum_{i=1}^{4}\sigma_{zz}^{(i)}(H_y). \tag{73}$$

Furthermore, the zero-magnetic-field electrical

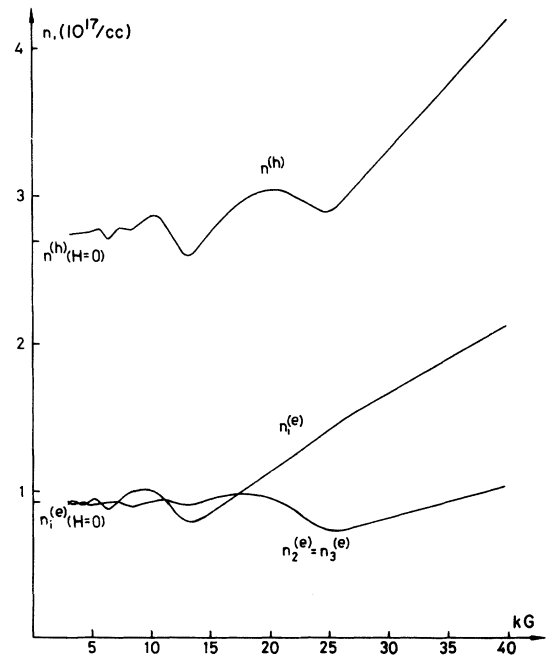

FIG. 1. Charge carrier density of single-crystal bismuth at $T=4.2\,^{\circ}\mathrm{K}$ vs H (parallel to the bisectrix axis). $n_1^{(e)}$ refers to the concentration of charge carriers in the electron ellipsoid with lighter cyclotron effective mass.

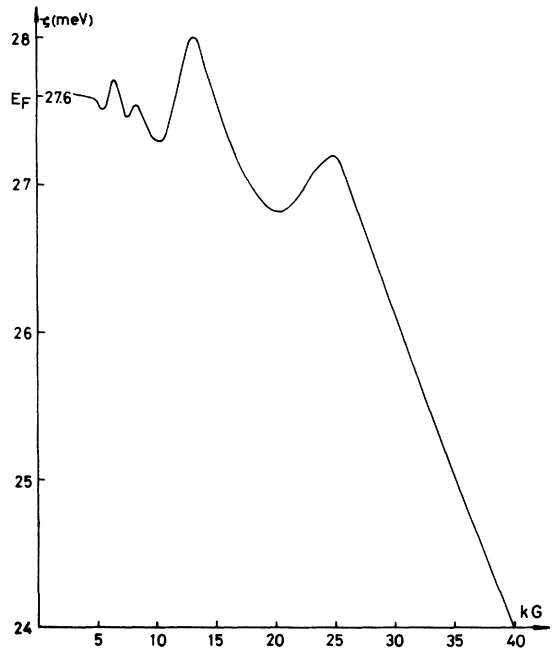

FIG. 2. Fermi energy of single-crystal bismuth at $T=4.2\,^{\circ}\mathrm{K}$ vs H (parallel to the bisectrix axis).

resistivity of single-crystal bismuth at $0\,^{\circ}\mathrm{K}$ can be found to be[28]

$$\rho_{zz}(0,0)=1\Big/\sum_{i=1}^{4}\sigma_{zz}^{(i)}(0,0), \tag{74}$$

$$\sigma_{zz}^{(i)}(0,0)=\frac{n^{(-)}e^2\tau_e(E_F)\mu_{zz}^{(i)}}{3(1+2E_F/E_G)} \quad (i=1,2,3),$$

$$\sigma_{zz}^{(4)}(0,0)=n^{(+)}e^2\tau_h(E_F)\mu_{zz}^{(4)}, \tag{75}$$

where $\tau_e(E_F)$ [or $\tau_h(E_F)\equiv\tau_h(E_0-E_F)$], E_F (or E_0-E_F), and $n^{(-)}$ (or $n^{(+)}$) are the zero-field relaxation time, Fermi energy, and the concentration of the electrons (or the holes) at $0\,^{\circ}\mathrm{K}$, respectively.

Numerical values of ρ/ρ_0 [$\equiv\rho_{zz}(H_y,T)/\rho_{zz}(0,0)$] at $T=4.2\,^{\circ}\mathrm{K}$ versus a magnetic field H_y from 5 to 26 kG have been calculated with the aid of an IBM 1130 computer. The result is illustrated in Fig. 3, in which the nine dots denote the experimental data of de Haas *et al.*[29] In this calculation, the zero-field relaxation times are taken to be

$$\tau_e(E_F)\cong 2.26\times10^{-10}\ \text{sec},\quad \tau_h(E_F)\cong 1.24\times10^{-10}\ \text{sec}. \tag{76}$$

It is noted that in DP's work,[10] the ρ/ρ_0-vs-H_y curve was calculated with $\tau_e=\tau_h=4\times10^{-10}$ sec. In the comparison of their magnetoresistance curve with the present one, we see two noticeable differences: (i) Our curve shows more oscillations; (ii) the oscillation amplitudes in our curve are much

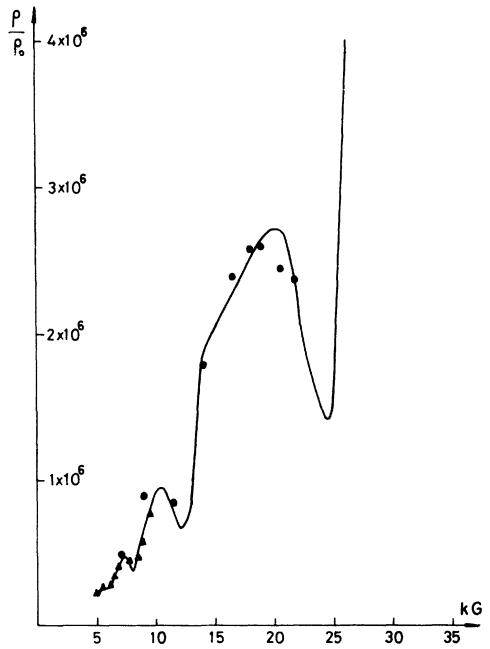

FIG. 3. Computed transverse magnetoresistance curve of single-crystal bismuth at $T=4.2\,^{\circ}\mathrm{K}$ vs H (5 to 26 kG, parallel to the bisectrix axis) when the electric field $\vec{F}$ is along the trigonal axis. The nine dots represent the experimental data of de Haas *et al.* (Ref. 29). Triangles are recent experimental values obtained by P. W. Chao (private communication).

larger. [In Fig. 3, the magnetoresistance maxima with $(\rho/\rho_0)\times 10^6 = 0.274,\ 0.467,\ 0.964,\ 2.74$ occur approximately at $H_y = 5.5,\ 7.5,\ 10.5,\ 20$ kG while the minima with $(\rho/\rho_0)\times 10^6 = 0.251,\ 0.377,\ 0.674,\ 1.43$ occur approximately at 6, 8, 12, 24.5 kG, respectively. Also included in this figure are some recent low-field experimental values obtained by P. W. Chao (private communication).]

VIII. REMARKS ON OSCILLATORY AND ASYMPTOTIC BEHAVIOR

From our results of calculation as shown in Figs. 1–3, all the quantities n_i, ζ, and ρ contain both an oscillatory as well as a monotonic variation with the magnetic field. The oscillatory part may be understood in the usual way as in the case of SP electrons while the monotonic part can be more complicated. Since the experimental curves are always due to a superposition of the two parts, the relative minima in the magnetoresistance curve do not necessarily coincide with the minima in the oscillatory part. The difference in position of the mininum which depends on the contribution due to the monotonic part can become quite sizable in some semimetals.

If we ignore the monotonic field dependence and spin splitting, Eqs. (47) and (71) give the approximate oscillations in $\sigma_{xx}^{(i)}$ and n_i, respectively, ($i = 1, 2, 3, 4$) with periods in $1/H$ as

$$\Delta^{(i)}(1/H_y) = \frac{e\hbar}{m_{cy}^{(i)} c\zeta(1+\zeta/E_G)} \quad \text{(electrons, } i=1,2,3\text{)},$$
$$\Delta^{(4)}(1/H_y) = \frac{e\hbar}{m_{cy}^{(4)} c(\Delta-\zeta)} \quad \text{(holes)}. \tag{77}$$

These results are in accord with those calculated from the simple Onsager relation[31]

$$\Delta(1/H) = 2\pi e\hbar/cS_{\max}, \tag{78}$$

where $S_{\max}$ is the extremal cross-section area of the Fermi ellipsoid in a plane perpendicular to the field $\vec{H}$. Using the parameters given by SBR with $\zeta \sim 27.6$ meV, we obtain from (77)

$$\Delta^{(1)}(1/H_y) \approx 0.082\ \text{kG}^{-1},$$
$$\Delta^{(2),(3)}(1/H_y) \approx 0.041\ \text{kG}^{-1}, \tag{79}$$
$$\Delta^{(4)}(1/H_y) \approx 0.0005\ \text{kG}^{-1}.$$

These values are consistent with the oscillations shown in Figs. 1 and 3 (Δ lies somewhere between 0.038 and 0.049 kG^{-1}), except for $\Delta^{(4)}$.

The asymptotic behavior of n_i, ζ, and ρ in high magnetic fields can be understood through Eq. (71). For the present case, H parallel to the bisectix axis, the orbital-cyclotron effective masses of electrons are greater than their corresponding spin-procession effective masses, $m_{cy}^{(1)} : m_{sy}^{(1)} = 0.0084 : 0.0079$, $m_{cy}^{(2),(3)} : m_{sy}^{(2),(3)} = 0.0168 : 0.0158$ (once again using values given by SBR). Thus, for these conduction electrons, the lowest energy level will decrease if we increase the magnetic field. According to Eq. (19), the quantum numbers n, S, k_z must be so chosen that the value in the radicand remains non-negative, or the allowed energy levels be greater than $-\frac{1}{2}E_G$ measured from the bottom of the conduction band. Under these conditions, more and more electrons will reside on the lowest level in an increasing magnetic field as the degeneracy in each level increases. Consequently, we obtain from (71) for the charge neutrality condition at low temperatures

$$\sum_{i=1,2,3} (\Delta m^{(i)})^{1/2}\Omega_y^{(i)}[\zeta(1+\zeta/E_G) - \hbar(\Omega_y^{(i)} - \omega_y^{(i)})/2]^{1/2}$$
$$= (\Delta m^{(4)})^{1/2}\Omega_y^{(4)} \sum_{n,S} \times[(E_0-\zeta) - (n+\tfrac{1}{2})\hbar\Omega_y^{(4)} - S\tfrac{1}{2}\hbar\omega_y^{(4)}]^{1/2}. \tag{80}$$

The Fermi energy ζ is field dependent. One assumes further that in the extremely high-field limit: $\zeta(1+\zeta/E_G) \ll \hbar(\omega_y^{(i)} - \Omega_y^{(i)})$ and the holes all reside on the lowest Landau level $n=0$, $\omega_y^{(4)} \ll \Omega_y^{(4)}$, hence (80) reduces to the form

$$\zeta = E_0 - AH, \tag{81}$$

where

$$A = \frac{e\hbar}{2cm_{cy}^{(4)}} + \left\{\sum_{i=1,2,3}\left[\frac{\Delta m^{(i)}}{\Delta m^{(4)}}\left(\frac{1}{m_{sy}^{(i)}} - \frac{1}{m_{cy}^{(i)}}\right)\frac{e\hbar}{2c}\right]^{1/2} \Big/ \frac{m_{cy}^{(i)}}{m_{cy}^{(4)}}\right\}^2 \tag{82}$$

in qualitative agreement with Fig. 2.

From (71), we also find that n_i goes as $H_y^{3/2}$ in this extreme limit. This accounts qualitatively for the rise in high fields of n_i's in Fig. 1, although quantitative agreement cannot be expected because the conditions we have assumed for the extreme-high-field limit are not well satisfied in Fig. 1.

To look for the asymptotic behavior of ρ at low temperatures in the extreme-high-field region, we make use of Eqs. (47), (63), and (65) ($y \to z$, $z \to y$) in conjunction with (81). From these relations one obtains

$$\sigma_{xx}^{(i)}(H_y),\ \sigma_{zz}^{(i)}(H_y) \sim (1+2\zeta/E_G)^2, \quad i=1,2,3,$$
$$\sigma_{yy}^{(i)}(H_y) \sim H_y(1+2\zeta/E_G)^{-2},$$

$$\sigma_{xx}^{(4)}(H_y),\ \sigma_{zz}^{(4)}(H_y) \sim \text{constant},$$

$$\sigma_{yy}^{(4)}(H_y) \sim H_y, \tag{83}$$

hence the transverse magnetoresistance as shown in Fig. 3 should take the form

$$\rho_{zz} \propto \left(\sum_{i=1}^{4} \sigma_{zz}^{(i)}(H_y)\right)^{-1} \propto \left[\alpha\left(1+\frac{2\zeta}{E_G}\right)^2+\beta\right]^{-1}, \tag{84}$$

where α and β are two constants. As ζ decreases with increasing H according to (81), ρ thereby increases with H in the extreme limit.

From (84), we observe an effect in the transverse magnetoresistance strictly due to the nonparabolicity. In the case of parabolic band ($E_G \to \infty$), ρ_{zz} shows saturation in the extreme limit. The final increase in ρ_{zz} comes solely from the fact that E_G is finite.

IX. CONCLUSION

We have performed a quantum-mechanical study of the galvanomagnetic effects of ENP electrons in a strong magnetic field along an arbitrary direction with respect to the Fermi ellipsoid. The difficulties due to nonzero off-diagonal effective masses and the nonparabolicity in the dispersion relation have both been overcome. Agreement of our calculated curve for the transverse magnetoresistance of single-crystal bismuth with the experimental data indicates that the electronic properties of bismuth can be satisfactorily described by the ENP model, although some experiments and theories[11,18,32,33] are in favor of more complicated models for the bismuth electrons. Magnetoresistance in the elastic impurity scattering region of a nonparabolic-band or bismuth-type metal in an arbitrary orientation with respect to the electric and magnetic fields at any temperature can in principle, be calculated by a simple extension of our derived results. It is hoped that comparison between the experimental and calculated results will help to reveal more information on the electronic structure of these metals.

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