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Magnetoconductivity of Dirac electrons in bismuth

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Abstract. The magnetoconductivity of bismuth is theoretically investigated on the basis of the Kubo formula to interpret the longstanding mystery of linear magnetoresistance in bismuth. First, the magnetoconductivity for the isotropic Dirac model is studied. It is found that the inverse magnetoconductivity increases quadratically at low magnetic fields and is saturated at high fields. This high field property is in contrast to that obtained by the semi-classical theory, where the inverse magnetoconductivity keeps quadratic increase. Next, the magnetoconductivity for the extended Dirac model, which is a realistic model for bismuth, is studied. The inverse magnetoconductivity so obtained is not saturated, but is reduced at high fields. Implications of present results to the linear magnetoresistivity of bismuth are discussed.

1. Introduction

In 1928, Kapitza reported that the magnetoresistance of bismuth increases linearly with respect to the external magnetic field [1]. Next year, he further reported such a linear dependence can be observed in various materials, which is known as "Kapitza's linear law" [2–5]. The linear magnetoresistance was a mystery at that time since the all existing theory predicted a quadratic dependence at small fields and a saturating behavior at high fields. This problem was partly solved by Lifshits and Peschanskii for the case with open Fermi surface [6]. Much later, it was shown by Abrikosov that the magnetoresistance becomes linear at extremely high magnetic fields, in the so-called quantum limit, where only the lowest Landau level is occupied, by taking into account the infinite order of impurity scattering beyond the Born approximation [5, 7]. The theory of Abrikosov seems to succeed to give a reasonable explanation for the linear magnetoresistance on bismuth. However, it is well known that the effective Hamiltonian of electrons in bismuth is given by the form equivalent to the Dirac Hamiltonian and the carrier density greatly varies as a function of the magnetic field due to the charge neutrality condition of compensated metals [8–10]. These specific features of bismuth are indispensable to explain various properties of bismuth, such as the angle resolved quantum oscillation [8, 9] and diamagnetism [11], but they were not taken into account in the Abrikosov's theory.

In this work, we investigate the magnetoconductivity of bismuth by taking into account the quantum effect of whole Landau levels on the basis of the Kubo formula [12], the Dirac dispersion, the spatial anisotropy, and the field dependence of the Fermi energy, aiming at giving a possible interpretation to the Kapitza's linear law.

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2. Theory

We consider the isotropic Dirac Hamiltonian under an external magnetic field [10, 13–15]:

$$\mathscr{H} = \begin{pmatrix} \Delta & i\gamma\boldsymbol{\pi}\cdot\boldsymbol{\sigma} \\ -i\gamma\boldsymbol{\pi}\cdot\boldsymbol{\sigma} & -\Delta \end{pmatrix}, \tag{1}$$

where 2Δ is the energy gap, γ is the isotropic velocity, and $\boldsymbol{\sigma}$ is the Pauli matrix. $\boldsymbol{\pi} = -i\boldsymbol{\nabla} + (e/c)\boldsymbol{A}$, where $\boldsymbol{A}$ is the vector potential. The eigenenergy of this Hamiltonian is given by

$$E^{\mathrm{iso}}_{n,\sigma}(k_z) = \pm\sqrt{\Delta^2 + 2\Delta\left\{\left(n + \frac{1}{2} + \frac{\sigma}{2}\right)\omega_{\mathrm{c}} + \frac{k_z^2}{2m_{\mathrm{c}}}\right\}}, \tag{2}$$

where the cyclotron frequency is defined as

$$\omega_{\mathrm{c}} = \frac{eB}{m_{\mathrm{c}}c} = \frac{eB\gamma^2}{c\Delta}. \tag{3}$$

Even if we take into account the anisotropy of the velocity, the above isotropic model is essentially valid only with a replacement $m_{\mathrm{c}} \to m_h$ in Eq. (2) [9, 15, 16]. It is a remarkable characteristic of Dirac electron system that the lowest Landau level, $E_{\mathrm{LLL}} = E_{n=0,\sigma=-1}$, is fixed at the initial energy even at high magnetic fields [10]. Note that the cyclotron mass $m_{\mathrm{c}} = \Delta/\gamma^2$ is much less than the bare electron mass, m, in the case of bismuth, e. g., $m_{\mathrm{c}}/m \simeq 0.0019$ for the field parallel to the bisectrix axis [9]. This is the reason why we can reach quantum limit at relatively low magnetic field.

The complete and normalized wave function has the form

$$\psi = \sqrt{\frac{E+\Delta}{2E}}\begin{pmatrix} \chi_{\mathrm{u}} \\ \dfrac{-i\gamma(\boldsymbol{\pi}\cdot\boldsymbol{\sigma})\chi_{\mathrm{u}}}{E+\Delta} \end{pmatrix}, \tag{4}$$

where χ_{u} is a wave function of free electrons under a magnetic field [13]. The matrix elements of the velocity operator, which is given by $v_i = \partial\mathscr{H}/\partial k_i$, are calculated as

$$\begin{aligned} \langle\psi|v_i|\psi'\rangle &= \sqrt{\frac{(E+\Delta)(E'+\Delta)}{4EE'}}\begin{pmatrix} \chi_{\mathrm{u}} & \dfrac{i\gamma(\boldsymbol{\pi}\cdot\boldsymbol{\sigma})\chi_{\mathrm{u}}}{E+\Delta} \end{pmatrix}\begin{pmatrix} 0 & i\gamma\sigma_i \\ -i\gamma\sigma_i & 0 \end{pmatrix}\begin{pmatrix} \chi'_{\mathrm{u}} \\ \dfrac{-i\gamma(\boldsymbol{\pi}\cdot\boldsymbol{\sigma})\chi'_{\mathrm{u}}}{E'+\Delta} \end{pmatrix} \\ &= \gamma^2\sqrt{\frac{(E+\Delta)(E'+\Delta)}{4EE'}}\begin{pmatrix} \chi_{\mathrm{u}} & \dfrac{\sigma_i(\boldsymbol{\pi}\cdot\boldsymbol{\sigma})}{E'+\Delta} + \dfrac{(\boldsymbol{\pi}\cdot\boldsymbol{\sigma})\sigma_i}{E+\Delta}\chi'_{\mathrm{u}} \end{pmatrix}. \end{aligned} \tag{5}$$

After some straightforward calculations, we obtain

$$\langle\psi|\boldsymbol{v}|\psi'\rangle = \frac{\gamma^2}{2\sqrt{EE'(E+\Delta)(E'+\Delta)}}\langle\chi_{\mathrm{u}}|(E+E'+2\Delta)\boldsymbol{\pi} + i(E-E')(\boldsymbol{\pi}\times\boldsymbol{\sigma})|\chi'_{\mathrm{u}}\rangle. \tag{6}$$

Then the matrix elements for v_x is given by

$$\begin{aligned} \langle\psi|v_x|\psi'\rangle &= \frac{\gamma^2 A(E,E')}{2\sqrt{2}}\langle\chi_{\mathrm{u}}|(E+E'+2\Delta)(\pi^+ + \pi^-) \\ &\quad +(E-E')\left\{(\pi^+ - \pi^-)\sigma_z - \pi_z(\sigma^+ - \sigma^-)\right\}|\chi_{\mathrm{u}}\rangle, \end{aligned} \tag{7}$$

where $A(E,E') = [EE'(E+\Delta)(E'+\Delta)]^{-1/2}$, $\pi_\pm \equiv (v_x \pm iv_y)/\sqrt{2}$, and $\sigma_\pm \equiv (\sigma_x \pm i\sigma_y)/\sqrt{2}$. The operator $\pi_\pm$ changes the orbital quantum number $n \to n \pm 1$, while $\sigma_\pm$ changes the spin quantum number $\sigma \to \sigma \pm 1$. The only good quantum number is $j = n + 1/2 + \sigma$, and the operator v_x changes j as $j \to j \pm 1$, namely, orbital and spin quantum number cannot be changed simultaneously.

The diagonal conductivity σ_{xx} is given on the basis of the Kubo formula as [12, 17]

$$\sigma_{xx}(\omega) = \frac{e^2}{i\omega}\left[\Phi_{xx}(\omega+i\delta) - \Phi_{xx}(0+i\delta)\right], \tag{8}$$

$$\Phi_{xx}(i\omega_\lambda) = -T\sum_{n,i,j}\langle i|v_x|j\rangle\langle j|v_x|i\rangle \mathscr{G}(i\tilde{\varepsilon}_n)\mathscr{G}(i\tilde{\varepsilon}_n - i\omega_\lambda), \tag{9}$$

where $\varepsilon_n = (2n+1)\pi T$, $\omega_\lambda = 2\pi\lambda T$ (n,λ: integer). Here we introduced the effect of impurity scattering, Γ, as $i\tilde{\varepsilon}_n = i\varepsilon_n + i\Gamma\varepsilon_n/|\varepsilon_n|$. For the Green function part,

$$F(i\omega_\lambda) = -T\sum_n \mathscr{G}(i\tilde{\varepsilon}_n)\mathscr{G}(i\tilde{\varepsilon}_n - i\omega_\lambda) = -T\sum_n \frac{1}{i\tilde{\varepsilon}_n - E'}\frac{1}{i\tilde{\varepsilon}_n - i\omega_\lambda - E}, \tag{10}$$

the summation with respect to ε_n can be carried out as

$$F(\omega) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dx \quad f(x)\left[\frac{1}{x+\omega-E'+i\Gamma}\frac{1}{x-E+i\Gamma} - \frac{1}{x+\omega-E'+i\Gamma}\frac{1}{x-E-i\Gamma}\right.$$
$$\left. + \frac{1}{x-E'+i\Gamma}\frac{1}{x-\omega-E-i\Gamma} - \frac{1}{x-E'-i\Gamma}\frac{1}{x-\omega-E-i\Gamma}\right]. \tag{11}$$

(ω_λ was analytically continued as $i\omega_\lambda \to \omega$.) The contributions from the second and third terms of Eq. (11) correspond to the "Fermi surface term", and that from the first and fourth terms correspond to the "Fermi sea term".

For the interband transition, we have

$$\begin{aligned}\Phi_{xx}^{\rm cv} = \frac{e^2\gamma^4 N_{\rm L}}{8}\sum_{n,k_z,\sigma}{}' \Bigg[& F(\omega,-E_{n,\sigma},E_{n+1,\sigma})(A^{\rm cv}_{n+1\sigma,n\sigma})^2 m\omega_{\rm c}(n+1)\left[(E_{n+1,\sigma}-E_{n,\sigma}+2\Delta)+\sigma(E_{n+1,\sigma}+E_{n,\sigma})\right]^2 \\ & + F(\omega,-E_{n,\sigma},E_{n-1,\sigma})(A^{\rm cv}_{n-1\sigma,n\sigma})^2 m\omega_{\rm c} n\left[(E_{n-1,\sigma}-E_{n,\sigma}+2\Delta)-\sigma(E_{n-1,\sigma}+E_{n,\sigma})\right]^2 \\ & + 2F(\omega,-E_{n,\sigma},E_{n,-\sigma})(A^{\rm cv}_{n-\sigma,n\sigma})^2 k_z^2(E_{n,-\sigma}+E_{n,\sigma})^2 \Bigg] \\ & + \frac{e^2\gamma^2}{2}F(\omega,-E_{0\downarrow},E_{0\uparrow})\frac{(E_{0\uparrow}+E_{0\downarrow})}{E_{0\uparrow}},\end{aligned} \tag{12}$$

where $\sum'_{n,k_z,\sigma}$ denotes summations with respect to n, k_z and σ except for $n=0, k_z=0, \sigma=-1$ of the valence band, and we omitted the k_z dependences in energy. $N_{\rm L}$ is the degrees of the Landau-level degeneracy, $N_{\rm L} = eB/2\pi c = \omega_{\rm c}\Delta/2\pi\gamma^2$. $A^{\rm cv}_{n+1\sigma,n\sigma}$ means $A(E_{n+1,\sigma}, -E_{n,\sigma})$. ("c" and "v" abbreviate conduction and valence bands, respectively.) The first and second term corresponds to the orbital transition, and the third term to the spin transition, which appear also in the Wolff's theory [13]. The fourth term is a new term only appears in the interband transition (not appear in the Wolff's theory). The total conductivity is calculated both from the intra- and inter-band contributions.

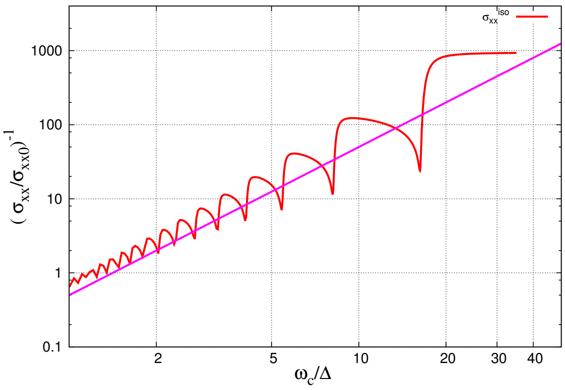

Figure 1. Inverse magnetoconductivity of the isotropic Dirac model as a function of magnetic field, ω_c/Δ, for $E_F/\Delta = 5.8$, $\Gamma/\Delta = 0.02$. The straight line shows B^2-dependence.

3. Results

3.1. Isotropic Dirac model

The results of the inverse magnetoconductivity for the isotropic Dirac model is shown in Fig. 1 as a function of ω_c/Δ. Here we fixed the Fermi energy to be $E_F/\Delta = 5.8$, where E_F is measured from the center of the band gap. There are clear quantum oscillations, which cannot be obtained by the semi-classical theory. When the Fermi energy E_F touches the minimum of the sub bands, $\sigma_{xx}^{\mathrm{iso}}$ shows a peak structure (appears as a dip in the plot of $1/\sigma_{xx}^{\mathrm{iso}}$). The peak width is widened by the impurity scattering Γ. $1/\sigma_{xx}^{\mathrm{iso}}$ exhibits B^2 dependence with the exception of the quantum oscillation in the weak field region, $\omega_c/\Delta \lesssim 15$. This is consistent with the semi-classical transport theory for free electrons[18],

$$\sigma_{xx}^{\mathrm{semi}}(B) = \frac{ne^2\tau}{m^*}\frac{1}{1+\omega_c^2\tau^2}, \tag{13}$$

where, $\tau = 1/2\Gamma$. The system reaches the quantum limit for $\omega_c/\Delta \gtrsim 17$, where only the lowest Landau level is occupied. Beyond the quantum limit, $1/\sigma_{xx}^{\mathrm{iso}}$ is saturated by the field. This is in contrast to the semi-classical result, where $1/\sigma_{xx}$ keeps quadratic increase.

3.2. Model for bismuth

Next, we consider the anisotropy and the change of the Fermi energy E_F according to the "extended Dirac model", whose energy is given as [9, 19]

$$E_{n,\sigma}^{\mathrm{ex}}(k_z) = \sqrt{\Delta^2 + 2\Delta\left\{\left(n+\frac{1}{2}+\frac{\sigma}{2}\right)\omega_c + \frac{k_z^2}{2m_h}\right\}} + \frac{g'\sigma}{2}\frac{\beta_0}{2}B, \tag{14}$$

where m_h is the effective mass along the magnetic field, and $\beta_0 = e/mc$. This model also takes into account the spin splitting and the shift of the lowest Landau level by introducing the g'-term in Eq. (14) [9, 20, 21]. This model has succeeded in giving good agreements with experiments on bismuth [9, 19]. The anisotropy is taken into account in ω_c and m_h. The field dependences of E_F (shown in the left panel of Fig. 2) is calculated so as to satisfy the charge neutrality condition [9].

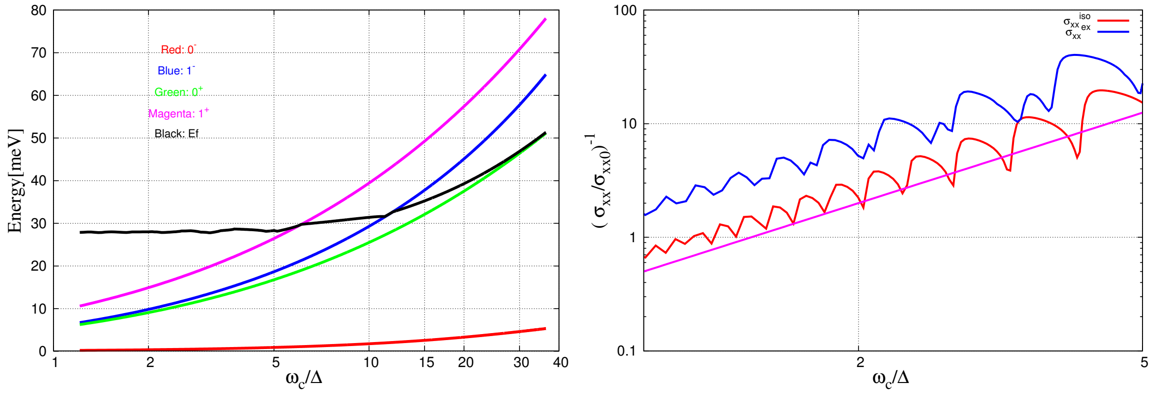

Figure 2. (left) Field dependence of the Fermi energy and Landau levels $E^{\rm ex}_{0,\pm}$ and $E^{\rm ex}_{1,\pm}$ for the extended Dirac model. (right) Inverse magnetoconductivity for the extended and isotropic Dirac models at low fields.

The result of the inverse magnetoconductivity so obtained is shown in the right panel of Fig. 2 for the magnetic field parallel to the trigonal axis. Since $E_{\rm F}$ does not vary so much at low fields, the properties of $\sigma^{\rm ex}_{xx}$ is basically the same as that of $\sigma^{\rm iso}_{xx}$. At high fields, on the other hand, $E_{\rm F}$ changes drastically as $E_{\rm F} \propto B$ in bismuth due to the charge neutrality condition [8, 9] and the effect of the g'-term becomes more relevant. Thus the properties of $\sigma^{\rm ex}_{xx}$ becomes different from those of $\sigma^{\rm iso}_{xx}$ as shown in Fig. 3. $1/\sigma^{\rm ex}_{xx}$ is not saturated but greatly reduced at high fields in contrast to the saturated $1/\sigma^{\rm iso}_{xx}$. This reduction in $1/\sigma^{\rm ex}_{xx}$ is a precursor to the quantum limit. For the field parallel to the trigonal axis, the second lowest Landau level, $E_{0,+}$, approaches $E_{\rm F}$, but cannot cross $E_{\rm F}$ even at high fields since both $E_{\rm F}$ and $E_{0,+}$ increases in almost the same way [9]. The system keeps the state just before entering the quantum limit, namely, $1/\sigma^{\rm ex}_{xx}$ keeps the dip structure at high fields. Consequently, the quantum effect and the change of $E_{\rm F}$ make the behavior of conductivity completely different from that of semi-classical one.

In order to understand the behavior of magnetoresistance, we need to calculate the magnetic field dependence of Hall conductivity, $\sigma_{xy}(B)$. Moreover, we also need to estimate the contributions not only from electrons, but also from holes for bismuth. According to the semi-classical theory, the total magnetoresistance exhibits unsaturated $\rho^{\rm semi}_{xx} \propto B^2$ behavior at high fields when the carrier numbers of electrons and holes are equal. This consequence is obtained from $1/\sigma^{\rm semi}_{xx} \propto B^2$ at high fields. Our result of $1/\sigma^{\rm ex}_{xx}$ exhibit the drastic reduction in $1/\sigma^{\rm ex}_{xx}$ at high fields. Therefore, it is naively expected that the $\rho^{\rm Bi}_{xx}$ will be reduced from the value o $\rho^{\rm semi}_{xx}$ at high fields and become close to $\rho_{xx} \propto B$ behavior.

4. Conclusion

We have investigated the magnetoconductivity of Dirac electrons in bismuth on the basis of the Kubo formula. For the isotropic Dirac model, $1/\sigma^{\rm iso}_{xx}(B) \propto B^2$ at low fields, which is consistent with the semi-classical results for free electrons. In the quantum limit, on the other hand, $1/\sigma^{\rm iso}_{xx}$ is saturated. This is contrast to the semi-classical result. We have also calculated the magnetoconductivity for electrons in bismuth based on the extended Dirac model. We have took into account the spacial anisotropy, the spin splitting, and the field dependences of the Fermi energy $E_{\rm F}$. $1/\sigma^{\rm ex}_{xx} \propto B^2$ at low fields, whereas $1/\sigma^{\rm ex}_{xx}$ is drastically reduced at high fields. This reduction in $1/\sigma^{\rm ex}_{xx}$ is significantly contrast to the semi-classical result, which keeps quadratic

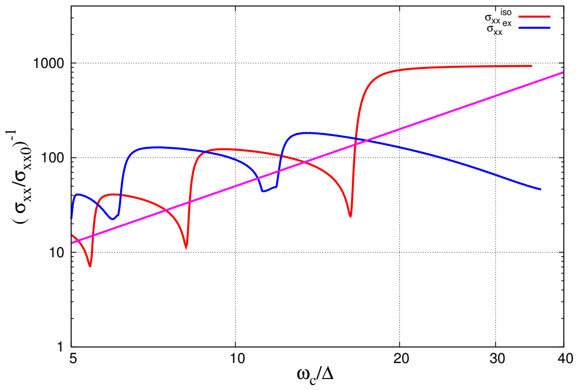

Figure 3. Inverse magnetoconductivity for the extended and isotopic Dirac models at high fields.

increase. Consequently, the magnetoconductivity of bismuth will be reduced from the semi-classical value $\rho_{xx}^{\rm semi} \propto B^2$ toward $\rho_{xx} \propto B$. We believe such a conclusion is useful to interpret the Kapitza's linear law in bismuth.

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