Corrections to the magnetoresistance formula for semimetals with Dirac electrons: The Boltzmann equation approach validated by the Kubo formula

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Abstract. The magnetoresistance (MR) in semimetals with Dirac (or Weyl) electrons and free holes is investigated on the basis of the Boltzmann theory. The MR is modified from the conventional results with free electron and holes in a very complex way due to the correction of the Dirac dispersion. The obtained formula explicitly includes the magnetic field dependence, which is very useful for the analysis of experimental results. In order to verify the validity of our results, the results obtained by the Boltzmann approach are compared with those by the Kubo theory. It is revealed that, by taking into account the field dependence of carrier density, the MR obtained by the Boltzmann theory almost perfectly agrees with that based on the Kubo theory even in the high-field region (in the quantum limit) except for the quantum oscillations. It is also shown that the MR in semimetals increases linearly with respect to the field in the quantum limit due to the drastic change of the carrier density, which is a significant characteristic of semimetals.

Keywords: *magnetoresistance, Dirac electrons, Weyl fermions, Boltzmann equation, Kubo formula*

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1. Introduction

Large and non-saturating magnetoresistance (MR) was first reported in semimetal bismuth by Kapitza in 1928 [1]. According to the Kapitza's report, the MR in bismuth keeps increasing linearly with respect to a magnetic field. In the last few years, the large and non-saturating MR has been attracting renewed interest since the observation in semimetal WTe_2, where the MR increases quadratically [2]. The interests are rapidly expanding related to the unusual transport phenomena in topological materials, such as in Cd_3As_2 [3], WP_2 [4], NbP [5], and LaBi [6]. A remarkable characteristic of these semimetals is that the Dirac (or Weyl) electrons of linear dispersion coexist with the nearly free holes of quadratic dispersion (figure 1).

For the analysis of the experimental data of MR, the semiclassical theory based on the Boltzmann equation is very useful and powerful even for the leading-edge MR studies [2, 6, 7, 8, 9]. What makes the analysis of MR very complex is the fact that the experimentally obtained physical quantity is the magnetoresistivity, $\hat{\rho}$, which is given in the tensor form. Theoretically, on the other hand, the conductivity tensor, $\hat{\sigma}$, is first calculated, and then, we have to calculate the inverse tensor of $\hat{\sigma}$ to compare with experiments. Therefore, in order to analyze experimental data of MR, it is of the prime importance to obtain a formula where the field dependence is clearly indicated not in $\hat{\sigma}$ but in $\hat{\rho}$. For this purpose, the approach based on the Boltzmann equation is appropriate and convenient. Note that the approach based on the Kubo formula is difficult to see the explicit field dependence of $\hat{\rho}$. This is why the Kubo formula is not so useful to analyze the experimental data, even though the result is rigorous.

However, the Boltzmann theory used in the previous analysis is basically for the semimetals with free electrons and holes, both of which have quadratic dispersions; the situation is different from the materials of current interest. The validity of the conventional

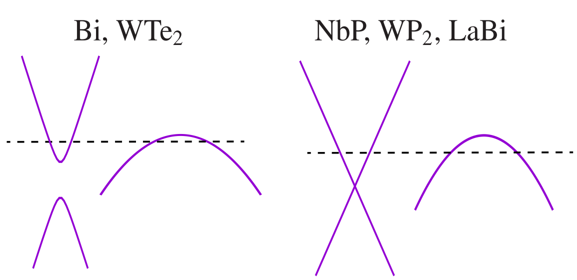

Figure 1. Schematic illustration of the band structure of semimetals with free holes and (left) Dirac electrons; (right) Weyl electrons. Cd_3As_2, the so-called Dirac semimetal, is not covered in the present paper since it has only one type of carrier.

Boltzmann theory with quadratic carriers is not well established for such systems. For example, it is well known that, when the electron (n) and hole (p) carriers with parabolic dispersions are perfectly compensated, $n = p$, the MR increases with the square of the magnetic field and does not saturate in the strong field limit [10]. When the compensation is not perfect, $n \neq p$, the MR saturates at a certain value of magnetic field. Then, what will happen if the system has Dirac electrons? It is not so straightforward to predict the property of MR in semimetals where Dirac electrons with linear dispersion and free holes with quadratic dispersion coexist since the symmetry between electron and hole carriers is broken.

In this paper, we obtain the analytic formula of MR in the system with Dirac (or Weyl) electrons and free holes based on the Boltzmann theory. The magnetoconductivity of Dirac electrons needs to be corrected from the conventional magnetoconductivity for the quadratic dispersion. The correction $\lambda_{\varepsilon_{\rm F}}$ appears in a complex way in the magnetoresistivity ρ_{xx} and the Hall resistivity ρ_{xy} depending on the magnitude of magnetic field.

It is also the purpose of this paper to establish the validity of the Boltzmann theory in the strong field region by comparing with the results obtained by the Kubo theory. When the magnetic field is sufficiently large, whole carriers are confined into the lowest Landau level, the so-called quantum limit. At such high fields, the effect of the Landau quantization plays a crucial role, which cannot be taken into account by the semiclassical Boltzmann theory in principle. Especially, in the case of semimetals, the carrier density changes drastically in the quantum limit due to the charge neutrality. (For example, the carrier density of bismuth changes five times larger at high fields [11].) This drastic change of carriers must affect the MR directly. Naively, the Boltzmann theory cannot be valid in such a high-field region. However, here we show that the approach based on the Boltzmann theory gives results almost perfectly agree (except for the quantum oscillation in ρ_{xx}) with the results obtained by the Kubo theory, where the Landau quantization and quantum effect on the transport coefficients are rigorously taken into account, only by considering the field dependence of carrier density. Based on this approach, it reveals that the MR increases linearly, $\rho_{xx} \propto B^1$, in the quantum limit.

The rest of this paper is organized as follows. Section 2 describes the formulation of the conductivity for the Dirac electrons. In section 3, we compare the MR with and without the correction of the Dirac dispersion in the two-band model. The magnetoconductivity near and beyond the quantum limit is described in section 4. We present the result of

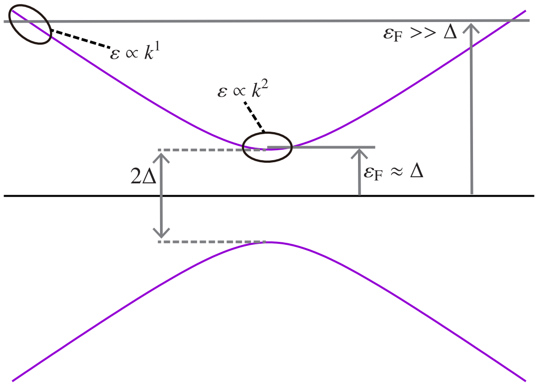

Figure 2. Relation between the band dispersion of the Dirac electron and the Fermi-energy.

the magnetoconductivity by considering the magnetic field dependence of carrier density in this section. The linear MR is obtained based on the theory introduced in section 4. Our conclusion is presented in section 5.

2. Magnetoconductivity in the Dirac (or Weyl) electrons

We derive the conductivity $\hat{\sigma}^{\mathrm{D}}$ for the anisotropic Wolff model, which is the common Hamiltonian to the system with strong spin-orbit coupling [12, 13]. The Wolff Hamiltonian is given by

$$\mathscr{H} = \Delta\gamma_4 + i\hbar\boldsymbol{k}\cdot\left[\sum_{i=1}^{3}\boldsymbol{W}(i)\gamma_4\gamma_i\right], \tag{1}$$

where $\boldsymbol{k}$ is the wave vector measured from an extremum of the dispersion. Δ is the half of the band gap (figure 2). γ_i is the 4×4 Dirac matrix of the form

$$\gamma_{i=1,2,3} = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \tag{2}$$

$$\gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{3}$$

where σ_i is the Pauli spin matrix. $\boldsymbol{W}(i)$ is related to the matrix elements of the velocity operator for the same spin, $\boldsymbol{t}$, and for the opposite spin, $\boldsymbol{u}$, as

$$\boldsymbol{W}(1) = \mathrm{Im}(\boldsymbol{u}), \tag{4}$$

$$\boldsymbol{W}(2) = \mathrm{Re}(\boldsymbol{u}), \tag{5}$$

$$\boldsymbol{W}(3) = \mathrm{Im}(\boldsymbol{t}). \tag{6}$$

The information of the strong spin-orbit coupling is included in $\boldsymbol{W}(i)$. Because of this strong spin-orbit couplings, the Dirac electrons exhibit specific properties, such as the large anisotropic g-factor [14, 15] and the spin transport phenomena [16, 17, 18]. On the other hand, for the electric conductivity and the Hall conductivity, the effect of spin-orbit coupling is negligibly small [19]. Therefore, the spin-orbit coupling does not affect directly the magnetoresistance except for the modification of the energy dispersion. The modification of the energy dispersion is appropriately considered in the present Boltzmann approach as follows.

The energy of the anisotropic Wolff model (equation (1)) is

$$\pm\varepsilon^{\mathrm{D}} = \pm\sqrt{\Delta^2 + \Delta\hbar^2\boldsymbol{k}\cdot\hat{\alpha}\cdot\boldsymbol{k}}, \tag{7}$$

where $\hat{\alpha}$ is the inverse mass tensor given by $\alpha_{ij} = \left[\sum_\mu W_i(\mu)W_j(\mu)\right]/\Delta$. The velocity of ε^{D}, i.e., the velocity of the Dirac electron ($\boldsymbol{v}^{\mathrm{D}}$) is given as

$$\boldsymbol{v}^{\mathrm{D}} = \frac{1}{\hbar}\frac{\partial\varepsilon^{\mathrm{D}}}{\partial\boldsymbol{k}} = \lambda_\varepsilon\boldsymbol{v}^{\mathrm{Q}}, \tag{8}$$

$$\lambda_\varepsilon = \frac{\Delta}{\varepsilon^{\mathrm{D}}}. \tag{9}$$

Here, $\boldsymbol{v}^{\mathrm{Q}}$ is the velocity of the carriers with quadratic dispersion defined by

$$\boldsymbol{v}^{\mathrm{Q}} = \hat{\alpha}\cdot\hbar\boldsymbol{k}. \tag{10}$$

The dimensionless parameter λ_ε expresses the correction for the Dirac electrons. In this paper, the values for the Dirac electrons are denoted by “D”, and these for the free holes with the quadratic dispersions are denoted by “Q”.

The Boltzmann equation under an electric field $\boldsymbol{E}$ and a magnetic field $\boldsymbol{B}$ is given as,

$$-\frac{e}{\hbar}(\boldsymbol{E} + v\times\boldsymbol{B})\cdot\nabla_{\boldsymbol{k}}f = -\frac{f - f_0}{\tau}, \tag{11}$$

by introducing the relaxation time τ, which is assumed to be constant throughout the paper. Here, e is the elementary charge ($e > 0$). f is the Fermi-Dirac distribution function which is represented by the thermal equilibrium distribution f_0 and $\boldsymbol{v_k}$ as [20, 21]

$$f = f_0 + \boldsymbol{F}\cdot\boldsymbol{v_k}\frac{\partial f_0}{\partial\varepsilon}. \tag{12}$$

$\boldsymbol{F}$ is the vector which depends on $\boldsymbol{E}$, $\boldsymbol{B}$, and the energy ε. From equations (7)-(12), $\boldsymbol{F}$ can be obtained as [20, 21]

$$\boldsymbol{F}^{\mathrm{D}} = e\tau\left(\hat{1} - e\tau\lambda_\varepsilon\hat{B}\cdot\hat{\alpha}\right)^{-1}\cdot\boldsymbol{E} \tag{13}$$

by introducing the magnetic field in terms of the 3×3 matrix [22, 23]:

$$\hat{B} = \begin{pmatrix} 0 & -B_z & B_y \\ B_z & 0 & -B_x \\ -B_y & B_x & 0 \end{pmatrix}. \tag{14}$$

The current density $\boldsymbol{j} = -(e/4\pi^3)\int\boldsymbol{v_k}f\mathrm{d}\boldsymbol{k}$ is described as follows:

$$\begin{aligned}\boldsymbol{j}^{\mathrm{D}} &= -\frac{e}{4\pi^3}\int\boldsymbol{v_k}^{\mathrm{D}}\left(\boldsymbol{F}^{\mathrm{D}}\cdot\boldsymbol{v_k}^{\mathrm{D}}\right)\frac{\partial f_0}{\partial\varepsilon}\mathrm{d}\boldsymbol{k} \\ &= \frac{e^2\tau}{4\pi^3}\int\mathrm{d}\boldsymbol{k}\left(-\frac{\partial f_0}{\partial\varepsilon}\right)\boldsymbol{v_k}^{\mathrm{D}} \\ &\quad\times\left[\left(\hat{1} - e\tau\lambda_\varepsilon\hat{B}\cdot\hat{\alpha}\right)^{-1}\cdot\boldsymbol{v_k}^{\mathrm{D}}\right]\cdot\boldsymbol{E}.\end{aligned} \tag{15}$$

In the low-temperature limit, $-\partial f_0/\partial\varepsilon$ becomes $\delta(\varepsilon - \varepsilon_{\mathrm{F}})$, where ε_{F} is the Fermi energy. From equations (8)-(10) and (15) becomes

$$\boldsymbol{j}^{\mathrm{D}} = \lambda_{\varepsilon_{\mathrm{F}}} ne \left(\hat{\mu}^{-1} - \lambda_{\varepsilon_{\mathrm{F}}}\hat{B}\right)^{-1} \cdot \boldsymbol{E}, \tag{16}$$

where n is the carrier density and $\hat{\mu} = e\tau\hat{\alpha}$ is the mobility tensor. Finally, the magnetoconductivity $\hat{\sigma}^{\mathrm{D}}$ for the Dirac electrons is obtained from equation (16) in the form:

$$\hat{\sigma}^{\mathrm{D}} = \lambda_{\varepsilon_{\mathrm{F}}} ne \left(\hat{\mu}^{-1} - \lambda_{\varepsilon_{\mathrm{F}}}\hat{B}\right)^{-1}. \tag{17}$$

This is the core formula of our work, including the correction of $\lambda_{\varepsilon_{\mathrm{F}}}$. Note that the magnetoconductivity for the free electrons is described as [22, 23]

$$\hat{\sigma}^{\mathrm{Q}} = ne \left(\hat{\mu}^{-1} - \hat{B}\right)^{-1}. \tag{18}$$

Equation (17) becomes equivalent to equation (18) in the limit of $\lambda_{\varepsilon_{\mathrm{F}}} \to 1$ ($\varepsilon_{\mathrm{F}} \to \Delta$), i.e., the so-called non-relativistic limit, where equation (7) becomes quadratic in $\boldsymbol{k}$ as is depicted in figure 2,

$$\varepsilon^{\mathrm{D}} \to \varepsilon^{\mathrm{Q}} = \Delta + \frac{\hbar^2}{2}\boldsymbol{k}\cdot\hat{\alpha}\cdot\boldsymbol{k}. \tag{19}$$

Equation (17) is also valid for the Weyl electrons by replacing $\lambda_{\varepsilon_{\mathrm{F}}}\mu$ as follows (the energy of Weyl electron is $\varepsilon^{\mathrm{w}} = \pm\hbar v_{\mathrm{F}}|\boldsymbol{k}|$):

$$\lambda_{\varepsilon_{\mathrm{F}}}\mu \to \frac{e\tau v_{\mathrm{F}}}{\hbar k_{\mathrm{F}}} \tag{20}$$

Hereafter, although we show results only for the Dirac electrons, they are also valid for the Weyl electrons only by considering the above transformation. The explicit forms for Weyl electrons are given in Appendix A.

3. MR with the fixed carrier densities

In this section, we discuss the MR in semimetals, especially, the case of the two-band model which has the Dirac electrons and the free holes, $\hat{\sigma}^{\mathrm{D+Q}} = \hat{\sigma}^{\mathrm{D}}_{\mathrm{e}} + \hat{\sigma}^{\mathrm{Q}}_{\mathrm{h}}$. Note that the so-called Dirac semimetals, e.g. $\mathrm{Cd_3As_2}$ [24], are not covered in the present paper since the Dirac semimetals have only one type of carrier at zero temperature. We assume the isotropic mobility tensor for electron and hole carriers $\mu_{ij} = \mu_0\delta_{ij}$ and $\nu_{ij} = \nu_0\delta_{ij}$, respectively. The elements of equation (17) are

$$\sigma^{\mathrm{D}}_{xx} = (\mu_0 + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_x^2)g^{\mathrm{D}}, \tag{21}$$

$$\sigma^{\mathrm{D}}_{yy} = (\mu_0 + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_y^2)g^{\mathrm{D}}, \tag{22}$$

$$\sigma^{\mathrm{D}}_{zz} = (\mu_0 + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_z^2)g^{\mathrm{D}}, \tag{23}$$

$$\sigma^{\mathrm{D}}_{yx} = (\lambda_{\varepsilon_{\mathrm{F}}}\mu_0^2 B_z + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_y B_x)g^{\mathrm{D}}, \tag{24}$$

$$\sigma^{\mathrm{D}}_{zy} = (\lambda_{\varepsilon_{\mathrm{F}}}\mu_0^2 B_x + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_z B_y)g^{\mathrm{D}}, \tag{25}$$

$$\sigma^{\mathrm{D}}_{xz} = (\lambda_{\varepsilon_{\mathrm{F}}}\mu_0^2 B_y + \lambda^2_{\varepsilon_{\mathrm{F}}}\eta B_z B_x)g^{\mathrm{D}}, \tag{26}$$

$$g^{\mathrm{D}} = \lambda_{\varepsilon_{\mathrm{F}}} ne \left[1 + \lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2\left(B_x^2 + B_y^2 + B_z^2\right)\right]^{-1}, \tag{27}$$

$$\eta = \det(\hat{\mu}) = \mu_0^3. \tag{28}$$

The other elements of $\hat{\sigma}^{\mathrm{D}}$ can be easily obtained from the Onsager relation, $\sigma^{\mathrm{D}}_{ij}(\boldsymbol{B}) = \sigma^{\mathrm{D}}_{ji}(-\boldsymbol{B})$.

From these equations, the magnetoconductivity $\sigma^{\mathrm{D+Q}}_{xx} = \sigma^{\mathrm{D}}_{\mathrm{e}xx} + \sigma^{\mathrm{Q}}_{\mathrm{h}xx}$ and the Hall conductivity $\sigma^{\mathrm{D+Q}}_{yx} = \sigma^{\mathrm{D}}_{\mathrm{e}yx} + \sigma^{\mathrm{Q}}_{\mathrm{h}yx}$ are obtained in the forms:

$$\sigma^{\mathrm{D+Q}}_{xx} = \sigma^{\mathrm{D+Q}}_{yy} = \frac{e\left[n\lambda_{\varepsilon_{\mathrm{F}}}\mu_0 + p\nu_0 + (p\lambda_{\varepsilon_{\mathrm{F}}}\mu_0 + n\nu_0)\lambda_{\varepsilon_{\mathrm{F}}}\mu_0\nu_0 B^2\right]}{(1+\lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2B^2)(1+\nu_0^2B^2)}, \tag{29}$$

$$\sigma^{\mathrm{D+Q}}_{yx} = -\frac{e\left[(p\nu_0^2 - n\lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2)B + (p-n)\lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2\nu_0^2B^3\right]}{(1+\lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2B^2)(1+\nu_0^2B^2)}. \tag{30}$$

Here, the magnetic field is set to be parallel to the z-axis ($\boldsymbol{B} = (0, 0, B)$). Correspondingly, the magnetoresistivity $\rho^{\mathrm{D+Q}}_{xx}$ and the Hall resistivity $\rho^{\mathrm{D+Q}}_{yx}$ are obtained:

$$\rho^{\mathrm{D+Q}}_{xx} = \rho^{\mathrm{D+Q}}_{yy} = \frac{1}{e}\frac{n\lambda_{\varepsilon_{\mathrm{F}}}\mu_0 + p\nu_0 + \lambda_{\varepsilon_{\mathrm{F}}}\mu_0\nu_0B^2(n\nu_0 + p\lambda_{\varepsilon_{\mathrm{F}}}\mu_0)}{(n\lambda_{\varepsilon_{\mathrm{F}}}\mu_0 + p\nu_0)^2 + \lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2\nu_0^2B^2(p-n)^2}, \tag{31}$$

$$\rho^{\mathrm{D+Q}}_{yx} = -\rho^{\mathrm{D+Q}}_{xy} = \frac{1}{e}\frac{(p\nu_0^2 - n\lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2)B + \lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2\nu_0^2B^3(p-n)}{(n\lambda_{\varepsilon_{\mathrm{F}}}\mu_0 + p\nu_0)^2 + \lambda^2_{\varepsilon_{\mathrm{F}}}\mu_0^2\nu_0^2B^2(p-n)^2}. \tag{32}$$

We obtain the analytic forms of $\rho_{xx}(B)$ and $\rho_{yx}(B)$, where their field dependences are clearly indicated. (See also Appendix A where we described the case with the Weyl electrons and the free holes.)

Figures 3(a) and 3(b) show the magnetic field dependences of $\rho^{\mathrm{D+Q}}_{xx}$ and $\rho^{\mathrm{D+Q}}_{yx}$ for $\lambda_{\varepsilon_{\mathrm{F}}} = 0.20$ (solid line), 1.00 (broken line) with $n = p = 1.0\times10^{17}\mathrm{cm}^{-3}$, $\mu_0 = 100\mathrm{T}^{-1}$ and $\nu_0 = 10\mathrm{T}^{-1}$. It is clarified that the properties of $\rho^{\mathrm{D+Q}}_{xx}$ for $\lambda_{\varepsilon_{\mathrm{F}}} = 1.00$ and 0.20 are qualitatively the same, but quantitatively different. At weak fields ($B < 0.5$T), they are independent of the field (figure 3(a)). The magnitude of $\rho^{\mathrm{D+Q}}_{xx}(\lambda_{\varepsilon_{\mathrm{F}}} = 0.20)$ is about three times "larger" than that of $\rho^{\mathrm{D+Q}}_{xx}(\lambda_{\varepsilon_{\mathrm{F}}} = 1.00)$ (the insets of figures 3(a) and 3(c)). This quantitative difference should be crucial when one analyzes the experimental data. The magnitude of $\rho^{\mathrm{D+Q}}_{yx}(\lambda_{\varepsilon_{\mathrm{F}}} = 0.20)$ is about twice "smaller" than that of $\rho^{\mathrm{D+Q}}_{yx}(\lambda_{\varepsilon_{\mathrm{F}}} = 1.00)$ (the insets of figures 3(b) and 3(d)). This difference can be seen in the whole region of the field for $n = p$, while it can be seen only in the weak field region for $n \neq p$ (the inset of figure 3(d)). Note that, in the case of $n/p = 0.98$, the signs of $\rho^{\mathrm{D+Q}}_{yx}$ are inverted at $B \sim 0.6$T for $\lambda_{\varepsilon_{\mathrm{F}}} = 0.20$ and at $B \sim 0.7$T for $\lambda_{\varepsilon_{\mathrm{F}}} = 1.00$. After the sign change, $\rho^{\mathrm{D+Q}}_{yx}(\lambda_{\varepsilon_{\mathrm{F}}} = 0.20)$ takes almost the same value as $\rho^{\mathrm{D+Q}}_{yx}(\lambda_{\varepsilon_{\mathrm{F}}} = 1.00)$. The behaviors of $\rho^{\mathrm{D+Q}}_{xx}$ and $\rho^{\mathrm{D+Q}}_{yx}$

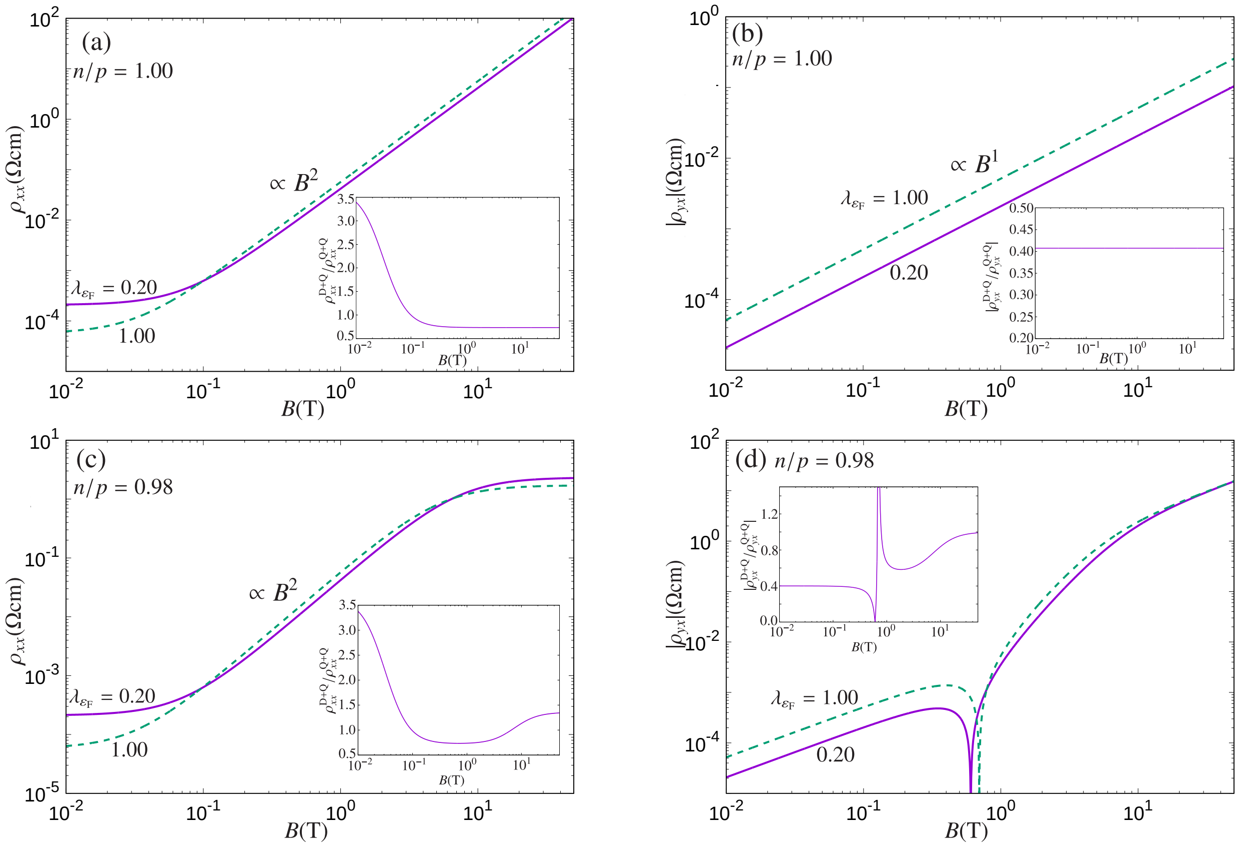

Figure 3. Field dependence of (a,c) the magnetoresistivity $\rho_{xx}^{\mathrm{D+Q}}$, (b,d) the Hall resistivity $\rho_{yx}^{\mathrm{D+Q}}$, with the correction $\lambda_{\varepsilon_{\mathrm{F}}} = 0.20$ (solid line) and without the correction $\lambda_{\varepsilon_{\mathrm{F}}}$ =1.0 (broken line). The insets show the ratio of the results for $\lambda_{\varepsilon_{\mathrm{F}}} = 0.20$ to those for $\lambda_{\varepsilon_{\mathrm{F}}} = 1.0$. The electron carrier n is $1.00 \times 10^{17}\mathrm{cm}^{-3}$ (a, b) and $0.98 \times 10^{17}\mathrm{cm}^{-3}$ (c, d). The hole carrier (p) is $1.0 \times 10^{17}\mathrm{cm}^{-3}$ μ_0, ν_0 are $100\mathrm{T}^{-1}$, $10\mathrm{T}^{-1}$, respectively.

can be understood more clearly if we take the limit of weak and strong fields.

At weak fields ($\lambda_{\varepsilon_{\mathrm{F}}}^2 \mu_0^2 B^2 \ll 1, \nu_0^2 B^2 \ll 1$), equations (31) and (32) become

$$\rho_{xx}^{\mathrm{D+Q}} = \frac{1}{e\nu_0} \frac{1}{(n\lambda_{\varepsilon_{\mathrm{F}}}\kappa + p)}, \tag{33}$$

$$\rho_{yx}^{\mathrm{D+Q}} = \frac{1}{e} \frac{\left(p - n\lambda_{\varepsilon_{\mathrm{F}}}^2 \kappa^2\right) B}{(p + n\lambda_{\varepsilon_{\mathrm{F}}}\kappa)^2}, \tag{34}$$

where κ expresses the ratio of the electron mobility to the hole mobility, $\kappa = \mu_0/\nu_0$. It is clear from equations (33) and (34) that the quantitative change due to the correction $\lambda_{\varepsilon_{\mathrm{F}}}$ is enhanced both by κ and the deviation from the perfect compensation. From equation (34), the Hall coefficient $R_{\mathrm{H}}^{\mathrm{D+Q}}$ is obtained:

$$R_{\mathrm{H}}^{\mathrm{D+Q}} = \frac{1}{e} \frac{p - \lambda_{\varepsilon_{\mathrm{F}}}^2 n\kappa^2}{(p + \lambda_{\varepsilon_{\mathrm{F}}} n\kappa)^2}. \tag{35}$$

Equation (35) is similar to the Hall coefficient of a system with electrons and holes as a free electron, given by [25]:

$$R_{\mathrm{H}}^{\mathrm{Q+Q}} = \frac{1}{e} \frac{p - n\kappa^2}{(p + n\kappa)^2}. \tag{36}$$

It should be emphasized here that the Hall coefficient $R_{\mathrm{H}}^{\mathrm{D+Q}}$ includes the correction for the Dirac electron $\lambda_{\varepsilon_{\mathrm{F}}}$, while $R_{\mathrm{H}}^{\mathrm{D}}$ does not for the one-band model. (See Appendix B.)

At strong fields ($\lambda_{\varepsilon_{\mathrm{F}}}^2 \mu_0^2 B^2, \nu_0^2 B^2 \gg 1$), equations (31) and (32) become as follows:

$$\rho_{xx}^{\mathrm{D+Q}} = \begin{cases} \dfrac{\nu_0}{ne} \dfrac{\lambda_{\varepsilon_{\mathrm{F}}}\kappa B^2}{1 + \lambda_{\varepsilon_{\mathrm{F}}}\kappa} & \text{for} \quad n = p \\[2ex] \dfrac{1}{e\nu_0} \dfrac{n + p\lambda_{\varepsilon_{\mathrm{F}}}\kappa}{(n-p)^2 \lambda_{\varepsilon_{\mathrm{F}}}\kappa} & \text{for} \quad n \neq p \end{cases} \tag{37}$$

$$\rho_{yx}^{\mathrm{D+Q}} = \begin{cases} \dfrac{1}{ne\nu_0} \dfrac{(1 - \lambda_{\varepsilon_{\mathrm{F}}}\kappa)B}{1 + \lambda_{\varepsilon_{\mathrm{F}}}} & \text{for} \quad n = p \\[2ex] -\dfrac{B}{(n-p)e} & \text{for} \quad n \neq p \end{cases} \tag{38}$$

$\rho_{xx}^{\mathrm{D+Q}}$ increases as $\rho_{xx}^{\mathrm{D+Q}} \propto B^2$ when n and p are completely equal $n = p$ (figure 3(a)). Despite the fact that Dirac electron and free hole have different band dispersions, $\rho_{xx}^{\mathrm{D+Q}}$ and $\rho_{xx}^{\mathrm{Q+Q}}$ increase with B^2 for $n = p$. When $n \neq p$, $\rho_{xx}^{\mathrm{D+Q}}$ is saturated (figure 3(c)) and the form of $\rho_{yx}^{\mathrm{D+Q}}$ is the same as $\rho_{yx}^{\mathrm{Q+Q}}$[25]. The $\lambda_{\varepsilon_{\mathrm{F}}}$ dependences of the magnetoresistivities $\rho_{ij}^{\mathrm{D+Q}}$ and

Table 1. Summary of the formulae of magnetoresistivity. ρ_{ij}^{D} is the magnetoresistivity for Dirac electrons, and $\rho_{ij}^{\mathrm{D+Q}}$ is that for semimetals with Dirac electrons and quadratic holes. $\lambda_{\varepsilon_\mathrm{F}} = \Delta/\varepsilon_\mathrm{F}$ is the correction due to the Dirac dispersion. When $\lambda_{\varepsilon_\mathrm{F}} \to 1$, the results of $\rho_{ij}^{\mathrm{D+Q}}$ become consistent with the conventional results with quadratic electrons and holes, $\rho_{ij}^{\mathrm{Q+Q}}$. $\kappa = \mu_0/\nu_0$ expresses the asymmetry between the electron mobility μ_0 and the hole mobility ν_0.

	One band model		Two band model			
			$n \neq p$		$n = p$	
	ρ_{xx}^{D}	ρ_{yx}^{D}	$\rho_{xx}^{\mathrm{D+Q}}$	$\rho_{yx}^{\mathrm{D+Q}}$	$\rho_{xx}^{\mathrm{D+Q}}$	$\rho_{yx}^{\mathrm{D+Q}}$
Weak fields	$\dfrac{1}{ne\lambda_{\varepsilon_\mathrm{F}}\mu_0}$	$-\dfrac{B}{ne}$	$\dfrac{1}{e\nu_0}\dfrac{1}{p+n\lambda_{\varepsilon_\mathrm{F}}\kappa}$	$\dfrac{1}{e}\dfrac{(p-n\lambda_{\varepsilon_\mathrm{F}}^2\kappa^2)B}{(p+n\lambda_{\varepsilon_\mathrm{F}}\kappa)^2}$	$\dfrac{1}{ne\nu_0}\dfrac{1}{1+\lambda_{\varepsilon_\mathrm{F}}\kappa}$	$\dfrac{1}{ne}\dfrac{(1-\lambda_{\varepsilon_\mathrm{F}}\kappa)B}{1+\lambda_{\varepsilon_\mathrm{F}}\kappa}$
Strong fields	$\dfrac{1}{ne\lambda_{\varepsilon_\mathrm{F}}\mu_0}$	$-\dfrac{B}{ne}$	$\dfrac{1}{e\nu_0}\dfrac{n+p\lambda_{\varepsilon_\mathrm{F}}\kappa}{(n-p)^2\lambda_{\varepsilon_\mathrm{F}}\kappa}$	$-\dfrac{B}{(n-p)e}$	$\dfrac{\nu_0}{ne}\dfrac{\lambda_{\varepsilon_\mathrm{F}}\kappa B^2}{1+\lambda_{\varepsilon_\mathrm{F}}\kappa}$	$\dfrac{1}{ne\nu_0}\dfrac{(1-\lambda_{\varepsilon_\mathrm{F}}\kappa)B}{1+\lambda_{\varepsilon_\mathrm{F}}}$

Table 2. Corrected mobilities and relaxation times of bismuth at 4.23 K. The upper line is the values obtained by Hartman using the conventional formula for the quadratic dispersion, and the lower line is the corrected values with $\lambda_{\varepsilon_\mathrm{F}} = 0.215$.

	$\mu_1(\mathrm{T}^{-1})$	$\mu_2(\mathrm{T}^{-1})$	$\mu_3(\mathrm{T}^{-1})$	$\tau_1 \times 10^{-10}$(s)	$\tau_2 \times 10^{-10}$(s)	$\tau_3 \times 10^{-10}$(s)
Hartman [26]	11000	220	6780	4.4	21.6	4.4
Corrected value	51000	1390	31000	20	100	19

the Hall coefficient $R_\mathrm{H}^{\mathrm{D+Q}}$ are summarized in table 1.

It should be emphasized here that the correction $\lambda_{\varepsilon_\mathrm{F}}$ is a correction to the conventional formula of magnetoresistance expressed in terms of the mobility since the mobility is introduced assuming the quadratic dispersion. If the formula is expressed in terms of the values at the Fermi surface, such as the Fermi velocity v_F and the Fermi wavenumber k_F, we do not need to correct the formula (cf. Appendix A). In addition, the experimentally observed magnetoresistance at low enough temperature is not directly affected by the existence of the Dirac point away from the Fermi level.

The correction $\lambda_{\varepsilon_\mathrm{F}}$ will be crucial when one estimates the mobility or the relaxation time from the experimentally obtained data of magnetoresistance. In most cases, the mobility is estimated by using the conventional formula like equation (18). However, in the case of semimetal with Dirac electrons, we should use equation (17). Consequently, the mobility should be corrected by a factor of $1/\lambda_{\varepsilon_\mathrm{F}}$. In the case of bismuth, $\lambda_{\varepsilon_\mathrm{F}} = 0.215$ ($\Delta = 7.65$ meV and $\varepsilon_\mathrm{F} = 35.5$ meV [11]). Then, the "true" mobilities should be $1/\lambda_{\varepsilon_\mathrm{F}} = 4.65$ times larger than the mobility estimated by the conventional formula. As an example, we listed the corrected mobilities and relaxation times for the experimental data by Hartman [26]. In the case of $\mathrm{WTe_2}$, which has the Dirac holes [2, 27], the correction is $\lambda_{\varepsilon_\mathrm{F}} \simeq 0.083$ ($\Delta \simeq 2.5$ meV and $\varepsilon_\mathrm{F} \simeq 30$ meV by the Supplemental Material of [28]). Thus, the mobilities and the relaxation times should be corrected by a factor of $1/\lambda_{\varepsilon_\mathrm{F}} \simeq 12.0$ as well.

4. MR with the field dependence of the carrier densities

At weak magnetic fields, the Fermi energy ε_F and carrier densities n and p do not change in three-dimensional systems. This is because carrier energy is not quantized clearly. At magnetic fields near the quantum limit, on the other hand, the carrier energies are clearly quantized in the Landau levels. ε_F, n and p of semimetals drastically change with magnetic field in order to keep the charge neutrality [11, 29, 30, 31]. This tendency becomes more significant when the difference between electron and hole mobilities becomes large, such as in bismuth. In this section, we extend the approach adopted in the last section by considering the field dependence of carrier densities $n(B)$ and $p(B)$, and also calculate the magnetoconductivity based on the Kubo formula for Dirac electrons, which is represented as $\hat{\sigma}^{\mathrm{KD}}$, to check the validity of the Boltzmann approach.

4.1. Field dependence of the carrier

The eigenenergies of the Wolff model under magnetic fields and of holes in free electrons with the Zeeman splitting are [11, 13, 12, 30]

$$\varepsilon^{\mathrm{D}} = \sqrt{\Delta^2 + 2\Delta\left[\left(l + \frac{1}{2} + \frac{\sigma}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m_z}\right]}, \quad (39)$$

$$\varepsilon_0 + \Delta - \varepsilon^{\mathrm{Q}} = \left(l + \frac{1}{2}\right)\hbar\Omega_\mathrm{c} + \frac{\hbar^2 k_z^2}{2M_z} + \sigma\frac{g}{2}\mu_\mathrm{B}B, \quad (40)$$

where l is an index of the Landau levels and σ is the sign of the spin ($\sigma = \pm 1$). k_z is the wavenumber

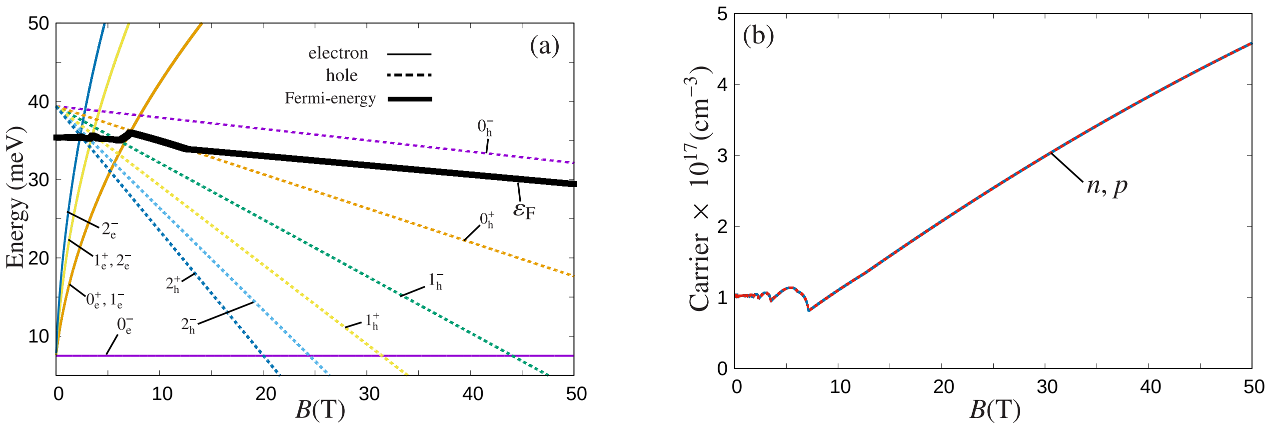

Figure 4. Field dependence of (a) the energies, and (b) the electron and hole carriers $(n(B), p(B))$. $l^{\pm}$ on the left is the Landau index. The solid line and broken line represent the Landau level of the electron and the hole, respectively. The solid thick line is the Fermi-energy ε_{F}.

parallel to the magnetic field. ε_0 is the energy difference between the bottom of the Dirac electron band and the top of the hole band, g is the g-factor for the hole. $m_z(M_z)$ and $\omega_{\mathrm{c}}(\Omega_{\mathrm{c}})$ are the effective mass parallel to the magnetic field and the cyclotron frequency for electrons (holes), respectively. In the following, we set $\Delta = 7.5\mathrm{meV}$, $\varepsilon_0 = 2\Delta$, $g = 5$, $m_{\mathrm{c}}/m_0 = m_z/m_0 = 0.01$ and $M_{\mathrm{c}}/m_0 = M_z/m_0 = 0.2$. The formula of carrier density under a magnetic field is represented as

$$n(B) = \frac{eB}{2\pi^2}\sum_{l\sigma}\hbar k_{\mathrm{F}}(l,\sigma). \tag{41}$$

The charge neutrality condition $(n = p)$ is given by

$$\sum_{l\sigma} k_{\mathrm{F}}^{\mathrm{e}}(l,\sigma) = \sum_{l'\sigma'} k_{\mathrm{F}}^{\mathrm{h}}(l',\sigma'), \tag{42}$$

where $k_{\mathrm{F}}^{\mathrm{e}}(k_{\mathrm{F}}^{\mathrm{h}})$ is the Fermi wavenumber of electrons (holes). All carriers occupy the lowest Landau level in the quantum limit $(l,\sigma) = (0,-1)$, so that equation (42) is changed as

$$k_{\mathrm{F}}^{\mathrm{e}} = k_{\mathrm{F}}^{\mathrm{h}}. \tag{43}$$

Figure 4(a) shows the magnetic field dependence of the Fermi-energy ε_{F} and figure 4(b) shows the carrier densities $n(B)$ and $p(B)$. The electrons and holes reach the quantum limit at $B \simeq 7\mathrm{T}$ and $B \simeq 12.5\mathrm{T}$, respectively. ε_{F} decreases by conserving the charge neutrality condition $(n = p)$. In contrast, the carrier densities $n(B)$ and $p(B)$ increase linearly as the Landau degeneracy $eB/2\pi^2$ increases (figure 4(b)).

Finally, we replace the carrier density n which is independent of the magnetic field in equations (21) and (24) with the field-dependent carrier density $n(B)$ so obtained (equation (41)). Then the results considered the magnetic field-dependence of the carrier density are obtained as shown in figure 5 (Here we used the relations: $\rho_{xx}^{\mathrm{D}} = \sigma_{xx}^{\mathrm{D}}/[(\sigma_{xx}^{\mathrm{D}})^2 + (\sigma_{yx}^{\mathrm{D}})^2]$, $\rho_{yx}^{\mathrm{D}} = -\sigma_{yx}^{\mathrm{D}}/[(\sigma_{xx}^{\mathrm{D}})^2 + (\sigma_{yx}^{\mathrm{D}})^2)]$).

4.2. Verification by the Kubo theory

The validity of the above procedure can be verified by comparing the calculation based on the Kubo theory [32], where the transport coefficients can be calculated in a fully quantum way together with the Landau quantization. For the Dirac electrons, the magnetoconductivity ($\sigma_{\mu\nu}^{\mathrm{KD}}$, "K" denotes the Kubo formula) is given by [13, 16]

$$\sigma_{\mu\nu}^{\mathrm{KD}} = \frac{1}{i\omega}\left[\Phi_{\mu\nu}^{\mathrm{D}}(\omega) - \Phi_{\mu\nu}^{\mathrm{D}}(0)\right], \tag{44}$$

$$\Phi_{xx}^{\mathrm{D}} = \frac{e^2 v^4 N_{\mathrm{L}}}{8}\sum_{lk\sigma}(f_1^{\mathrm{D}} + f_2^{\mathrm{D}} + f_3^{\mathrm{D}}) + f_4^{\mathrm{D}}, \tag{45}$$

$$\Phi_{yx}^{\mathrm{D}} = \frac{e^2 v^4 N_{\mathrm{L}}}{8}\sum_{lk\sigma}(f_1^{\mathrm{D}} - f_2^{\mathrm{D}} - \sigma f_3^{\mathrm{D}}) + f_4^{\mathrm{D}}. \tag{46}$$

Here, the Landau degeneracy is $N_{\mathrm{L}} = eB/2\pi\hbar$ and the functions $f_{1\to 4}^{\mathrm{D}}$ are given by

$$\begin{aligned} f_1^{\mathrm{D}} &= \Xi(\omega,\varepsilon_{l\sigma},\varepsilon_{l+1\sigma})\left(\Lambda_{l\sigma}^{l+1\sigma}\right)^2 m_c\hbar\omega_c(l+1) \\ &\quad\times[(\varepsilon_{l+1\sigma} + \varepsilon_{l\sigma} + 2\Delta) + \sigma(\varepsilon_{l+1\sigma} - \varepsilon_{l\sigma})]^2, \end{aligned} \tag{47}$$

$$\begin{aligned} f_2^{\mathrm{D}} &= \Xi(\omega,\varepsilon_{l\sigma},\varepsilon_{l-1\sigma})\left(\Lambda_{l\sigma}^{l-1\sigma}\right)^2 m_c\hbar\omega_c l \\ &\quad\times[(\varepsilon_{l-1\sigma} + \varepsilon_{l\sigma} + 2\Delta) - \sigma(\varepsilon_{l-1\sigma} - \varepsilon_{l\sigma})]^2, \end{aligned} \tag{48}$$

$$f_3^{\mathrm{D}} = 2\Xi(\omega,\varepsilon_{l\sigma},\varepsilon_{l-\sigma})\left(\Lambda_{l\sigma}^{l-\sigma}\right)^2\hbar^2 k_z^2(\varepsilon_{l-\sigma} - \varepsilon_{l\sigma})^2, \tag{49}$$

$$f_4^{\mathrm{D}} = \frac{e^2 v^2 N_{\mathrm{L}}}{2}\Xi(\omega)\frac{\varepsilon_{0+} - \varepsilon_{0-}}{\varepsilon_{0+}}, \tag{50}$$

$$\Lambda_a^b(\varepsilon_a,\varepsilon_b) = [\varepsilon_a\varepsilon_b(\varepsilon_a + \Delta)(\varepsilon_b + \Delta)]^{-1/2}. \tag{51}$$

The terms f_1 and f_2 originate from the "orbital transition" and f_3 from the "spin transition". f_4 is the contribution from $(l,k,\sigma) = (0,0,-1)$.

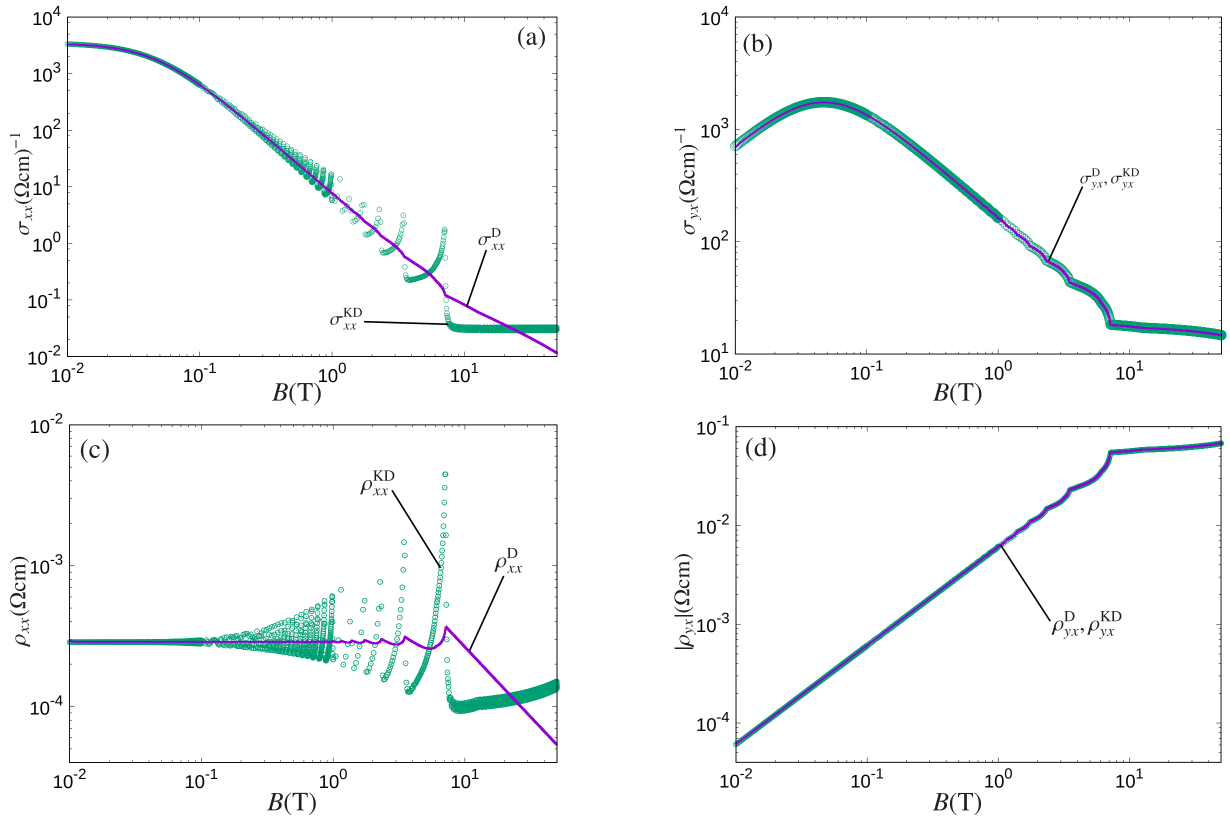

Figure 5. Field dependence of (a) the magnetoconductivity σ^{D}_{xx}, (b) the Hall conductivity σ^{D}_{yx}, (c) the magnetoresistivity ρ^{D}_{xx} and (d) the Hall resistivity ρ^{D}_{yx} for the Dirac electrons. The symbols are the results based on the Kubo theory ($\sigma^{\mathrm{KD}}_{ij}, \rho^{\mathrm{KD}}_{ij}$) and the solid lines are these based on the Boltzmann theory ($\sigma^{\mathrm{D}}_{ij}, \rho^{\mathrm{D}}_{ij}$). The parameters are set to be $\Delta = 7.5$meV, $m_{\mathrm{c}}/m_0 = 0.01$, $\mu_0 = 100\mathrm{T}^{-1}$. The longitudinal mass is equal to cyclotron mass ($m_{\mathrm{c}} = m_z$).

The contribution from the two one-particle Green's functions Ξ becomes as follows [13]:

$$\begin{aligned}\Xi(\omega, \varepsilon_a, \varepsilon_b) &= \frac{\mathrm{i}}{2\pi} \\ &\times \Bigg\{ \frac{1}{\omega + \varepsilon_b - \varepsilon_a + \mathrm{i}\Gamma} \Big[\ln(\varepsilon_{\mathrm{F}} - \varepsilon_b - \mathrm{i}\Gamma) \\ &\quad - \ln(\varepsilon_{\mathrm{F}} - \omega - \varepsilon_b - \mathrm{i}\Gamma) \\ &\quad + \ln(\varepsilon_{\mathrm{F}} - \varepsilon_a + \mathrm{i}\Gamma) \\ &\quad - \ln(\varepsilon_{\mathrm{F}} + \omega - \varepsilon_a + \mathrm{i}\Gamma) \Big] \\ &- \frac{1}{\omega + \varepsilon_b - \varepsilon_a} \Big[\ln(\varepsilon_{\mathrm{F}} - \varepsilon_b + \mathrm{i}\Gamma) \\ &\quad - \ln(\varepsilon_{\mathrm{F}} - \omega - \varepsilon_b - \mathrm{i}\Gamma) \\ &\quad + \ln(\varepsilon_{\mathrm{F}} - \varepsilon_a - \mathrm{i}\Gamma) \\ &\quad - \ln(\varepsilon_{\mathrm{F}} + \omega - \varepsilon_a + \mathrm{i}\Gamma) \Big] \Bigg\}, \end{aligned} \tag{52}$$

where Γ is related to τ and μ in the form

$$\Gamma = \frac{\hbar}{2\tau} = \frac{e\hbar}{2m\mu}. \tag{53}$$

We set the value of Γ for electrons to be consistent with the calculations in the previous sections. The field dependence of energy is identical to figure 4(a). The magnetoconductivities so obtained, $\sigma^{\mathrm{KD}}_{ij}$, are plotted in figure 5 together with the results based on the Boltzmann theory plus field-dependent $n(B)$. Here we set the following parameters: $\Delta = 7.5$meV, $m_c/m_0 = m_z/m_0 = 0.01$, $\mu_0 = 100\mathrm{T}^{-1}$. Figure 5(b) clearly shows that the Hall conductivity by the Boltzmann approach with the correction $\lambda_{\varepsilon_{\mathrm{F}}}$ and $n(B)$, σ^{D}_{yx} (solid line), agrees perfectly with that based on the Kubo formula $\sigma^{\mathrm{KD}}_{yx}$ (circles) even in the quantum limit: a rather surprising result. For the magnetoconductivity, it also agrees quantitatively with $\sigma^{\mathrm{KD}}_{xx}$ in the strong field region, although σ^{D}_{xx} does not exhibit the quantum oscillations. Consequently, we can conclude that the Boltzmann approach with the correction for the Dirac electrons, $\lambda_{\varepsilon_{\mathrm{F}}}$, and the field dependence of carriers, $n(B)$, can give correct results even in the quantum limit except for the quantum oscillations. It should be noted here that the amplitude of the quantum oscillation in the actual measurements is indistinct and not so clear as in figure 5(a) because of the smearing by the temperature or electron-electron, electron-phonon, and impurity scatterings [1, 33, 34].

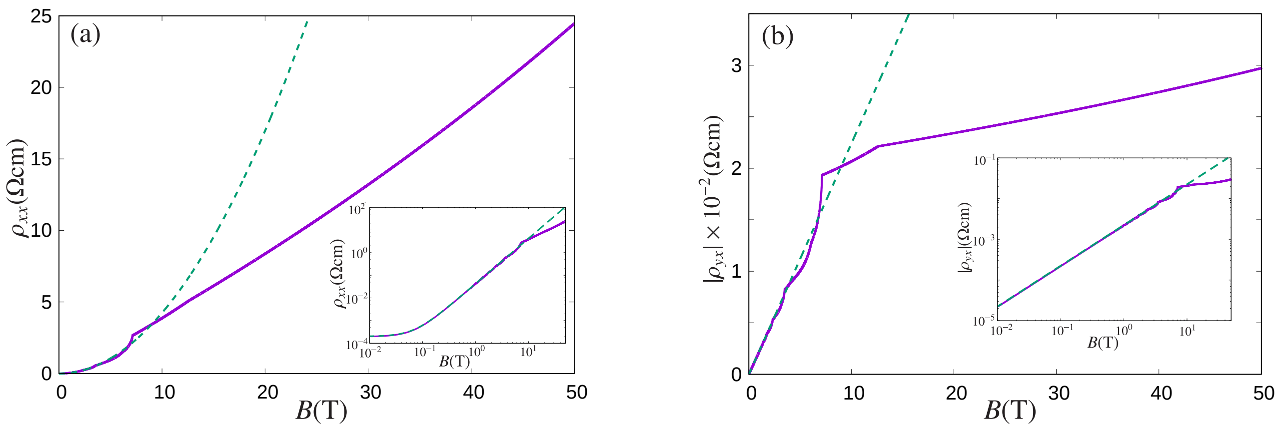

Figure 6. Field dependence of (a) the magnotoresistivity, $\rho_{xx}^{\mathrm{D+Q}}$, (b) the Hall resistivity, $\rho_{yx}^{\mathrm{D+Q}}$. The solid line is the result with the field dependence of carrier densities $n(\boldsymbol{B}), p(\boldsymbol{B})$ and $\lambda_{\varepsilon_{\mathrm{F}}}$. The broken line is the result without the field dependence of n, p and $\lambda_{\varepsilon_{\mathrm{F}}} = 0.2119$ ($n = p = 1.0 \times 10^{17}\mathrm{cm}^{-3}$). The insets are the logarithmical plot of each figure. The electron and hole carriers are $n(B) = p(B)$ at any magnetic fields. The mobilities μ_0 and ν_0 are $100\mathrm{T}^{-1}$ and $10\mathrm{T}^{-1}$, respectively.

Therefore, the present Boltzmann approach should be useful in the practical analysis of the experimental data, even though it does not indicate the quantum oscillations.

One may think that, if we have the rigorous results by the Kubo theory, the results based on the Boltzmann approach are needless. However, it is very hard to understand the field dependence of MR and the effect of the correction due to the Dirac dispersion directly from the formula by the Kubo theory. On the other hand, it is very easy and simple to understand them from the formula by the Boltzmann approach. This is the merit of the Boltzmann approach for the analysis of the experimental results. An example of such an easy and transparent treatment is given in the next sub-section.

4.3. Linear magnetoresistance in the quantum limit

In this sub-section, we argue the properties of MR in the quantum limit based on our Boltzmann approach with the Dirac correction $\lambda_{\varepsilon_{\mathrm{F}}}$ and the field-dependence of carriers $n(B)$. As is discussed in the last section, the carrier density of semimetals drastically changes in the quantum limit. Because of this, the MR changes its property in the quantum limit as is shown in figure 6. $\rho_{xx}^{\mathrm{D+Q}}$ increases linearly with respect to B in the quantum limit of the electron ($B > 7\mathrm{T}$) (figure 6(a)) and the magnetic field dependence of $\rho_{yx}^{\mathrm{D+Q}}$ becomes very small (figure 6(b)). The origin of these properties can be easily understood based on our results of equations (37) and (38) as follows. $\rho_{xx}^{\mathrm{D+Q}}$ and $\rho_{yx}^{\mathrm{D+Q}}$ have the following dependence:

$$\rho_{xx}^{\mathrm{D+Q}} = \frac{\mu_0}{n(B)e}\frac{\lambda_{\varepsilon_{\mathrm{F}}} B^2}{1+\lambda_{\varepsilon_{\mathrm{F}}}\kappa}, \tag{54}$$

$$\rho_{yx}^{\mathrm{D+Q}} = \frac{1}{n(B)e}\frac{(1-\lambda_{\varepsilon_{\mathrm{F}}}\kappa)B}{1+\lambda_{\varepsilon_{\mathrm{F}}}\kappa}. \tag{55}$$

The carrier density $n(B)$ has linear dependence $n(B) \propto B^1$ in the quantum limit ($B > 7\mathrm{T}$), so $\rho_{xx}^{\mathrm{D+Q}}$ and $\rho_{yx}^{\mathrm{D+Q}}$ become

$$\rho_{xx}^{\mathrm{D+Q}} \propto \frac{B^2}{n(B)} = B^1, \tag{56}$$

$$\rho_{yx}^{\mathrm{D+Q}} \propto \frac{B^1}{n(B)} = B^0. \tag{57}$$

What we show here is simply that the MR in semimetals increases linearly with respect to the magnetic field in the quantum limit if we assume the relaxation time is constant. This conclusion would be common to semimetals with Dirac (or Weyl) electrons and nearly free holes since $n(B) \propto B$ is quite general in the quantum limit of semimetals. Of course, however, we should further consider the various effects, such as the energy and the field dependence of relaxation time, into our theory in order to resolve the longstanding problem of linear MR, which is one of the recent hot topics [35, 36, 37, 38, 39, 40, 41, 42, 43, 44].

5. Summary

We studied the magnetoresistance (MR) in semimetals with Dirac (or Weyl) electrons and nearly free holes. It is shown that the magnetoconductivity of Dirac electrons is corrected by the factor $\lambda_{\varepsilon_{\mathrm{F}}} = \Delta/\varepsilon_{\mathrm{F}}$ which does not appear in the formula for the free electrons. Due to this correction $\lambda_{\varepsilon_{\mathrm{F}}}$, the magnetoresistivity and the Hall resistivity with the Dirac electrons and quadratic holes are modified qualitatively from the conventional results with quadratic electrons and holes. This qualitative correction should play a crucial role in the analysis of the experimental data. In our formula of magnetoconductivity based on the Boltzmann theory, the correction due to the Dirac dispersion and the field dependence is clearly indicated, which makes the analysis of experimental data easier and more transparent than the usage of the Kubo formula.

The gap between the semi-classical and quantum approaches for the magnetoconductivities of Dirac electrons is removed. The validity of our approach based on the Boltzmann theory including the field dependence of carrier is verified by the calculation based on the Kubo formula for Dirac electrons. It is rather surprising that the magnetoconductivity by the Boltzmann approach perfectly agrees with that by the Kubo formula even in the quantum limit only by taking into account the field dependence of carrier, except for the quantum oscillations. By this verification, we can safely utilize our semiclassical formula even for the semimetals with Dirac electrons in the quantum limit. In the previous studies [7, 29, 45], the MR of bismuth has been analyzed by using the formula of free electron carriers for two bands. The analysis can be quantitatively corrected by considering the correction ($\lambda_{\varepsilon_{\rm F}}$) found in the present work. In order to obtain the quantitative evaluation of MR in actual semimetals, we further need to take into account the anisotropy and the field dependence of the mobility.

With our formula considering the field-dependent carriers, it is revealed that the MR in semimetals increases linearly with respect to the magnetic field in the quantum limit. The origin of this linear MR is the fact that the carrier density is proportional to the magnetic field in the quantum limit of semimetals; $\rho_{xx}^{D+Q} \propto B^2/n(B) \propto B^1$. This result is obtained by assuming the relaxation time to be constant. It is known that the relaxation time depends on the energy and the magnetic field, which should be taking into account to resolve the longstanding problem of linear MR. Nevertheless, the simple understanding for the linear MR obtained in the present work would give a good starting point of the future investigation.

Acknowledgement

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Appendix A. MR of Weyl electrons and free holes

By replacing $\lambda_{\varepsilon_{\rm F}}\mu_0 \to e\tau v_{\rm F}/\hbar k_{\rm F}$, we obtain the conductivity and resistivity for the Weyl electron and the free hole from equations (29)-(32), as follows:

$$\begin{aligned}
\sigma_{xx}^{\rm W+Q} &= \sigma_{yy}^{\rm W+Q} \\
&= \frac{e\left[n\mu_{\rm w} + p\nu_0 + (p\mu_{\rm w} + n\nu_0)\mu_{\rm w}\nu_0 B^2\right]}{(1+\lambda_{\varepsilon_{\rm F}}^2\mu_0^2B^2)(1+\nu_0^2B^2)}, \qquad (A.1)\\
\sigma_{yx}^{\rm W+Q} &= -\frac{e\left[(p\nu_0^2 - n\mu_{\rm w}^2)B + (p-n)\mu_{\rm w}^2\nu_0^2B^3\right]}{(1+\mu_{\rm w}^2B^2)(1+\nu_0^2B^2)}.
\end{aligned}$$

$$\begin{aligned}
\rho_{xx}^{\rm W+Q} &= \rho_{yy}^{\rm D+Q} \\
&= \frac{1}{e}\frac{n\mu_{\rm w} + p\nu_0 + \mu_{\rm w}\nu_0B^2(n\nu_0 + p\mu_{\rm w})}{(n\mu_{\rm w}+p\nu_0)^2 + \mu_{\rm w}^2\nu_0^2B^2(p-n)^2}, \qquad (A.2)\\
\rho_{yx}^{\rm W+Q} &= -\rho_{xy}^{\rm D+Q} \\
&= \frac{1}{e}\frac{(p\nu_0^2 - n\mu_{\rm w}^2)B + \mu_{\rm w}^2\nu_0^2B^3(p-n)}{(n\mu_{\rm w}+p\nu_0)^2 + \mu_{\rm w}^2\nu_0^2B^2(p-n)^2}, \qquad (A.3)\\
\mu_{\rm w} &= \frac{e\tau v_{\rm F}}{\hbar k_{\rm F}}. \qquad (A.4)
\end{aligned}$$

In the case of the Weyl semimetal, we cannot define the mobility in principle since the effective mass is exactly zero. That's why we redefined the mobility of Weyl semimetal $\mu_{\rm w}$ only by using $v_{\rm F}$ and $k_{\rm F}$.

Lastly, we comment on the experimentally obtained mobility of NbP, which is known as Weyl semimetal. In the previous work [5], they estimate the mobility by using the relation $\mu = R_{\rm H}/\rho_{xx}$, assuming the single carrier of Weyl electron. From a viewpoint of our correct formula of (A.1)-(A.4), this evaluation is correct if one assumes $\nu_0 = 0$. Therefore, their estimated value of the mobility is not needed to be corrected. Furthermore, they evaluate both $k_{\rm F}$ and the cyclotron mass $m_{\rm c}$ from the frequency of the Shubnikov-de Haas oscillation and defined the Fermi velocity as $v_{\rm F} = \hbar k_{\rm F}/m_{\rm c}$. With these definitions, the conventional formula of mobility $\mu = e\tau/m^*$ corresponds to the correct mobility $\mu_{\rm w}$ if we assume $m^* = m_{\rm c}$. Therefore, the evaluated values of $\mu_{\rm w}$, $k_{\rm F}$ and $v_{\rm F}$ (table A1) are totally consistent with each other. In fact, the relaxation time evaluated from $\tau = \hbar k_{\rm F}/ev_{\rm F} = 2.13 \times 10^{-10}$s is consistent with that from $\tau = \mu m_c/e = 2.16 \times 10^{-10}$s.

Appendix B. MR of the one band model with the Dirac electrons

From equations (21)-(26), the magnetoresistivity $\rho_{xx}^{\rm D}$ and the Hall resistivity $\rho_{yx}^{\rm D}$ are obtained as follows ($B = (0, 0, B)$):

$$\rho_{xx}^{\rm D} = \rho_{yy}^{\rm D} = \frac{\sigma_{xx}^{\rm D}}{(\sigma_{xx}^{\rm D})^2 + (\sigma_{yx}^{\rm D})^2} = \frac{1}{ne\lambda_{\varepsilon_{\rm F}}\mu_0}, \qquad (B.1)$$

Table A1. Parameters of NbP obtained in [5], which are consistent with our modified definition of mobility for Weyl electrons $\mu_{\rm w}$. m_0 is the bare mass of the electron.

$k_{\rm F}$(Å^{-1})	m_c/m_0	$v_{\rm F} \times 10^5$(m/s)	μ(T^{-1})
0.0312	0.076	4.8	500

$$\rho_{yx}^{\mathrm{D}} = -\frac{\sigma_{yx}^{\mathrm{D}}}{(\sigma_{xx}^{\mathrm{D}})^2 + (\sigma_{yx}^{\mathrm{D}})^2} = -\frac{B}{ne}. \tag{B.2}$$

One can clearly see the field dependences of ρ_{xx}^{D} and ρ_{yx}^{D}, which are what we desired to obtain. It is found that ρ_{xx}^{D} does not depend on B but its amplitude is modified by the factor of $\lambda_{\varepsilon_{\mathrm{F}}}$ (figure B1), whereas ρ_{yx}^{D} is proportional to B but not modified by $\lambda_{\varepsilon_{\mathrm{F}}}$. The ratios of ρ_{xx}^{D} to ρ_{xx}^{Q} and ρ_{yx}^{D} to ρ_{yx}^{Q} are ($\rho_{ij}^{\mathrm{D}}(\lambda_{\varepsilon_{\mathrm{F}}} \to 1) = \rho_{ij}^{\mathrm{Q}}$):

$$\frac{\rho_{xx}^{\mathrm{D}}}{\rho_{xx}^{\mathrm{Q}}} = \frac{\rho_{yy}^{\mathrm{D}}}{\rho_{yy}^{\mathrm{Q}}} = \frac{1}{\lambda_{\varepsilon_{\mathrm{F}}}}, \tag{B.3}$$

$$\frac{\rho_{yx}^{\mathrm{D}}}{\rho_{yx}^{\mathrm{Q}}} = 1. \tag{B.4}$$

In addition, the Hall coefficient for the Dirac electron $R_{\mathrm{H}}^{\mathrm{D}}$ is obtained as

$$R_{\mathrm{H}}^{\mathrm{D}} = -\frac{1}{ne}, \tag{B.5}$$

for the Dirac electron. Therefore, the Hall coefficient $R_{\mathrm{H}}^{\mathrm{D}}$ is exactly the same as the Hall coefficient for the free electron, $R_{\mathrm{H}}^{\mathrm{Q}}$. This is consistent with the result for graphene (massless Dirac $\Delta = 0$)[46].

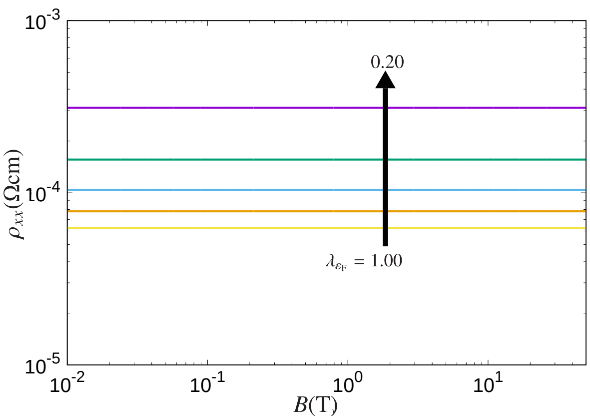

Figure B1. Field dependence of the magnetoresistivity ρ_{xx}^{D} with the different correction factor $\lambda_{\varepsilon_{\mathrm{F}}} = 0.2, 0.4, 0.6, 0.8, 1.0$. n and μ_0 are set to be $1.0 \times 10^{17}\mathrm{cm}^{-3}$ and $100\mathrm{T}^{-1}$, respectively.

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