Rapid Communications

Intrinsic magnetoresistance in three-dimensional Dirac materials with low carrier density

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Negative longitudinal and positive in-plane transverse magnetoresistance have been observed in most topological Dirac/Weyl semimetals and some other topological materials. Here, we present a quantum theory of intrinsic magnetoresistance for three-dimensional Dirac fermions at a finite and uniform magnetic field B. In a semiclassical regime, it is shown that the longitudinal magnetoresistance is negative and quadratic of a weak field B while the in-plane transverse magnetoresistance is positive and quadratic of B. The relative magnetoresistance is inversely quartic of the Fermi wave vector and only determined by carrier density, irrelevant to the external scatterings in the weak scattering limit. This intrinsic anisotropic magnetoresistance is measurable in systems with low carrier density and high mobility. In the quantum oscillation regime a formula for the phase shift in Shubnikov–de Haas oscillation is present as a function of the mobility and the magnetic field, which is helpful for experimental data analysis.

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Introduction. Magnetoresistance is the value change of electric resistance of a material in an applied magnetic field, and depends on the mutual orientation of the electric current and the magnetic field. In a sufficient weak field, the origin of the magnetoresistance is highly related to the Lorentz force experienced by charge carriers in the magnetic field and the spin-dependent scattering of electrons [1,2]. Recently, a positive in-plane transverse and negative longitudinal magnetoresistance have been observed in topological Dirac and Weyl semimetals [3–13], and some other metallic materials [14–17]. Especially, the negative longitudinal magnetoresistance in Dirac and Weyl semimetals attracts great interest as its physical origin is possibly related to the chiral anomaly [18–20], a purely quantum mechanical effect, of three-dimensional Weyl fermions in electric and magnetic fields [21–25]. Several mechanisms without chiral anomaly are also proposed for conventional and topological metals [26–28]. On the other hand, while the touching points of conduction and valence bands in the Weyl semimetals are protected topologically, the Dirac semimetals are located between conventional and topological insulators [29–31]. A small lattice distortion or external field can open a small energy gap in the band structure. Furthermore, narrow-gap semiconductors are also well described by the Kane model [32] in which the conduction and valence bands are strongly coupled together. A class of gapless topological semimetals, and narrow-gap semiconductors or topological materials can be well described by an effective multiband Dirac model [33–35]. In this class of materials, when the Fermi energy is located above the bottom of the conduction band, the transport properties are also affected by the existence of valence bands as well as the conduction band. The strong band coupling in these materials produces prosperous physics of the Berry phase in electron dynamics [36,37].

In this Rapid Communication, we propose an intrinsic origin of magnetoresistance of three-dimensional Dirac fermions in a finite magnetic field in the framework of the Kubo formula with the help of full Landau levels. In the semiclassical regime, the quadratic corrections of a magnetic field are found to both longitudinal and in-plane transverse resistivity and the electrical mobility. As a consequence, the relative magnetoresistivity is quartic of the ratio of the Fermi wavelength (the reciprocal of the Fermi wave vector) to the magnetic length. In the weak scattering limit the magnetoresistivity is only determined by the carrier density, and irrelevant to the external scatterings. Thus we call it the intrinsic magnetoresistivity. The effect becomes measurable when the Fermi wavelength is comparable with the magnetic length, i.e., the carrier density is low such that the Fermi level crosses near the Weyl nodes for the Dirac semimetals and is close to the bottom of the conduction bands for the narrow-gap semiconductors or topological insulators. In the quantum oscillatory regime, a formula for the phase shift is presented as a function of the mobility and the magnetic field, which will be useful for data analysis.

Model and the Kubo-Streda formula for conductivity. To illustrate the effect of the intrinsic magnetoresistivity, we start with the Dirac Hamiltonian in a finite magnetic field, which describes either the Dirac semimetals or the narrow-gap semiconductors and topological materials,

$$\mathcal{H} = \begin{bmatrix} \Delta & v\hbar\sigma\cdot(\mathbf{k}-e\mathbf{A}) \\ v\hbar\sigma\cdot(\mathbf{k}-e\mathbf{A}) & -\Delta \end{bmatrix}. \tag{1}$$

Here, v is the effective velocity and 2Δ is the energy gap between the conduction band and valence band. σ_α ($\alpha = x, y, z$) are the Pauli matrices. Without loss of generality, we assume the magnetic field is applied along the z direction. The vector potential is then chosen as $\mathbf{A} = (-By, 0, 0)$. We focus on the situation in which the Fermi level μ is above the energy gap 2Δ. In the absence of a magnetic field, the Fermi level μ is related to the Fermi wave vector k_f, $\mu^2 = \Delta^2 + (\hbar v k_f)^2$,

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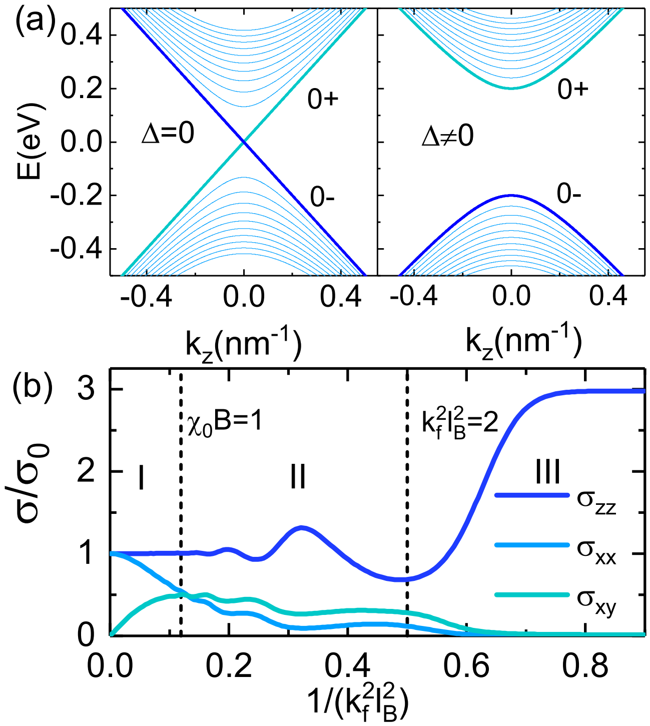

FIG. 1. (a) The band structure of Dirac fermions for the gapless case $\Delta = 0$ (the left panel) and the massive case $\Delta \neq 0$ (the right panel). (b) The conductivity as a function of a magnetic field for massless Dirac fermions. The shown dimensionless magnetic field scales (vertical dashed lines) indicate the borders of the different regimes: (I) the semiclassical regime ($\chi_0 B < 1$); (II) quantum oscillation regime ($\chi_0 B > 1$); (III) the quantum limit regime ($k_f l_B < \sqrt{2}$).

or the Fermi wavelength $1/k_f$. In a finite field, the energy spectrum has the form $\varepsilon_n^\zeta = \zeta\sqrt{v^2\hbar^2k_z^2 + 2n(\hbar v/l_B)^2 + \Delta^2}$, where $l_B = \sqrt{\hbar/eB}$ is the magnetic length and $\zeta = \pm 1$ is the band index and each band is doubly degenerate in energy for $n = 1, 2, \ldots$, and nondegenerate for $n = 0$, as shown in Fig. 1(a).

We consider the short-range pointlike impurities $U = u_0 \sum_l \delta(\mathbf{r} - \mathbf{R}_l)$ with the impurity concentration n_i. In this work, we utilize the Kubo-Streda formula [38] to calculate the matrix element of the conductivity tensor,

$$\sigma_{\alpha\beta} = \frac{\hbar e^2}{2\pi V}\sum_k \int_{-\infty}^{+\infty} d\xi n_F(\xi)\mathrm{Tr}\bigg[\hat{v}^\alpha \frac{dG^R}{d\xi}\hat{v}^\beta(G^A - G^R) - \hat{v}^\alpha(G^A - G^R)\hat{v}^\beta\frac{dG^A}{d\xi}\bigg], \tag{2}$$

where V is the volume of the system, $\hat{v}^\alpha \equiv \frac{1}{\hbar}\frac{\partial \mathcal{H}}{\partial k_\alpha}$ is the velocity operator along the α direction with $\alpha = x, y, z$, $n_F(\xi) = [1 + \exp(\frac{\xi - \mu}{k_B T})]^{-1}$ is the Fermi-Dirac distribution with k_B being the Boltzmann constant and T being the absolute temperature, and $G^{R/A}(\xi) = \frac{1}{\xi - \mathcal{H} \pm i\gamma}$ are the retarded and advanced Green's functions. In the Born approximation, the scattering time $\tau = \frac{\hbar}{2\gamma} = \frac{\hbar}{2\pi N_f n_i u_0^2}$ with the density states $N_f = \frac{\mu k_f}{\pi \hbar^3 v^3}$ at the Fermi level. With the help of the eigenfunctions of the Landau levels, all the elements of the conductivity tensor can be expressed as a series summation over the Landau index n at zero temperature [see Eqs. (S13), (S14), and (S19) in Ref. [39]].

The calculated longitudinal conductivity σ_{zz}, in-plane transverse conductivity $\sigma_{xx} = \sigma_{yy}$, and the Hall conductivity σ_{xy} are plotted in Fig. 1(b), which can be divided into three different regimes: (I) the semiclassical regime, (II) the quantum oscillation regime, and (III) the quantum limit regime. In the semiclassical regime, the energy band broadening width γ is larger than the energy spacing of two adjacent Landau levels near the Fermi level, i.e., $\chi_0 B < 1$, with the mobility $\chi_0 = e\hbar v^2/(2\gamma\mu)$. Thus the Shubnikov–de Haas oscillations will be smeared out by the disorder effect in this regime. In the quantum oscillation regime $\chi_0 B > 1$, the Landau levels near the Fermi level μ will be well separated from each other and the quantum oscillations become distinct. Further increasing the magnetic field $k_f l_B < \sqrt{2}$, all the charge carriers will be confined into the lowest Landau level, which is also called the quantum limit.

Intrinsic magnetoresistivity. In the semiclassical regime, the longitudinal magnetoconductivity is usually thought to be absent in the approximation of a spherical Fermi surface. In the weak field limit we find that $\sigma_{zz} = \sigma_0 = \frac{e^2v^2k_f^3}{3\pi^2\mu}\tau$ and $\sigma_{xx} = \frac{\sigma_0}{1+(\chi_0 B)^2}$. In this case, although the transverse conductivity decays with the magnetic field, both the longitudinal and transverse magnetoresistivity is absent, $\rho_{xx} = \rho_{zz} = 1/\sigma_0$ [2]. However, a detailed calculation of the series summation of the conductivity tensor at a finite field shows a quantum correction to either the conductivity or the mobility. We perform the summation over the Landau levels with the help of the Hurwitz zeta function $\zeta(s, z) = \sum_n (n + z)^{-s}$ and the digamma function $\psi(z)$, and then utilize the asymptotic expansion of the digamma function and Hurwitz zeta function for a large z, $\psi(z) = \log z - \frac{1}{2z} - \frac{1}{12z^2} + \cdots$ and $\zeta(2, z) = \frac{1}{z} + \frac{1}{2z^2} + \frac{1}{6z^3} + \cdots$, keeping up to the $(k_f l_B)^{-4}$ terms, to evaluate the conductivity (see Sec. S5 in Ref. [39] for the calculation).

After some cumbersome but straightforward calculations, we find that the longitudinal conductivity is expressed as $\sigma_{zz} = \sigma_0[1 - \frac{c_z}{(k_f l_B)^4}]$ and the transverse conductivity as $\sigma_{xx} = \frac{\sigma_0}{1+\chi^2 B^2}[1 - \frac{c_x}{(k_f l_B)^4}]$ with the mobility $\chi = \chi_0[1 + \frac{c_\chi}{(k_f l_B)^4}]$. The mobility is derived from the ratio of the Hall conductivity to the transverse conductivity, $\chi = \sigma_{xy}/\sigma_{xx} B$. The quadratic correction is consistent with the Casimir-Onsager reciprocity relation $\sigma_{\alpha\alpha}(B) = \sigma_{\alpha\alpha}(-B)$ as a consequence of the time-reversal symmetry [40]. The dimensionless parameter $1/(k_f l_B)$ can be understood as the ratio of the Fermi wavelength $\lambda_f = 1/k_f$ to the magnetic length l_B. The Fermi wave vector k_f is determined by the carrier density ϱ, i.e., $k_f = (3\pi^2\varrho)^{1/3}$. Comparisons of these semiclassical formulas and the numerical results are shown in Figs. 2(a) and 2(c) for massless and massive Dirac fermions, respectively. We find that the semiclassical formulas for conductivity are in a good agreement with the numerical results in the whole semiclassical regime.

The magnetoresistivity $\rho_{\alpha\alpha}(B)$ is derived from the inverse of the conductivity tensor. Here, we stress the importance of the complete set of the conductivity tensor to produce accurate and correct behaviors of the magnetoresistivity. Denote the relative magnetoresistivity by $\delta\rho_{\alpha\alpha} = \rho_{\alpha\alpha}(B)/\rho(0) - 1$. In a

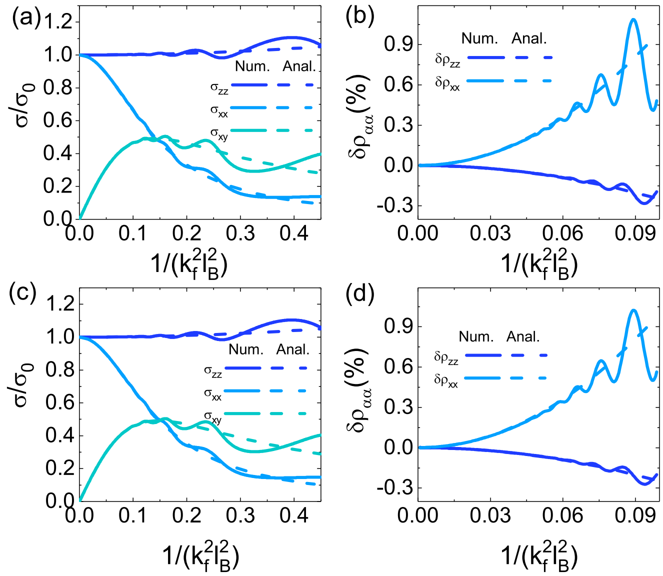

FIG. 2. (a) The magnetoconductivity and (b) magnetoresistivity for massless Dirac fermions ($\Delta = 0$). The dashed lines are the explicit numerical results and the solid lines are the corresponding analytic results in the semiclassical regime. (c) The magnetoconductivity and (d) magnetoresistivity for massless Dirac fermions ($\Delta/\hbar v k_f = 0.3$). The broadening width is $\frac{\gamma}{\hbar v k_f} = 0.07$. $k_f = 0.13\ \mathrm{nm}^{-1}$ throughout the work. The calculated coefficients are $c_x = 1$ and $c_z = -\frac{1}{4}$ for both the massless and massive case.

weak field, the relative magnetoresistivity can be expressed as

$$\delta\rho_{\alpha\alpha}(B) = \frac{c_\alpha}{(l_B k_f)^4} = c_\alpha\left(\frac{B}{2B_F}\right)^2, \tag{3}$$

with $B_F = \frac{\hbar}{2e}k_f^2$. The formula is also in good agreement with the numerical results as shown in Figs. 2(b) and 2(d). The relative magnetoresistivity is the main result in this work. Here, we want to emphasize the highly similar behaviors of the magnetoresistivity for massless and massive fermions as shown in Fig. 2.

The dimensionless coefficients c_α ($\alpha = x, y, z, \chi$) are functions of the broadening width γ, the chemical potential μ, and the energy gap Δ. The general expressions for c_α are given by Eqs. (S35)–(S37) in Ref. [39]. In the weak scattering limit, i.e., $\gamma\mu \ll \hbar^2 v^2 k_f^2$, keeping up to the $(\frac{\gamma}{v\hbar k_f})^2$ and $(\frac{\mu\gamma}{v^2\hbar^2 k_f^2})^2$ terms, one obtains

$$c_x = c_y \approx 1 + \frac{3}{4}\left(1 - \frac{8\mu^2}{v^2\hbar^2 k_f^2}\right)\frac{\gamma^2}{v^2\hbar^2 k_f^2}, \tag{4}$$

$$c_z \approx -\frac{1}{4} + \frac{1}{2}\frac{\gamma^2}{v^2\hbar^2 k_f^2}, \tag{5}$$

$$c_\chi \approx -\frac{3}{4} + \frac{3}{4}\left(1 + \frac{2\mu^2}{v^2\hbar^2 k_f^2}\right)\frac{\gamma^2}{v^2\hbar^2 k_f^2}. \tag{6}$$

When $\gamma \to 0$, $c_x = 1$, $c_z = -1/4$, and $c_\chi = -3/4$. In this case, the magnetoresistivity is only determined by the Fermi wave vector k_f, irrelevant to the band gap. Thus the magnetoresistivity is determined by the electronic band structure. A similar intrinsic longitudinal magnetoconductivity was pro-

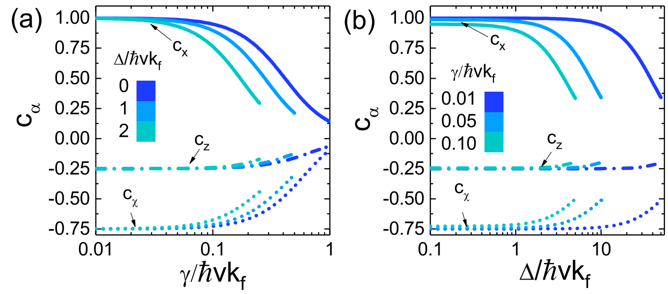

FIG. 3. The dimensionless coefficients (c_α) of the magnetoresistivities and electric mobility as a function of (a) the broadening width with different energy gaps and (b) energy gaps with different broadening widths. All of the lines are plotted with the constraint of $\hbar^2 v^2 k_f^2 > 2\Delta\gamma$, i.e., in the semiclassical regime.

duced by the Abelian Berry curvature in the semiclassical theory for gapless Dirac fermions [26], where the intrinsic component is obtained by collecting the contribution from the linear order of relaxation time. The coefficient $c_z = -2/15$, different from that in Eq. (5). The quantitative difference may be traced to the miscounting of the quadratic corrections of equal order in the semiclassical theory. For the massive case, when projecting the full four-dimensional Dirac space onto the two degenerate Bloch bands (positive energy branch), all the relevant information will be encoded into a matrix form of an SU(2) non-Abelian gauge field which will appear in the equation of motion for the wave packet [36,37]. The non-Abelian gauge field can provide a mechanism for the intrinsic magnetoresistivity here.

The intrinsic effect can be suppressed by the strong impurity scattering. For a fixed Fermi wave vector, the calculated coefficients as functions of the broadening width γ and the gap Δ are shown in Fig. 3. For a weak scattering $\gamma < 0.1\hbar v k_f$, the coefficients are rather robust against γ, but decay quickly for a large γ. However, for a strong disorder scattering the validity of the Born approximation is a question. The effect becomes strong when the carrier density is low and the electric mobility is high. The characteristic field for this intrinsic magnetoresistivity is one magnetic quantum flux $\phi_0 = h/2e$ per Fermi wavelength area $\pi\lambda_f^2$. For a density $\varrho = \varrho_0 \times 10^{16}/\mathrm{cm}^3$, the field is about $2B_F \approx 2.92\varrho_0^{2/3}$ T. Recent discovered Weyl and Dirac semimetals [3] may provide samples with a low carrier density and high mobility as the Fermi level is expected to cross near the Weyl nodes, which are good candidates for measuring the intrinsic effect.

Phase shift in the quantum oscillation regime. The quantum oscillation in regime II is known as the Shubnikov–de Haas oscillation, which is described by the Lifshitz-Kosevich formula [41]. By introducing the Dingle factor $\lambda_D = \pi/(\chi_0 B)$ for the Lorentz distribution function in the series summation in the conductivity, which is a function of the mobility χ_0 and the magnetic field B, the relative oscillatory part of conductivity is approximately described by

$$\delta\rho_{\alpha\alpha}^{\mathrm{os}} = \frac{d_\alpha}{k_f l_B \cos 2\pi\phi(B)}\mathrm{Li}_{\frac{1}{2}}\left(e^{-\frac{\pi}{\chi_0 B}}\right)\cos\left[2\pi\left(\frac{B_F}{B} + \phi(B)\right)\right], \tag{7}$$

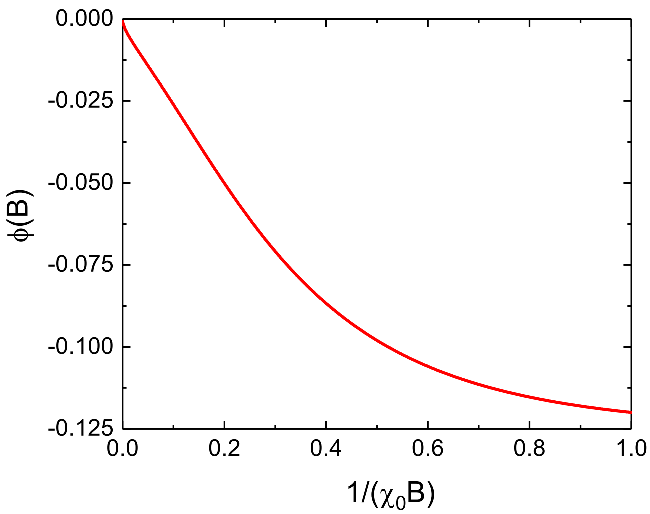

FIG. 4. The phase shift $\phi(B)$ as a function of $1/(\chi_0 B)$.

with the prefactors $d_x = 7\sqrt{2}/4$ and $d_z = \sqrt{2}$. $\mathrm{Li}_s(z)$ is the polylogarithm function of order s and argument z. ϕ_B is not a constant, but a slowly varying phase shift as a function of the Dingle factor,

$$2\pi\phi(B) = \arctan\left\{\frac{\mathrm{Re}\left[\sqrt{2}\exp\left(i\frac{3\pi}{4}\right)\mathrm{Li}_{\frac{1}{2}}\left(ie^{-\frac{\pi}{\chi_0 B}}\right)\right]}{\mathrm{Li}_{\frac{1}{2}}\left(e^{-\frac{\pi}{\chi_0 B}}\right)}\right\}. \quad (8)$$

In the quantum oscillation regime, the field B is confined by $\chi_0 B_F > \frac{B_F}{B} > 1$, and the value of the Dingle factor is between $\pi/(\chi_0 B_F)$ and π. As a consequence, the phase shift continuously varies from almost 0 to -0.238π as shown in Fig. 4. For a specific range of a measurable magnetic field B, the value of $\phi(B)$ is mainly determined by the mobility. In the massless case $\Delta = 0$, usually the mobility can be very large and the factor $\pi/\chi_0 B_F = 4\pi\gamma/(v\hbar k_f)$ is quite small, and the phase shift almost equal to zero for B has the same or less order of B_F. However, for a large gap $\Delta/v\hbar k_f \gg 1$, $\pi/\chi_0 B_F = 4\pi\gamma\Delta/(v\hbar k_f)^2$ and the phase shift is close to $-\pi/4$. In practice, $\phi(B)$ and B_F can be obtained from the Landau level fan diagram (see Fig. 1 in Ref. [39]). It is noted that the phase shift is only a function of the Dingle factor regardless of whether or not the Dirac fermions are gapless.

Magnetoconductivity in the quantum limit. When the magnetic field grows sufficient large ($k_f \ell_B \ll 1$), only the Landau level of $n = 0$ is partially filled, i.e., the system is in the quantum limit regime [42]. So we only need to consider the $n = 0$ term in Eqs. (S13) and (S14) in Ref. [39]. In this case, the chemical potential varies with the magnetic field as $\mu = \sqrt{(2\pi^2 l_B^2 \hbar v \varrho)^2 + \Delta^2}$ and the scattering time is evaluated as $\tau = \frac{2\pi^3 \ell_B^4 \hbar^3 v^2 \varrho}{n_i u_0^2 \sqrt{(2\pi^2 \ell_B^2 \hbar v \varrho)^2 + \Delta^2}}$ in the Born approximation. The longitudinal and transverse conductivities satisfy a relation approximately [39],

$$\sigma_{xx}\sigma_{zz} \simeq \frac{e^4}{2\pi^2 l_B^2 h^2}. \quad (9)$$

The longitudinal conductivity is $\sigma_{zz} = \frac{e^2 v^2 \varrho \tau}{\mu}$. For the massless case of $\Delta = 0$, $\tau = \frac{\pi \ell_B^2 \hbar^2 v}{n_i u_0^2}$ and $\mu = 2\pi^2 \ell_B^2 \hbar v \varrho$. The resulting conductivity $\sigma_{zz} = \frac{e^2 \hbar}{2\pi} \frac{v^2}{n_i u_0^2}$ and $\sigma_{xx} \propto B$, which are consistent with the results for massless Dirac fermions in Refs. [43–45]. For the large massive case of $\Delta \gg 2\pi^2 \ell_B^2 \hbar v \varrho$, $\tau = \frac{\pi \ell_B^2 \hbar^2 v}{n_i u_0^2 \Delta}$ and $\mu \simeq \Delta$. The conductivity $\sigma_{zz} \approx \frac{2\pi^3 e^2 \hbar^3 v^4 l_B^4 \varrho^2}{n_i u_0^2 \Delta^2} \propto \frac{1}{B^2}$. This result is consistent with the results in semiconductors with a low carrier density [24]. Following from Eq. (9), the corresponding transverse magnetoconductivity is found to be $\sigma_{xx} \propto B^3$.

Discussions. The negative longitudinal and positive in-plane transverse magnetoresistivity reflect the anisotropic magnetotransport in the Dirac materials. The difference of the two resistivities $\rho_{zz} - \rho_{xx} = \frac{c_z - c_x}{\sigma_0} \frac{B^2}{(2B_F)^2}$ leads to a general relation between the electric field $\mathbf{E}$ and charge current density $\mathbf{j}$,

$$\mathbf{E} = \rho_\perp \mathbf{j} + \frac{c_z - c_x}{\sigma_0} \frac{(\mathbf{j}\cdot\mathbf{B})\mathbf{B}}{(2B_F)^2} + \rho_\perp \chi \mathbf{B}\times\mathbf{j}, \quad (10)$$

with $\rho_\perp = \frac{1}{\sigma_0}(1 + c_x \frac{B^2}{(2B_F)^2})$. In the x-z plane constructed by $\mathbf{B}$ and $\mathbf{j}$, it follows that the resistivity $\rho_{ij} = \rho_\perp \delta_{ij} + \frac{c_z - c_x}{\sigma_0} \frac{B_i B_j}{(2B_F)^2}$. The diagonal resistivity is anisotropic as a function of the angle φ between the magnetic field and electric current density, i.e., anisotropic magnetoresistivity (AMR), $\rho_{zz} = \frac{1}{\sigma_0}(1 + \frac{c_z + c_x}{2} \frac{B^2}{(2B_F)^2} + \frac{c_z - c_x}{2} \frac{B^2}{(2B_F)^2} \cos 2\varphi)$, and the off-diagonal or planar Hall resistivity is $\rho_{xz} = \rho_{zx} = \frac{c_z - c_x}{2\sigma_0} \frac{B^2}{(2B_F)^2} \sin 2\varphi$. This effect was recently discussed and explored in the Dirac semimetals [46–50].

Before ending this Rapid Communication, several remarks are in order. (1) The present work uses the Kubo' s linear response theory in the full Landau level representation. The Green's functions and the physical operators in the formula of the conductivity in Eq. (2) are calculated in the Landau level representation. Hence, it is a full quantum mechanical calculation and goes beyond the existing semiclassical theory based on the wave packet dynamics [37]. Usually the semiclassical theory is limited to a sufficiently weak magnetic field, and cannot capture the physics in a strong field. However, the formula in Eq. (2) is valid in the whole magnetic field regime. Besides the intrinsic magnetoresistivity, it also gives the quantum oscillatory behaviors of the magnetoresistivity, which connects the semiclassical regime and the quantum limit regime smoothly. (2) The intrinsic magnetoresistivity exists for either massless or massive Dirac fermions. The existence of negative magnetoresistivity in the massive Dirac fermions excludes the mechanism of the chiral anomaly, which is only available for the massless Dirac fermions [3,4]. In other words, negative magnetoresistivity cannot simply be regarded as a signature of the chiral anomaly. (3) The massless and massive Dirac fermions have Abelian and non-Abelian Berry curvatures, respectively. For the case of non-Abelian Berry curvature, how to calculate the magnetotransport properties by using the semiclassical theory is still an open and challenging issue. The present work provides a general approach to study the magnetotransport property for both Abelian and non-Abelian cases. (4) The intrinsic magnetoresistivity exists for either longitudinal or transverse fields. The positive transverse and negative longitudinal magnetoresistivity have been widely observed simultaneously in topological materials with a low carrier density and high mobility [9,51,52].

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