Magnetococonductivity of type-II Weyl semimetals

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Type-II Weyl semimetals are characterized by the tilted linear dispersion in the low-energy excitations, mimicking Weyl fermions but with manifest violation of the Lorentz invariance, which has intriguing quantum transport properties. The magnetococonductivity of type-II Weyl semimetals is investigated numerically based on lattice models in parallel electric and magnetic field. We show that in the high-field regime, the sign of the magnetococonductivity of an inversion-symmetry-breaking type-II Weyl semimetal depends on the direction of the magnetic field, whereas in the weak field regime, positive magnetococonductivity is always obtained regardless of the magnetic field direction. We find that the weak localization is sensitive to the spatial extent of impurity potential. In time-reversal symmetry-breaking type-II Weyl semimetals, the system displays either positive or negative magnetococonductivity along the direction of band tilting, owing to the associated effect of group velocity, Berry curvature, and the magnetic field.

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I. INTRODUCTION

A Weyl semimetal [1–9] hosts linear energy dispersions through the Weyl points in the electronic band structure and displays interesting quantum properties, such as Fermi-arc surface states and the chiral anomaly [10–12]. As a manifestation of the chiral anomaly associated with a Weyl Fermion, positive magnetococonductivity [13] has been observed in Weyl semimetals [14–16]. Recently, type-II Weyl semimetals were theoretically proposed and soon realized in experiments [17–22]. Unlike the usual, or type-I, Weyl semimetals, the linear band dispersion near a Weyl node in type-II Weyl semimetals is significantly tilted, so that the Fermi surface encloses both electron and hole pockets. It is therefore important to examine the consequence of tilted Weyl-type dispersion from a microscopic viewpoint in order to understand the extraordinary properties of type-II Weyl semimetals [23–25]. An aim of the present work is to investigate theoretically the transport properties of type-II Weyl semimetals based on tight-binding models, with which the full extent of the band tilting in \(k\) space can be accessed. Both inversion-breaking type-II Weyl semimetals and time-reversal-breaking type-II Weyl semimetals are addressed in our calculations.

Indeed, as a result of the tilted dispersion, the chiral anomaly and likewise the positive magnetococonductivity are believed to be absent in some directions [17,23–25]. It is also intriguing to notice that the observed magnetococonductivity in type-II Weyl semimetals [26,27] shows both direction as well as sample dependencies. Evidently this suggests that the nature of impurity and localization also play crucial roles in the transport properties of type-II Weyl semimetals, which is also the case for type-I Weyl semimetals [28,29]. For type-II Weyl semimetals, the previous theoretical analyses are mainly based on the semiclassical Boltzmann approach [17,30–33]. Detailed analyses on the quantum transport and the effects of the impurity potential are still lacking. Therefore, a second aim of this work is then to systematically investigate the conductivity of type-II Weyl semimetals under magnetic field, combining a quantum mechanical linear-response theory based on the Kubo formula and a semiclassical approach based on the Boltzmann equation. In this approach, the effects of the range of impurity potentials and the quantum mechanical interference in the transport can be quantitatively analyzed with the tight-binding models.

We show that the Drude magnetococonductivity of the inversion-breaking type-II Weyl semimetals is positive in the weak magnetic field limit, while in the high field regime its sign is dependent on the magnetic field direction. These results are consistent with the recent experiments on WTe\(_2\) [26,27], and may also be justified theoretically. The quantum correction to the magnetococonductivity is found to be negative due to weak localization effect [34,35], and its magnitude decreases with an increasing magnetic field, indicating the suppression of weak localization. In particular, we demonstrate that the weak localization in type-II Weyl semimetals decreases with increasing spatial extent of impurity potential. Finally, a tight-binding model without time-reversal symmetry is analyzed. We find that the magnetococonductivity can be either positive or negative along the band tilting direction, which depends on the combined effect of group velocity, Berry curvature, and the direction of the magnetic field.

The paper is organized as follows. Section II demonstrates the magnetococonductivity of the inversion-breaking type-II Weyl semimetals, where the chiral anomaly and quantum oscillations are discussed. This is followed by an analysis of
The two-band Hamiltonian without a magnetic field is

\[ H = \sum_{i} c_{k,i}^{\dagger} \sigma_{\alpha}^{i} \mathbf{A}^{\alpha} c_{k,i}, \]

where \( V(R) \) stands for the impurity potential at site \( R \) produced by the impurity site \( R_i \). In this section, short-ranged impurity potential \( V(R - R_i) = u \delta_{R,R_i} \) is employed. In Sec. III, \( V(R - R') \) with finite spatial extent will be examined. The impurity sites are assumed to be randomly and uniformly distributed on the lattice, with a concentration \( n \). The self-consistent Born approximation is used to compute electron lifetimes. Subsequently, the Kubo formula will be used to calculate the Drude conductivity, in which the magnetic field enters into the Hamiltonian in Eq. (1) via the standard Peierls substitution. In the weak magnetic field limit, the semiclassical Boltzmann equation is used in place of the Kubo formula, as the magnetic supercells required by the Peierls substitution become excessively large. Further details of the model and the computational method can be found in the Appendix.

Drude conductivity along \( x/z \) direction. For the model under scrutiny the band dispersion across the Weyl nodes along the \( z \) direction displays a quadratic dependence on \( B \), which is taken into account by the Peierls substitution implemented with a \( 1 \times 1 \) magnetic supercell. \( \mathbf{A}^{\alpha} \) is related to the magnetic field by \( \mathbf{A}^{\alpha} = 2 \pi \mathbf{B} / \mathbf{B} \). The calculated Drude conductivity always decreases with increasing \( B \) when \( 25 < B < 75 \) T. In the relatively weak field limit the magnetococonductivity, obtained using the semiclassical Boltzmann equation, appears to be positive in both \( x \) and \( z \) direction, as displayed in the inset of Fig. 2. We have also examined the case when the Fermi level deviates slightly from half-filling, and found that the magnetococonductivity is qualitatively similar to the half-filling case (\( E_F = 0 \) eV), as described above.
transport experiments in WTe$_2$, where our calculated
different behaviors provide a microscopic reconciliation of two
Hamiltonian described by Eq. (1). The definition of
Landau levels only exist along the direction characterized
by the tilt direction. Reference [17] pointed out that the chiral
levels depend on the angle between applied magnetic field and
the magnetic field increases. A confirmation can be obtained
for the conductivity with oscillations is periodic on 1/B with a
relation of cos[2\pi (F/B + \phi)], where F is the frequency and
\phi is the phase shift. However, the calculated oscillations do not
exhibit single periodicity to be fitted with the Lifshitz-Kosevich
formula, possibly due to the complicated Fermi surfaces as
shown in Fig. 3(b). Indeed, the experiments have observed the
SdH oscillations with multiple frequencies in Weyl semimetals
hosting multiple Fermi pockets [15,39,40].

Furthermore, it is seen that the amplitude of the SdH oscillations
in $\sigma_{zz}$ becomes reduced as the impurity strength measured
by $u^2n$ increases. For sufficiently large values of $u^2n$, the SdH
oscillations become completely suppressed, as demonstrated in
Fig. 3(c). This reduction and eventual disappearance of the
SdH oscillations arises from the decrease of relaxation time at
large $u^2n$, which in turn leads to increasing broadening of the
Landau levels. This implies that the spectral oscillation that
causes SdH oscillation gets less sharp as the impurity scattering
is increased, resulting in weaker SdH oscillations. We expect
that the increase of interaction range, resulting in smaller

It has been demonstrated with a semiclassical approach
that the chiral anomaly of type-I Weyl fermions can lead to
a positive magnetoconductivity quadratic in $B$ in the presence
of parallel electric and magnetic fields [13]. In contrast to type-I
Weyl fermions, the general trend of the magnetoconductivity
of type-II Weyl fermions is separated into two regimes, as
indicated by our numerical calculations. In the quantum regime
(high field), the chiral anomaly induced positive magnetocon-
ductivity emerges only if the chiral Landau levels are formed
under the given magnetic field, as shown in Fig. 2. The previous
works [17,23–25] found that the existence of chiral Landau
levels depend on the angle between applied magnetic field and
the tilt direction. Reference [17] pointed out that the chiral
Landau levels only exist along the direction characterized
by a ratio $P > 1$ around the Weyl node [the $z$ direction in
Hamiltonian described by Eq. (1)]. The definition of $P$ is

$$P = (h/\hbar)^2 / [(h/\hbar)^2 + (h/\hbar)^2 + (h/\hbar)^2], \quad (4)$$

in which the numerator and the denominator represent the
square of potential energy and kinetic energy of the Weyl
fermions, respectively. However, in the low-field regime the
positive magnetoconductivity is shown to exist when $B$ is along
any arbitrary direction based on the Boltzmann approach, as
shown in the inset of Fig. 2. The numerical results are consistent
with the previous theoretical works [17,30,32]. These two
different behaviors provide a microscopic reconciliation of two
transport experiments in WTe$_2$, where our calculated $\sigma_{zz}$ and
$\sigma_{xx}$ in high field ($B > 25$ T) and weak field limit conform to
the two regimes, respectively [26,27,30].

Shubnikov–de Haas oscillations. The oscillations in $\sigma_{zz}$
shown in Fig. 2 is attributable to the Shubnikov–de Haas
(SdH) oscillations arising from the oscillation of relaxation
time, which in turn reflects the oscillation of spectra as the
magnetic field increases. A confirmation can be obtained
by computing the magnetoconductivity with the relaxation
time fixed to the value $\tau_0$ under zero magnetic field instead
of that derived from the self-consistent Born approximation

with actual magnetic field. The results indicate that $\sigma_{zz}(\tau_0)$
increases without any obvious oscillations as $B$ increases. In
order to focus on the oscillations, we remove the effect of
chiral anomaly by considering a relative conductivity $[\sigma_{zz} - \sigma_{zz}(\tau_0)]/\sigma_{zz}^0$, where $\sigma_{zz}^0$ is the conductivity under $B = 0$. The
relative conductivity is presented as a function of 1/B in
Fig. 3(a). According to the Lifshitz-Kosevich formula [38],
the conductivity with oscillations is periodic on 1/B with a
relation of $\cos[2\pi (F/B + \phi)]$, where $F$ is the frequency and
$\phi$ is the phase shift. However, the calculated oscillations do not
exhibit single periodicity to be fitted with the Lifshitz-Kosevich
formula, possibly due to the complicated Fermi surfaces as
shown in Fig. 3(b). Indeed, the experiments have observed the
SdH oscillations with multiple frequencies in Weyl semimetals
hosting multiple Fermi pockets [15,39,40].
relaxation time, could also suppress the SdH oscillations. These results and analyses provide an explanation to the experimental observation that the SdH oscillations displayed sample-dependent features at the same temperature and the same magnetic field [14]. Similarly, in experiment the rising sample-dependent features at the same temperature and the relaxation time, could also suppress the SdH oscillations.

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Lastly, we note that the calculated conductivity along \( x \) direction is always reduced by increasing magnetic field.

We can easily realize the transition from type-I to type-II Weyl fermions by increasing the tilt parameter \( \gamma \) in Eq. (1). In the low field regime, \( \sigma_{xx} \) and \( \sigma_{zz} \) show no qualitative changes when the system changes from type-I to type-II Weyl fermions according to our numerical results with Boltzmann approach. In the high field regime, the magnetococonductivity is shown in Figs. 4(a)–4(d), and the Fermi surface cuts are shown in Fig. 4(e). The tilt parameters \( \gamma = 1.6 \) and \( \gamma = 2.4 \) are chosen as two typical cases corresponding to type-I and type-II Weyl fermions, respectively, and \( \gamma = 2.0 \) is the critical point. Along the tilt \( z \) direction, the magnetococonductivity is always positive for these two cases. However, the behavior of \( \sigma_{xx} \) in type-I Weyl fermions is distinct from that in type-II Weyl fermions. In the type-II case (with \( \gamma = 2.4 \)), \( \sigma_{xx} \) is negative, whereas \( \sigma_{xx} \) is positive in the type-I case (with \( \gamma = 1.6 \)) according to our calculation. At the critical point with \( \gamma = 2.0 \), \( \sigma_{xx} \) is still positive, just like the case in type-I Weyl fermions. As \( \gamma \) increases in a small range from the critical point 2.0 to 2.2, the sign of \( \sigma_{xx} \) changes from positive to negative. These results demonstrate that the sign change of magnetococonductivity is not clear cut between these two types of fermions (type-I and type-II).

III. QUANTUM CORRECTION TO CONDUCTIVITY

The Drude conductivity presented above does not include the so-called weak (anti-)localization [34,35], while this type of quantum correction to the conductivity could play an important role in the transport especially in time-reversal invariant systems at low temperatures. When scattering mechanism is being considered, the inherent anisotropy in type-II Weyl fermions leads to a rather different symmetry classification from the isotropic Weyl fermions [41]. Consequently, the quantum correction to the Drude conductivity warrants careful scrutiny. This is achieved by solving the four-point Dyson equation corresponding to the maximally crossed diagrams [42], which is the leading order contribution to the quantum correction from the diagrammatic averaging of the Kubo formula over the ensemble of disorder configurations.

In Fig. 5(a) we present the computed quantum correction to conductivity (\( \delta \sigma_{zz} \)) of the tight-binding model in Eq. (1) along with a localized impurity potential, under zero magnetic field as a function of \( l_\phi \). \( l_\phi \) is the coherence length in \( z \) direction characterizing the inelastic scattering process, as shown in the Appendix. It is clear that \( \delta \sigma_{zz} \) is negative, indicating weak localization. The weak localization correction to conductivity in the anisotropic system theoretically takes the form [43]

\[
\delta \sigma_{zz} = \frac{e^2}{\hbar \pi^2} \alpha (\Gamma l_{\phi} - 1/l),
\]

with \( l \) denoting the mean-free path and \( \alpha = \frac{\sigma_{xx}}{\sqrt{\sigma_{xx} \sigma_{yy} \sigma_{zz}}} \). The effects of anisotropy are absorbed into the anisotropic coefficient \( \alpha \). Fitting the calculated \( \delta \sigma_{zz} \) versus \( l_\phi \) shown in Fig. 5(a) to the formula in Eq. (5) gives the fitted values \( \alpha = 0.41 \) and \( l = 5.85\sigma_0 \), which are quite different from \( \alpha \) given by \( \frac{\sigma_{xx}}{\sqrt{\sigma_{xx} \sigma_{yy} \sigma_{zz}}} = 0.43 \) and the mean-free path \( l = 8.89\sigma_0 \) determined by the relaxation time and the diffusion coefficient (see the Appendix). Since the quantum corrections do not have an intrinsic difference between tilt \( z \) direction and other directions, then we believe that the quantum corrections to conductivity along other directions are also negative. This is confirmed by our calculation of conductivity along \( z \) and \( x \) directions, and the quantum corrections along these two directions are found to be roughly proportional to the Drude conductivity along the corresponding direction.

To understand the mismatch between the fitted and the theoretically derived values of \( \alpha \) and \( l \), it is useful to analyze \( q \)-resolved conductivity change \( \delta \sigma_{zz}(q) \), which when integrated yield the total quantum correction to conductivity. Under the assumption that the diffusion coefficient is anisotropic but \( q \) independent, \( \sigma_{zz}(q) \) has \( \frac{e^2}{\hbar \pi^2} (D_{xx}/D_{zz} q_x^2 + D_{yy}/D_{zz} q_y^2 + q_z^2)^{-1} \) near the diffusion pole (\( q = 0 \)), where \( D_{xx}, D_{yy}, D_{zz} \) are diffusion coefficients. Rescaling the momenta as \( \tilde{q} \equiv \left( \frac{\sqrt{2\pi}}{\sigma_0} q_x, \frac{\sqrt{2\pi}}{\sigma_0} q_y, q_z \right) \), we have \( \delta \sigma_{zz}(\tilde{q}) = -e^2/(4\pi^3 h q_z^2) \), using the fact that the ratios of diffusion coefficients are equal to...
the ratios of conductivity via the Einstein relation. It is easy to find that the integral of $\sigma_{zz}(\tilde{q})$ exactly gives the relation shown in Eq. (5). The calculated $\delta\sigma_{zz}(\tilde{q})$ versus $\tilde{q}$ is presented in Fig. 6(a) in logarithmic coordinates. We find that when $\tilde{q}$ is small, the calculated $\delta\sigma_{zz}(\tilde{q})$ is almost the same for different $q$ with the same length and can be well fitted by the formula $\delta\sigma_{zz}(\tilde{q}) = -e^2/(4\pi^3\hbar^2q^2)$ describing the correction in the three-dimensional isotropic systems. However, for larger $\tilde{q}$ the calculated $\delta\sigma_{zz}(\tilde{q})$ deviates significantly from $\tilde{q}^{-2}$, and quite remarkably, are generally smaller than the corresponding values obtained by $\delta\sigma_{zz}(\tilde{q}) = -e^2/(4\pi^3\hbar^2q^2)$. This makes the fitted $l$ smaller than the theoretical value. By changing the parameters $\gamma$ to 0 and $t_1$ to $t$ in Eq. (1), a model of type-I Weyl fermions is obtained. The anisotropy of $\delta\sigma_{zz}(\tilde{q})$ is also found in type-I Weyl fermions as shown in Fig. 6(b) with the localized impurity potential $u_0^2n = 0.002\ eV^2$ and $E_F = 0.15\ eV$. Thus our results and analysis indicate that the anisotropic efficient $\alpha$ can only capture the anisotropy from the scattering processes associated with the small total momentum. Therefore, for both type-I and -II Weyl fermions with anisotropy, the quantum correction $\delta\sigma_{zz}(\tilde{q})$ originating from the scattering processes with large total momentum, can have significant dependence on high orders of $q$; that is, the diffusion coefficients are no longer constants but now become $q$ dependent.

It is known that weak localization, reflecting quantum interference between time-reversed paths, can be suppressed by the application of an external magnetic field. To account for the external magnetic field, $\delta\sigma_{zz}$ is computed by the Kubo formula in magnetic supercells in the high-field regime, and with a semiclassical approximation (details in the Appendix) in the low-field regime [35], respectively. The computed values of $\delta\sigma_{zz}$ are shown as a function of magnetic field $B$ in Fig. 5(b).

Indeed, as the addition of a magnetic field suppresses the weak localization, the conductivity increases quickly with increasing $B$. In fact, the quantum correction vanishes at around $B = 3\ T$ from the semiclassical calculations, which is consistent with the result of Kubo formula by computing the maximally crossed diagrams in supercells at the high-field limit.

The spatial extent of impurity potential has an important influence on the quantum correction to conductivity [44], which we now examine for the type-II Weyl fermion, by using the scattering Hamiltonian in Eq. (3) with finite ranges of impurity potential. We adopt a Gaussian-type impurity potential in order to model the influence of spatial range on this quantum correction. The impurity potential is independent of orbital, and is expressed as

$$V(R - R_0) = \alpha \prod_j \frac{a_0}{\sqrt{2\pi R_0^j}} e^{-R_j^2 |R_j^2/(2 R_0^j)^2)}, \quad (6)$$

where $R_j$ represents the component of $R$ along $j$ direction ($j = x, y, z$), and $R_0$ characterizes the spatial ranges in the three directions.

To focus on the quantum correction to conductivity contributed by the Weyl fermions, in evaluating the quantum correction from the maximally crossed diagrams we only include the $K$ points close to each Weyl point (distance between the $k$ points to nearby Weyl point smaller than $\pi/4a_0$) so as to exclude the contributions from the trivial Fermi pockets. In this time-reversal invariant system, the quantum interference is dominated by intervalley scattering between states related...
by time-reversal symmetry. As shown in Fig. 1, all four Weyl
nodes are located on the \( k_y \) = 0 plane and the extent of Fermi
surfaces around each Weyl point are small in the \( y \) direction. It
is therefore expected that the quantum correction depends more
sensitively on the spatial extent of impurity potential in the \( x-z \)
plane, than on the spatial extent along the \( y \) direction. For
this reason, it is sensible to devise the components of \( R_0 \) such
that \( R_0^x = 0 \) and \( R_0^y = R_0^z = D_0 \) to reduce computational
cost. The computed quantum correction to conductivity with the
same \( I_0 \) and \( t \) is seen to be suppressed by increasing the range
\( D_0 \) of impurity potentials, and finally vanishes as soon as \( D_0 \)
approaches the lattice constant \( a_0 \), as shown in Fig. 5(c). These
results imply that the long-range potential could destroy the
quantum interference between the scattering paths interrelated
by time-reversal symmetry. The quantum interference diminishes as the increase in spatial extent of the impurity
potential reduces intervalley scattering. The case \( R_0^y = D_0 \)
\((R_0^x \text{ and } R_0^y \to 0)\) is also computed for comparison, where the
correction \( \delta \sigma_{zz} \) does not change over \( R_0^y \) as expected.

IV. DRUDE CONDUCTIVITY OF
TIME-REVERSAL-BREAKING TYPE-II
WEYL SEMIMETALS

We now turn to a brief discussion of the magnetocon-
ductivity of time-reversal-breaking type-II Weyl semimetal.
It was pointed out that time-reversal-breaking type-I Weyl
semimetal could exhibit linear magnetoconductivity by in-
trouducing a band tilting term or by taking nonlinear terms
of the band dispersion into account [32,33]. If we consider
the magnetoconductivity from a semiclassical viewpoint, as
given in Eq. (A3), it is seen that Berry curvature can make a
crucial contribution. If a system preserves inversion symmetry,
we have \( \xi_k = \Omega_{-k} \) and \( v_k = -v_{-k} \), where \( \xi_k \) and \( v_k \) are
the Berry curvature and group velocity at wave vector \( \mathbf{k} \).
Upon the zone sum prescribed in Eq. (A3), it clearly leads
to a nonvanishing contribution to the magnetoconductivity
first order in \( B \). There is, however, no further constraint that
determines the sign of the magnetoconductivity. Indeed,
our calculations confirm that we can have a situation where
the magnetoconductivity along the band tilting direction is either
positive or negative in a time-reversal-breaking type-II Weyl
semimetal contrary to the conclusion drawn previously [30].

The minimal model of time-reversal-breaking type-II Weyl
fermions takes the following form [37]:

\[
H^T = c_\alpha^\dagger k_x h_T^\alpha \sigma_{\alpha \beta} c_{k\beta},
\]

in which

\[
\begin{align*}
h_T^0 &= \gamma (\cos k_x - \cos k_0), \\
h_T^1 &= -2t \sin k_y, \\
h_T^2 &= -m (2 - \cos k_x - \cos k_0). 
\end{align*}
\]

(8)

This model hosts two Weyl nodes at \(( \pm k_0, 0, 0)\) with \( k_0 = \pi/2 \). The dispersion of the Weyl nodes tilt in the \( x \) direction. We shall
examine two typical situations \( t_x = t \) and \( t_x = -t \), where
the components of the Berry curvature around the Weyl points
have opposite signs between these two cases, featuring opposite
chiralities. The band structures are depicted in Figs. 7(a) and

FIG. 7. Band structures and magnetoconductivity of time-
reversal breaking model when \( B \) is along the same direction of
\( E \). (a) and (b) Band structures of the Hamiltonian in Eq. (7) with
\( k_y = 0 \). The Weyl points are enclosed by red circles. We chose
\( m = 2t, \gamma = 3t, t = 0.1 \) eV, \( k_0 = \pi/2, a_0 = 6 \) Å, \( E_F = 0 \) eV for
(a) with \( t_x = t \) and for (b) with \( t_x = -t \). Magnetoconductivity shown
in (c) and (d) correspond to the band structures in (a) and (b),
respectively, where \( \sigma_{xx} \) and \( \sigma_{zz} \) represent the magnetoconductivity
with the magnetic field applied along \( x \) and \( z \) direction, respectively.
The red lines are the fitted results with \( \alpha B \). The localized impurity
potential satisfy \( u^2 n = 0.002 \) eV\(^2\).

7(b). Owing that the first-order terms of magnetoconductivity
in \( B \) are dependent on the sign of magnetic field, both the
parallel and antiparallel electric and magnetic field are
discussed.

The Drude conductivity is calculated by Kubo formula with
magnetic field applied by Peierls substitution with the
short-ranged impurity potential \( u^2 n = 0.002 \) eV\(^2\). The absence
of time-reversal symmetry destroys the quantum interference
between the scattering paths, making the quantum correction
negligible, thus it is not included here. The Drude conductivity
with \( E_F = 0 \) eV is shown in Fig. 7(c) with \( t_x = t \) and Fig. 7(d)
with \( t_x = -t \), where the magnetic field is applied along the
same direction with the electric field. The oscillatory pattern
of magnetoconductivity is once again a manifestation of the
SdH oscillations. The value of \( \sigma_{zz} \) decreases with increasing \( B \)
for both \( t_x = t \) and \( t_x = -t \). Besides, the value of \( \sigma_{xx} \) increases
linearly with \( B \) for \( t_x = t \), in accordance with previous work
based on the Boltzmann approach [30]. However, when \( t_x = -t \) the computed \( \sigma_{xx} \) is negative for a finite value of \( B \). In
contrast to the case that \( B \) and \( E \) are in the same direction, the
calculated \( \sigma_{xx} \) becomes decreasing for \( t_x = t \) and increasing
for \( t_x = -t \) with increasing \( B \), when the magnetic field is
applied in the opposite direction of the electric field. According
to our calculations, the positive magnetoconductivity appears
only if the following two conditions are met in the high field
regime. First, the ratio \( P \) defined in Eq. (4) is greater than
one along the direction of magnetic field [17] (\( x \) direction in
where (a) and (b) correspond to the magnitude. The lines represent $\Omega_{ak} \cdot v_{ak}$, where the line thickness represents the magnitude. The purple (blue) color marks that the sign of $\Omega_{ak} \cdot v_{ak}$ is positive (negative). The corresponding $v_{ak}(\Omega_{ak} \cdot v_{ak})$ are represented by red arrows. The lengths of arrows correspond to the magnitude.

this case). Second, the first-order terms in $B$ to magnetoconductivity should be positive, which corresponds to $B > 0$ for $t_x = t$ or $B < 0$ for $t_x = -t$ in the Hamiltonian described in Eq. (7).

To understand the results of $\sigma_{xx}$ from a perspective of semiclassical theory, we investigate the first-order terms of Eq. (A3), $B^n v_{nk}(\Omega_{nk} \cdot v_{nk})$, in which the signs and magnitudes of $\Omega_{nk} \cdot v_{nk}$, and $B^n$ are clearly all important. $\Omega_{nk} \cdot v_{nk}$ near the Weyl nodes is seen to dominate owing to the divergent $\Omega_{nk}$, and has opposite signs for $k$ and $-k$ as shown in Fig. 8. When multiplied by the factor $v_{nk}$, the resulted quantity $v_{nk}(\Omega_{nk} \cdot v_{nk})$ is dominated by the contributions from the Weyl nodes, which for $t_x = t$ is positive for the two Weyl nodes in Fig. 8(a). This results in a positive overall magnetoconductivity along $x$ direction for $B^x > 0$. In the case $t_x = -t$, the dominated first-order terms $v_{nk}(\Omega_{nk} \cdot v_{nk})$ are negative as shown in Fig. 8(b), and lead to negative overall magnetoconductivity along the $x$ direction for $B^x < 0$. Specifically, the Hamiltonian with $t_x = -t$ and $t_x = t$ can be connected by the transform $H_{n,k,k}' = -\sigma^2 H_{n,k,k}^s$, such that the first-order terms at momentum $(k_x + \pi, k_y, -k_z)$ with $t_x = -t$ and $(k_x, k_y, k_z)$ with $t_x = t$ are found to be of opposite sign. Thus the opposite sign of $\sigma_{xx}$ is obtained under the same $B$ with $t_x = \pm t$. These semiclassical expectations agree very well with our numerical results. And it is evaluated that the sign change of $B^x$ could also lead to the sign change of magnetoconductivity. These results quantitatively demonstrate that the magnetoconductivity of time-reversal-breaking type-II Weyl fermions can be either positive or negative along the band tilting direction, depending on the combined effect of group velocity, Berry curvature, and the magnetic field. This is quite different from the inversion-breaking Weyl semimetals, where only second-order terms of magnetic field survive, and the magnetoconductivity is always positive regardless of the sign of magnetic field. The above analysis can also be applied to explain the magnetoconductivity in Dirac semimetals, of which the magnetoconductivity is expected to exhibit no dependence on the sign of a magnetic field.

V. SUMMARY

To summarize, the magnetoconductivity of the type-II Weyl semimetals is systematically analyzed based on tight-binding models, in which the effects of magnetic field, spatial extent of the impurity potential, and quantum correction are taken into account. For the inversion-breaking type-II Weyl semimetal, the magnetoconductivity is always positive along the band tilting direction, whereas if the magnetic field is perpendicular to the band tilting direction, the magnetoconductivity is positive under relatively weak magnetic field and negative under high magnetic field due to the absence of chiral Landau levels. Along this direction (perpendicular to tilt direction), the magnetoconductivity undergoes a sign transition as tuning the tilt parameter $\gamma$ to crossover from type-I to type-II Weyl fermions. The accompanying SdH oscillations are found not to exhibit simple periodicity due to the complicated Fermi surfaces, and the oscillations can be suppressed by increasing the impurity potential or concentration. Taking into account the quantum correction to conductivity, our results indicate that weak localization is present and it should be described by anisotropic and $q$-dependent diffusion coefficients. It is found that the quantum correction increases with increasing magnetic field or increasing spatial extent of the impurity potential, either of which suppresses weak localization. For the time-reversal-breaking type-II Weyl semimetals, the sign of magnetoconductivity can be either positive or negative along the band tilting direction, which is determined by an interplay of group velocity, Berry curvature, and the magnetic field near Weyl nodes.

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APPENDIX: COMPUTATIONAL DETAILS

Drude conductivity. The impurities break translational symmetry, which result in scatterings between different $k$ points. To restore the symmetry, we adopt the impurity configuration averaged Green’s function with self-consistent Born approximation:

$$G(k) = [E_F - H_k - \Sigma(k)]^{-1},$$

$$\Sigma(k)_{nm} = \sum_{k' n_1 n_2} \langle H'_{n k n_2 k'} H'_{n_1 k' n_3} \rangle G_{n_1 n_2}(k'),$$

where $\langle \cdots \rangle$ represents the average over impurity configurations and $m, n, n_1, n_2$ are the band indices. The imaginary part of $\Sigma(k)_{nm}$ is directly related to the inverse of relaxation time by $\tau_{nk} = \hbar/2|\text{Im} \Sigma(k)_{nm}|$. In relatively high magnetic field, the formal Kubo formula is employed to calculate the conductivity, which takes the form

$$\sigma_{\mu \nu} = \frac{e^2 \hbar}{\pi V} \text{Tr} [\nu^\mu (\text{Im} \tilde{G}) \nu^\nu \text{Im} \tilde{G}].$$

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Here $V$ is the volume of the unit cell and $v^\mu$ is the velocity operator along $\mu$ direction. The magnetic field breaks the translational symmetry in real space, which is restored by Peierls substitution with a magnetic supercell in our calculations. When the magnetic field is weak, this Peierls substitution approach requires a large supercell that makes the computation intractable. Therefore, in the low-field regime, the conductivity ($B^2/E$) is obtained by the semiclassical Boltzmann approach, given by the formula [45]

$$\sigma_{\mu\mu} = \sum_n e^2 \int \frac{dk}{(2\pi)^3} D_{nk} \left( v^\mu_{nk} + \frac{eB^\mu}{\hbar} \Omega_{nk} \cdot v_{nk} \right)^2 \times \tau_{nk} \delta(\epsilon_{nk} - E_F),$$

(A3)

with $D_{nk} = \left[ 1 + (e/\hbar)(B \cdot \Omega_{nk}) \right]^{-1}$, $\Omega_{nk} \cdot v_{nk} = \epsilon_{nk}$, $\tau_{nk}$ are, respectively, the Berry curvature, group velocity, band energy, and relaxation time of the $n$th band at wave vector $k$. The angular dependence of relaxation time is ignored in our calculations. The Landau quantization is neglected in the semiclassical Boltzmann approach.

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