Introduction. A forty-year-old puzzle in transition metal pentatellurides ZrTe$_5$ and HfTe$_5$ is the anomalous peak in the temperature dependence of resistivity, which is accompanied by sign reverses of the Hall and Seebeck coefficients. We give a plausible explanation for these phenomena without assuming any phase transition or strong interaction effect. We show that due to intrinsic thermodynamics and diluteness of the conducting electrons in these materials, the chemical potential displays a strong dependence on the temperature and magnetic field. With that, we compute resistivity, Hall and Seebeck coefficients in zero field, and magnetoresistivity and Hall resistivity in finite magnetic fields, in all of which we reproduce the main features that are observed in experiments.

Model. Our discussions will focus on ZrTe$_5$ but they can be easily adapted to HfTe$_5$. ZrTe$_5$ is a highly anisotropic layered material. According to Ref. 11, the low-energy band structure contains a Dirac-like electron pocket at Γ point and four other electron pockets near Brillouin zone boundary. We model them by an anisotropic Dirac fermion and four identical anisotropic quadratic fermions[Fig. 1(a)]. The Dirac fermion has the well known relativistic dispersion $E = \pm \sqrt{m^2 + v^2 p_y^2 + v^2 p_z^2}$, where $m$ is the Dirac mass and $v_\alpha$ is the velocity in $\alpha$ direction, $\alpha = x, y, z$. The energy bottom of the quadratic fermions is $\Delta$, measured by an anisotropic Dirac fermion and four identical anisotropic quadratic fermions[Fig. 1(a)]. The total DOS is given respectively by

$$D_1(\epsilon) = 2\alpha_1|\epsilon|\sqrt{\epsilon^2 - m^2} \Theta(|\epsilon| - m),$$

$$D_2(\epsilon) = 2\alpha_2 \sqrt{\epsilon - \Delta} \Theta(\epsilon - \Delta),$$

where $\alpha_1 = 1/(2\pi^2\hbar^3 v_x v_y v_z)$, $\Theta(x)$ is the Heaviside step function, $\kappa = 4$ denotes the four copies of quadratic fermions, $\alpha_2 = \sqrt{2m_\pi^* m_\pi^* m_\pi^*/(2\pi^2 \hbar^3)}$, $m_\pi^*$ is the anisotropic effective mass of quadratic fermions, the factor 2 comes from spin degeneracy. The total DOS is

\[\text{FIG. 1. (a) Schematics of the low-energy band structure in ZrTe}_5. \text{ (b) Landau level bottoms of 3D Dirac and quadratic fermions with } B = 4T \text{ (energy in units of meV; see Fig. 2 for numerics). (c) Densities of states at } B = 0 \text{ and (d) at } B = 4T \text{ (smoothed by a small disorder).}\]
$D(\epsilon) = D_1(\epsilon) + D_2(\epsilon)$. We emphasize that the Dirac dispersion is PH symmetric, i.e., $D_1(\epsilon) = -D_1(-\epsilon)$. Presence of the quadratic fermions breaks the PH symmetry.\cite{22}

We also consider the effect of an external magnetic field $B = B\hat{z}$, under which electron eigenstates form Landau levels. Details on Landau levels of Dirac fermion can be found, e.g., in Refs. 23 and 24 or Supplemental Materials (SM)\cite{25}. The Landau level energy is given by $E_a = \lambda \sqrt{m^2 + \hbar^2 \omega_{c1}^2 N + v_z^2 p_z^2}$, where $N \geq 0$ is the Landau level index, $p_z$ is the momentum along $z$ direction, $\lambda = \pm 1$ represents the electron or hole branch respectively, $\omega_{c1} = \sqrt{2v_x v_y eB/\hbar}$ is relativistic cyclotron frequency and Zeeman splitting is neglected. Landau levels of quadratic fermions are textbook results, with the energy $E = \hbar \omega_{c2}(N+1/2) + p_z^2/2m_z^2 + \Delta$, where $\omega_{c2} = eB/(c \sqrt{m_z^2 m_y^2})$. The DOS’s are now given by

$$D_1(\epsilon, B) = a_1 \sum_{N \geq 0} \frac{d_N \hbar^2 \omega_{c1}^2 |\epsilon|}{2 \sqrt{\epsilon^2 - E_{N1}}} \Theta(|\epsilon| - E_{N1})$$

$$D_2(\epsilon, B) = k a_2 \sum_{N \geq 0} \frac{\hbar \omega_{c2}}{\sqrt{\epsilon^2 - E_{N2}}} \Theta(\epsilon - E_{N2})$$

where $d_N = 2 - \delta_{N,0}$, $E_{N1} = \sqrt{m^2 + \hbar^2 \omega_{c1}^2 N}$ and $E_{N2} = \hbar \omega_{c2}(N+1/2) + \Delta$. The latter two are the bottom energies of 3D Landau levels of the Dirac and quadratic fermions respectively. In the limit $B \to 0$, expressions in (2) reduce to those in (1).

Figure 1(b) plots the Landau level bottoms at $B = 4T$ to give readers a sense of level spacings, with numerics given in the caption of Fig. 2. We note that the Dirac fermion is “lighter” than the quadratic fermions, and thereby has bigger level spacings. Figure 1(c) and 1(d) show DOS’s in zero field and in a finite $B$ field respectively. Effect of disorder is neglected in our thermodynamic calculations. It will be included in our calculations of transport properties below.

Chemical potential $\mu(T, B)$. With the above DOS’s, we now study the $T$ and $B$ dependence of the chemical potential $\mu$. The particle number density $n(T, B, \mu)$ can be expressed as

$$n(T, B, \mu) = \int_0^\infty d\epsilon D(\epsilon, B) f_T(\epsilon - \mu)$$

$$+ \int_{-\infty}^0 d\epsilon D(\epsilon, B)[f_T(\epsilon - \mu) - 1],$$

where $f_T(\epsilon) = 1/[\exp(\epsilon/T) + 1]$ is the Fermi-Dirac distribution (Boltzmann constant $k_B$ is absorbed into $T$ throughout the paper). Charge neutrality is taken to be at $\epsilon = 0$. The density $n$ is fixed in a given 3D sample, so Eq. (3) should be understood as an integral equation that defines a function $\mu(T, B)$.

We solve Eq. (3) numerically by setting all the parameters in (1) and (2) to be comparable to experimentally measured values.\cite{10} The results are shown in Fig. 2. When $T$ varies in the range $0 \sim 25$meV and $B$ varies in the range $0 \sim 25T$, our calculation shows a significant variation in $\mu$, of the order of $E_F$, in agreement with the APRES observation\cite{11}. In particular, for $B = 0$, the chemical potential $\mu$ decreases monotonically from a positive $E_F$ into a negative value around $T_0 \approx 10$meV. One can show that this monotonic decreasing behavior occurs for a fairly general class of DOS’s — see SM\cite{25}. A monotonic behavior is also observed when $T \gtrsim \hbar \omega_{c1}$ for a finite $B$. When $T \lesssim \hbar \omega_{c1}$, quantum oscillations in $\mu$ can also be seen in Fig. 2(c), which however is not our focus.

The fact that $\mu$ changes so dramatically, compared to conventional metals, in the temperature regime $T \lesssim 25$meV and in experimentally accessible magnetic fields $B \lesssim 25T$ follows from two properties of ZrTe$_5$: (i) $E_F$ is small, approximately 25meV, i.e., conducting electrons are dilute; and (ii) the PH symmetry is broken at the
We begin with the longitudinal resistivity \( \rho_{xx}(T) \), Hall coefficient \( R_H(T) \) and Seebeck coefficient \( S_{xx}(T) \) with different Fermi energies. The level broadening constants are set by \( \Gamma_1 = 0.5 \text{ meV} \), estimated from experimental data in Ref. 10 and \( \Gamma_2 = 10 \Gamma_1 \) (see an estimate in SM[25] using Born approximation) throughout our calculations. Panels (b) and (d) show different contributions to the longitudinal conductivity \( \sigma_{xx} \) and Hall conductivity \( \sigma_{xy} \) at \( E_F = 25 \text{ meV} \) and panel (f) shows the density ratios \( n_{\text{Dirac}}/n \) and \( n_{\text{qual}}/n \) versus temperature.

Resistance, Hall and Seebeck coefficients. We now proceed to calculate transport coefficients and see if the above thermodynamic behaviors can result in the experimentally observed resistivity peak and other transport phenomena. We begin with the longitudinal resistivity \( \rho_{xx}(T) \), Hall coefficient \( R_H(T) \) and Seebeck coefficient \( S_{xx}(T) \) in zero magnetic field.

To calculate transport coefficients, we use the Kubo formula (see e.g. Refs. 26 and 27). Our calculations are standard and details are included in SM[25]. The Hall coefficient, defined by \( \rho_{xy} = R_H B \), is obtained by taking the \( B \to 0 \) limit of our finite-magnetic-field results. The Seebeck coefficient is computed by a generalized Mott formula that was obtained in Ref. 28. Here, we discuss how disorder is treated. Disorder is the only source of resistivity in our calculations as electron-phonon and electron-electron scattering are absent. It is included by an energy level broadening \( \Gamma_\alpha \) in the single-particle Green’s function

\[
G_\alpha(\omega) = \frac{1}{\omega - E_\alpha + i\Gamma_\alpha(\omega)}
\]

where \( E_\alpha \) is the energy associated with the single-particle eigenstate \( |\alpha\rangle \). We take a crude simplification: \( \Gamma_\alpha(\omega) = \Gamma_1 \) is a constant for all eigenstates of the Dirac fermion, and \( \Gamma_\alpha(\omega) = \Gamma_2 \) is also a constant for all eigenstates of the quadratic fermions. We will see that this somewhat oversimplified treatment produces surprisingly good results. So, we will not bother to apply more realistic disorder models such as Born approximation or self-consistent Born approximation[27, 29].

Evaluations of \( \rho_{xx}(T), R_H(T) \) and \( S_{xx}(T) \) are done numerically with an input of temperature-dependent \( \mu \) determined from Eq. (3). The results are shown in Fig. 3. Indeed, an anomalous peak appears in the longitudinal resistivity and the sign reverses in both the Hall and Seebeck coefficients, all of which occur around the temperature \( T_0 \). The shapes of the curves in Fig. 3(a), (c) and (e) agree very well with those in experiments.[1–5, 10, 15, 30]

To have a better understanding, we show different contributions to the longitudinal conductivity \( \sigma_{xx} \) and Hall conductivity \( \sigma_{xy} \) in Fig. 3(b) and (d). Contributions from intra-branch scatterings of the Dirac fermion \( \sigma_{xx}^{(1)}(\sigma_{xy}^{(1)}) \) and \( \sigma_{xy}^{(1)} \) dominate, and those from inter-branch scattering \( \sigma_{xx}^{(1)} \) and the quadratic fermions \( \sigma_{xx}^{(2)} \) are negligible in the temperature regime of our interests. Intuitively, the “relativistic” Dirac fermion moves much faster than the “non-relativistic” quadratic fermions, and so contributes more to the conductivity.[31] While they do not conduct much current, the quadratic fermions do serve as good thermodynamic reservoirs, as shown in Fig. 3(f). That is, they are thermodynamically activated, but not quite in transport.

Analytically, once we neglect the contributions from the quadratic fermions and inter-branch scattering of the Dirac fermion and focus on the regime \( T \gg \Gamma_1 \), the conductivities can be approximated by

\[
\sigma_{xx} \approx C_{xx} \sum_{\lambda = \pm} \int_0^\infty d\epsilon \frac{e^2 - m^2\epsilon^{3/2}}{\epsilon} \left[ -f_T(\lambda \epsilon - \mu) \right],
\]

\[
\sigma_{xy} \approx C_{xy} \sum_{\lambda = \pm} \int_0^\infty d\epsilon \frac{e^2 - m^2\epsilon^{3/2}}{\epsilon^2} \left[ \lambda f_T(\lambda \epsilon - \mu) \right],
\]

energy scale of \( \Delta \), and \( \Delta \approx E_F \). Generally speaking, variation of \( \mu \) is set by \( T/E_F \) and \( h\omega_{\text{ar}}/E_F \). Accordingly, a small \( E_F \) makes it easier to achieve a significant change in \( \mu \) by tuning \( T \) and \( B \). Nevertheless, without property (ii), one can show that the PH symmetry guarantees \( \mu > 0 \), if \( E_F > 0 \). Or equivalently, PH symmetry pushes the sign-reversing temperature \( T_0 \), defined by \( \mu(T_0, B) = 0 \), to infinity. To have a finite \( T_0 \), the PH symmetry must be broken. We will show below that \( T_0 \) is closely related to the sign-reversing temperature of the Hall and Seebeck coefficients. While the scale of \( T_0 \) is set by \( \Delta \), its precise value depends on \( E_F \), the effective masses \( m_\alpha^{*} \), magnetic field \( B \), etc. We note that in Fig. 2(b), \( T_0 \) barely displays a dependence on \( B \). However, there is actually a very weak quadratic correction, \( \delta T_0 \propto B^2 \), which we discuss in SM[25].

FIG. 3. Temperature dependence of the longitudinal resistivity \( \rho_{xx}(T) \), Hall coefficient \( R_H(T) \) and Seebeck coefficient \( S_{xx}(T) \) with different Fermi energies. The level broadening constants are set by \( \Gamma_1 = 0.5 \text{ meV} \) (estimated from experimental data in Ref. 10) and \( \Gamma_2 = 10 \Gamma_1 \) (see an estimate in SM[25] using Born approximation) throughout our calculations. Panels (b) and (d) show different contributions to the longitudinal conductivity \( \sigma_{xx} \) and Hall conductivity \( \sigma_{xy} \) at \( E_F = 25 \text{ meV} \) and panel (f) shows the density ratios \( n_{\text{Dirac}}/n \) and \( n_{\text{qual}}/n \) versus temperature.
where the coefficients are \( C_{xx} = v^2_1 \alpha_1 \hbar e^2/(3 \Gamma_1) \) and \( C_{xy} = e^3 \hbar^2 B v^2_1 \alpha_1/(6 \Gamma_1^2) \). The conductivity \( \sigma_{xy} \) can be obtained by replacing the index “x” with “y” in the expression of \( \sigma_{xx} \), and the resistivity is given by \( \rho_{\alpha\beta} = (\sigma^{-1})_{\alpha\beta} \). One can see that when \( \mu = 0 \), the Hall conductivity \( \sigma_{xy} \) is zero, which is a consequence of the PH symmetry of the Dirac fermion. The non-zero conductivity \( \sigma_{xy}^{(2)} \), though tiny, makes the sign-reversing temperature \( T_0 \) of \( R_H \) differ slightly away from the sign-reversing temperature \( T_0 \) of \( \mu \).

**Magnetoresistivity and Hall resistivity at finite \( B \).** The longitudinal resistivity \( \rho_{xx}(T, B) \) and Hall resistivity \( \rho_{yx}(T, B) \) in a finite magnetic field \( B \) are also calculated. The calculation is similar to the zero-field case: We first express the Kubo formula of the conductivity tensor \( \sigma_{\alpha\beta} \) in the Landau level basis, then input the chemical potential \( \mu(T, B) \) obtained from Eq. (3), and finally evaluate the conductivity numerically (see details in SM [25]).

Numerical results are shown in Fig. 4. Our focus is the high-field and high-temperature regime, i.e., \( T, \hbar \omega_c \gtrsim \Gamma_1 \). The curves of \( \rho_{xx} \) and \( \rho_{yx} \) as functions of \( T \) or \( B \) again show good agreements with experiments. Two features deserve some attention. First, the “anomalous” peak in \( \rho_{xx}(T) \) is largely enhanced by the magnetic field, which was initially observed in experiments in Ref. [32](see also [10, 30]). Theoretically, current conduction occurs when electrons/holes hop between two states, in the \( N \)-th and \( (N + 1) \)-th Landau levels respectively, whose energies overlap after disorder broadening. By increasing \( B \) such that Landau level spacing is larger than \( \Gamma_1 \), available states that overlap in energy greatly decrease, leading to enhancement of resistivity. For the same reason, \( \rho_{yx} \) is also enlarged by the magnetic field. Second, the temperature \( \tilde{T}_0 \) at which \( \sigma_{xy} = 0 \) (equivalently \( \rho_{yx} = 0 \)) increases as \( B \) increases (e.g., see experiments in Refs. [10, 30]). When \( B \) is large, \( \sigma_{xy}^{(2)} \) cannot be neglected as shown in the inset of Fig. 4(b). The underlying reason is that Landau level spacing is much smaller for the quadratic fermions than for the Dirac fermion, so \( \sigma_{xy}^{(1)} \) reduces faster than \( \sigma_{xy}^{(2)} \) as \( B \) increases. If \( \sigma_{xy}^{(2)} \) is neglected, \( \sigma_{xy} = 0 \) occurs at \( \mu = 0 \) and so \( \tilde{T}_0 = T_0 \) which has negligible \( B \) dependence. Now that \( \sigma_{xy}^{(2)} \) is non-negligible, its \( B \) dependence as well as the \( B \) dependence of other conductivity contributions make \( \tilde{T}_0 \) increases as \( B \) increases. This is also the reason behind the feature that \( \rho_{yx}(B) \) reverses the sign as \( B \) increases, for certain temperatures, as shown in Fig. 4(d).

**Discussions.** In summary, we have shown a plausible explanation for the long standing puzzle on the anomalous peak of resistivity as well as other related transport phenomena in dilute metals ZrTe5/HfTe5. While many aspects of this work can be improved, e.g., by a more realistic handling of disorder and by including electron-phonon coupling in high-temperature regime, we believe that our explanation captures the essence of the experimentally observed transport anomalies. Our study describes an interesting scenario that a minority current carrier may be thermodynamically very active, leading to intriguing interplay between equilibrium thermodynamics and transport properties. This work can be thought of as a microscopic theory of the phenomenological multi-carrier model that is commonly used to fit experimental data [10, 15, 30] For future studies, it is interesting to extend this work to other dilute metals such as SrTiO3[33].

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Appendix A: Properties of $\mu(T, B)$

In this section, we discuss some technical details and show additional properties regarding the chemical potential $\mu(T, B)$.

1. Monotonicity of $\mu(T)$ at $B = 0$

The chemical potential $\mu(T, B)$ is defined through the integral equation (3) by imposing a constant density $n$. Here we prove a general monotonic behavior of $\mu(T)$ at $B = 0$. We claim that $\mu(T)$ is monotonically decreasing, if $\mu(T)$ itself is non-negative and if the DOS $D(\epsilon)$ satisfies the following two conditions: (i) $D(\epsilon)$ is monotonically increasing for $\epsilon \geq 0$, and monotonically decreasing for $\epsilon \leq 0$ and (ii) $D(|\epsilon|) - D(-|\epsilon|) \geq 0$. The two conditions are satisfied in our low-energy model of $\text{ZrTe}_5$.

To prove the claim, we need to show $\partial \mu / \partial T |_{n} \leq 0$ when $\mu \geq 0$. This derivative can be alternatively written as

$$\frac{\partial \mu}{\partial T} |_{n} = -\left( \frac{\partial n}{\partial T} \right)_{\mu} \left( \frac{\partial n}{\partial \mu} \right)^{-1}$$

(A1)

With the expression (3) of the density $n(T, \mu)$, derivatives on the right-hand side of (A1) can be easily obtained. We have

$$\frac{\partial n}{\partial T} |_{\mu} = - \int_{-\infty}^{\infty} d\epsilon D(\epsilon) f_T'(\epsilon - \mu) \frac{\epsilon - \mu}{T} = \int_{0}^{\infty} d\epsilon [D(\epsilon + \mu) - D(-\epsilon + \mu)] \frac{f_T'(\epsilon)}{T}$$

(A2)

where $f_T'(x) = \partial f_T(x) / \partial x$. It is not hard to see that the integrand is always non-negative for $\epsilon \geq 0$, provided that conditions (i) and (ii) are satisfied. In addition,

$$\frac{\partial n}{\partial \mu} |_{T} = \int_{-\infty}^{\infty} d\epsilon D(\epsilon) [-f_T'(\epsilon - \mu)] > 0$$

(A3)

Combining all together, we immediately have $\partial \mu / \partial T |_{n} \leq 0$. The equality is achieved only in special cases, e.g., $D(\epsilon)$ is a constant function.

FIG. S1. (a) Zero-field chemical potential $\mu(T)$ with different Fermi energies $E_F$ in our model. Note that $E_F = 31$ and 34 meV are above the band bottom $\Delta = 30$ meV of the quadratic fermions. (b) The temperature $T_0(B)$ with $E_F = 25$ meV, at which $\mu$ reverses its sign. All other parameters are set to the same numerical values as in Fig. 2, if not mentioned here.
With this monotonic property, we see that starting at a positive $E_F$, $\mu$ will monotonically decrease as $T$ increases, until it becomes negative (it may continue to decrease after being negative). One may prove similar results in the opposite scenario of a negative $E_F$. We comment that this monotonicity extends to a finite $B$ field roughly when $T \gtrsim \hbar \omega_c$, where $\hbar \omega_c$ denotes a characteristic cyclotron energy. When $T \lesssim \hbar \omega_c$, the monotonicity is affected by quantum oscillation in $\mu$.

2. Sign-reversing temperature $T_0$

The sign-reversing temperature $T_0$, defined by $\mu(T_0, B) = 0$, depends on $n$, $B$ and a few other quantities. In experiments, different samples have different densities and so have different $T_0$’s. Fig. S1(a) shows $\mu(T)$ at $B = 0$ for different $n$'s. We observe that $T_0$ increases as $n$ increases (equivalently, as $E_F$ increases).

The magnetic field dependence $T_0(B)$ is quadratic to the lowest order [Fig. S1(b)]. To see that analytically, let us obtain an expression of $T_0(B)$ for a small $B$ field. Since $D_1(\epsilon, B)$ is PH symmetric, at $\mu = 0$, Eq. (3) reduces to

$$n = \int_0^{\infty} d\epsilon D_2(\epsilon, B) f_T(\epsilon) = \kappa \alpha_2 \sum_{N \geq 0} \int_0^{\infty} d\epsilon \frac{\hbar \omega_2}{\sqrt{\epsilon}} f_T(\epsilon + E_{N2})$$

(A4)

This equation determines $T_0(B)$. Recall that $\hbar \omega_2 = eB/\sqrt{m_x^2 m_y}$ and $E_{N2} = \hbar \omega_c(N + 1/2) + \Delta$. In the limit $B \to 0$, the summation over $N$ can be replaced by an integral

$$n = \kappa \alpha_2 \int_0^{\infty} d\omega \frac{1}{\sqrt{\omega}} f_T(\omega + \Delta)$$

(A5)

which determines the $T_0 \equiv T_0(0)$. Accordingly, $\delta T_0 = T_0(B) - T_0$ is the difference between the summation (A4) and the integral (A5). For a small $B$, this can be evaluated by Taylor expanding $f_T(\omega + E_{N2})$ in (A4) around $B = 0$ and $T = T_0$, and then take the continuum limit. One can check that the lowest order non-vanishing term is of $B^2$. After some calculations, we obtain

$$\delta T_0 = \frac{\hbar \omega_2^2}{24 T_0} g(\Delta/T_0)$$

(A6)

where $g$ is a dimensionless function

$$g(z) = \frac{\int_0^{\infty} dx f'(x + z)/\sqrt{x}}{\int_0^{\infty} dx dy [(x + y + z)/\sqrt{x}] f'(x + y + z)}$$

(A7)

Here $f(x) = 1/(e^x + 1)$ and $f'(x)$ is its first derivative. The function $g(z)$ is positive valued and monotonically decreasing as $z$ increases. For numerical values in the caption of Fig. 2, $\Delta/T_0 \approx 3.4$ and then $\delta T_0 \approx 3.3 \times 10^{-4} B^2$ with $B$ in units of Tesla and $\delta T_0$ in meV.

We comment that if the Landau level energy is $\hbar \omega_c(N + \nu) + \Delta$ with $\nu \neq 1/2$, the lowest order term in $\delta T_0$ will be linear in $B$. More precisely, $\delta T_0 \propto (\nu - 1/2) B$. Accordingly, $\nu = 1/2$ makes the linear correction vanishing. The situation $\nu \neq 1/2$ occurs in the presence of non-trivial Berry phase in Bloch wave functions.

Appendix B: Methods for computing transport coefficients

In this section, we describe details of the calculations on the transport coefficients. Most of our calculations are standard applications of the celebrated Kubo formula.

1. Generalities

We use the standard Kubo formula to compute the dc conductivity tensor $\sigma_{\alpha\beta}$, with $\alpha, \beta = x, y$ (see, for example, Ref. 26). Conductivities, both at zero and finite magnetic fields, will be calculated. We will neglect inter-band scattering between the Dirac and quadratic fermions, as well as scattering between the four copies of quadratic fermions, however contribution from scattering between the particle and hole branches of the Dirac fermion will be
the quadratic fermions at for properly chosen $E_1$ for a single-particle eigenstate $|\alpha\rangle$. We have defined $v_\alpha$ and $-v_\alpha$, where $K_\alpha(0)$ represents the diamagnetic response. In terms of Matsubara frequency $i\omega_n = i2\pi n T$, we have $K_\alpha(i\omega_n) = \frac{1}{V} \int_0^{1/T} \langle J_\alpha(\tau) J_\beta(0) \rangle$, where $V$ is the volume. The retarded Green’s function is then obtained by analytic continuation $i\omega_n \rightarrow \omega + i\delta$. Writing the Green’s function in the spectral representation, one finds that
\[
K_{\alpha\beta}(i\omega_n) = -\frac{e^2\hbar}{V} \sum_{ab} (v_{\alpha})_{ab} (v_{\beta})_{ba} \int \frac{d\epsilon_1}{2\pi} \frac{d\epsilon_2}{2\pi} A_{\alpha}(\epsilon_1) A_{\beta}(\epsilon_2) \frac{f_R(\epsilon_1) - f_R(\epsilon_2)}{i\omega_n + \epsilon_1 - \epsilon_2}
\]
where $(v_{\alpha})_{ab} = \langle a| \hat{v}_{\alpha} |b\rangle$ is the matrix element between two single-particle eigenstates $\{|a\rangle\}$. $A_{\alpha}(\epsilon)$ is the spectral function, and $f_R(\epsilon)$ is the Fermi-Dirac distribution. In the expression (B2), vertex correction to the two-particle Green’s function is neglected (which indeed vanishes in the case of Born approximation for $\delta$-function impurities[29]).

After analytic continuation $i\omega_n \rightarrow \omega + i\delta$, inserting (B2) into (B1), taking the limit $\omega \rightarrow 0$, one can show that the conductivity tensor is given by
\[
\sigma_{\alpha\beta} = \frac{e^2\hbar}{V} \sum_{ab} \{ \text{Re}[\langle v_{\alpha}\rangle_{ab} (v_{\beta})_{ba}] \mathcal{P}_{ab} - \text{Im}[\langle v_{\alpha}\rangle_{ab} (v_{\beta})_{ba}] \mathcal{Q}_{ab} \}
\]
where we have defined
\[
\mathcal{P}_{ab} = \int \frac{d\omega}{4\pi} A_{\alpha}(\omega) A_{\beta}(\omega) [-f_R(\omega)], \quad \mathcal{Q}_{ab} = \int \frac{d\omega}{2\pi} [A_{\alpha}(\omega) \mathcal{R}'_a(\omega) - A_{\beta}(\omega) \mathcal{R}'_a(\omega)] f_R(\omega)
\]
where $\mathcal{R}_a(\omega)$ is the real part of the single-particle Green’s function, and $\mathcal{R}'_a(\omega)$ is the first derivative of $\mathcal{R}_a(\omega)$. This formula can also be found in Ref. [28]. Note that $\mathcal{P}_{ab} = \mathcal{P}_{ba}$ and $\mathcal{Q}_{ab} = -\mathcal{Q}_{ba}$.

We will assume that the single-particle Green’s function has the following form
\[
G_{\alpha}(\omega) = \frac{1}{\omega - E_a + i\Gamma}
\]
for a single-particle eigenstate $|a\rangle$ with eigenenergy $E_a$. We take a crude assumption that the imaginary part $\Gamma$ of the self-energy is a constant ($\Gamma_1$ and $\Gamma_2$ for the Dirac and quadratic fermions respectively). Then,
\[
A_{\alpha}(\omega) = A(E_a - \omega) = \frac{2\Gamma}{(\omega - E_a)^2 + \Gamma^2}, \quad \mathcal{R}_{\alpha}(\omega) = \mathcal{R}(E_a - \omega) = \frac{\omega - E_a}{(\omega - E_a)^2 + \Gamma^2}
\]
This means $\mathcal{P}_{ab} = \mathcal{P}(E_a, E_b)$ and $\mathcal{Q}_{ab} = \mathcal{Q}(E_a, E_b)$. The level broadening $\Gamma$ is due to disorder scattering. For weak disorder, one generally uses Born approximation to obtain the self-energy, which leads to an energy dependent $\Gamma(\omega)$ that is proportional to the density of states $D(\omega)$ per band. Moreover, in the presence of strong magnetic field, self-consistent Born approximation is preferred[29]. Nevertheless, even with a constant $\Gamma$, we find our results can reproduce the main features of resistivity and magnetotransport observed in experiments. So, we will stick to constant $\Gamma$ for simplicity. At the same time, we do have computed the resistivity and Hall coefficient at zero field using Born approximation (results not shown here), which are qualitatively the same as those presented here. We estimate the ratio $\Gamma_2/\Gamma_1$ by taking the Born approximation which gives
\[
\frac{\Gamma_2}{\Gamma_1} = \frac{D_2(E_2)/\kappa}{D_1(E_1)}
\]
for properly chosen $E_2$ and $E_1$, and $D_1(\epsilon), D_2(\epsilon)$ are given in Eq. (1). We chose $E_1 = E_F$ and $E_2$ to be the average energy of the quadratic fermions at $T = T_0$. With the numerics in Fig. 2, we have $\Gamma_2/\Gamma_1 \approx 7$. In our calculations, we
set $\Gamma_2/\Gamma_1 = 10$. The specific ratio does not affect the results qualitatively on transport properties as long as it is not too small.

In the limit $\Gamma \ll T$, the function $f_T(\omega)$ is a smooth function compared with $A$ and $R$. Then, one can show that the following approximations hold

$$
\mathcal{P}_{ab} \approx \begin{cases} 
\mathcal{A}_0^b(E_a)[f_T^b(E_a) - f_T^b(E_b)]/2, & E_a - E_b \gg \Gamma \\
\mathcal{A}_0^b(E_a)[f_T^b(E_a)]/2, & E_a - E_b \ll \Gamma 
\end{cases}
$$

(B8)

where $\mathcal{A}_0^b$ means the spectral function with $\Gamma$ replaced by $2\Gamma$. Also,

$$
\mathcal{Q}_{ab} \approx \begin{cases} 
\mathcal{R}_0^b(E_a)f_T(E_a) - \mathcal{R}_0^b(E_b)f_T(E_b), & E_a - E_b \gg \Gamma \\
(\tau_1^{E_a} - \tau_1^{E_b})^2 [f_T^b(E_b)]^2, & E_a - E_b \ll \Gamma 
\end{cases}
$$

(B9)

Note that the energies $E_a, E_b$ in the above expressions are measured with respect to the chemical potential $\mu$.

2. Transport at $B = 0$

Let us now compute transport coefficients in zero field. We compute the temperature dependence of the resistivity $\rho_{xx}$, Hall coefficient $R_H$, and Seebeck coefficient $S_{xx}$. The Dirac fermion is described by the Hamiltonian

$$
H = m_n \tau_z \sigma_0 + v_x \hat{p}_x \tau_x \sigma_x + v_y \hat{p}_y \tau_y \sigma_0 + v_z \hat{p}_z \tau_z \sigma_x
$$

(B10)

where $\sigma_i$ and $\tau_i$ are Pauli matrices with $\sigma_i$ acting on spins. It is straightforward to obtain the eigenstates $|k\lambda\sigma\rangle$, where $\lambda = \pm 1$ denotes the particle and hole branches respectively and $\sigma = \pm 1$ denotes the spin state. The corresponding energy is $E_{k\lambda\sigma} = \lambda \sqrt{h^2 c^2 k_x^2 + h^2 v_y^2 k_y^2 + h^2 v_z^2 k_z^2 + m^2}$, which is independent of the spin index $\sigma$ since we have neglected the Zeeman coupling. Eigenstates of the anisotropic quadratic fermion are denoted as $|\lambda\sigma\rangle$ and the energy is $E_{k\sigma} = h^2 c^2 k_x^2/2m^*_x + h^2 v_y^2/2m^*_y + h^2 v_z^2/2m^*_z + \Delta$, where $\Delta$ is the bottom of the dispersion. According to Eq. (B3), the longitudinal conductivity $\sigma_{xx}$ can then be expressed as

$$
\sigma_{xx} = \frac{\hbar e^2}{3(2\pi)^3} \sum_{\nu, \nu'} \int d^3k \left|\langle \nu'| \hat{v}_x | \nu \rangle\right|^2 \mathcal{P}(E_{k\nu'} - \mu, E_{k\nu} - \mu)
$$

(B11)

where $\nu = \lambda\sigma$ or $\nu = \sigma$ for the Dirac and quadratic fermions respectively. In this expression, we have used the fact that $\hat{v}_x = i[H, x]/\hbar$ is diagonal in the index $k$, and have written out the the chemical potential $\mu$ explicitly. Calculations of the matrix element $\langle \nu'| \hat{v}_x | \nu \rangle$ is straightforward. After some simplifications, we obtain

$$
\sigma_{xx}^{(1)} = \frac{\hbar e^2}{3} \sum_{\lambda\lambda'} \int_0^\infty d\epsilon D_1(\epsilon) \mathcal{M}_{1,\lambda\lambda'}(\epsilon) \mathcal{P}(\lambda\epsilon - \mu, \lambda'\epsilon - \mu)
$$

(B12)

and

$$
\sigma_{xx}^{(2)} = \frac{\hbar e^2}{9} \int_0^\infty d\epsilon D_2(\epsilon) \mathcal{M}_2(\epsilon) \mathcal{P}(\epsilon - \mu, -\epsilon - \mu)
$$

(B13)

where $\sigma_{xx}^{(1)}$ and $\sigma_{xx}^{(2)}$ are contributions from the Dirac and quadratic fermions respectively, $D_1(\epsilon)$ are DOS’s given in Eq. (1), and

$$
\mathcal{M}_{1,\lambda\lambda'}(\epsilon) = \frac{1}{2} \left( \frac{\lambda\lambda'}{2} + \frac{\lambda\lambda'}{2} \frac{2m^2}{3\epsilon^2} \right), \quad \mathcal{M}_2(\epsilon) = \frac{2}{3} (\epsilon - \Delta)
$$

(B14)

The total conductivity is given by $\sigma_{xx} = \sigma_{xx}^{(1)} + \sigma_{xx}^{(2)}$. The conductivities $\sigma_{xy}^{(i)}$ can be obtained simply by replacing $x$ with $y$ in the above expressions.

The Hall conductivity $\sigma_{xy}$ under a finite magnetic field $B$ is obtained below in Eqs. (B23) and (B24) in Sec. B 3. We derive the Hall coefficient simply by considering small $B$ and separating out the piece that is linear in $B$. We obtain the following expressions

$$
\sigma_{xy}^{(1)} = \frac{e^3 h^2 B}{c} \sum_{\lambda\lambda'} \int_0^\infty d\epsilon D_1(\epsilon) \frac{\lambda\lambda'}{\epsilon} \frac{\partial Q}{\partial E_b}(\lambda\epsilon - \mu, \lambda'\epsilon - \mu)
$$

(B15)

and

$$
\sigma_{xy}^{(2)} = \frac{e^3 h^2 B}{c} \int_0^\infty d\epsilon D_2(\epsilon) \frac{1}{m^*_x m^*_y} \frac{\partial Q}{\partial E_b}(\epsilon - \mu, -\epsilon - \mu)
$$

(B16)
where $\partial Q(E_\alpha, E_\beta)/\partial E_\beta$ is the first derivative of $Q(E_\alpha, E_\beta) \equiv Q_{ab}$ defined in (B4). The total Hall conductivity is $\sigma_{xy} = \sigma_{xy}^{(1)} + \sigma_{xy}^{(2)}$, and $\sigma_{xx} = -\sigma_{xy}$. The resistivity tensor is given by $\rho_{\alpha\beta} = (\hat{\sigma}^{-1})_{\alpha\beta}$ and the Hall coefficient $R_H$ is given by $\rho_{xy} = R_H B$. Numerical evaluations of the expressions (B12), (B13), (B15) and (B16) are performed with varying temperature $T$ and the chemical potential $\mu(T)$ determined by Eq. (3). The results are shown in Fig. 3.

The above expressions of $\sigma_{xy}^{(1)}$ and $\sigma_{xy}^{(2)}$ can be simplified using the following facts: (i) We will set the level broadening $\Gamma_1 = 0.5$ meV, which satisfies $\Gamma_1 \ll T$ in most part of the temperature regime that we are interested in, so the approximations (B8) and (B9) are applicable; (ii) the inter-branch contributions to $\sigma_{xx}$ is small compared to intra-branch contributions in the whole temperature regime that we are interested in, and so they can be neglected. The simplification has been checked numerically and works very well. Then, we have the following simplified expressions

\begin{equation}
\sigma_{xx}^{(1)} \approx \frac{e^2}{\lambda B} \int_{m - \Delta/2}^{m + \Delta/2} d\epsilon \frac{d\epsilon}{\epsilon} \left[ -f_T''(\epsilon) - f_T''(-\epsilon) \right]
\end{equation}

\begin{equation}
\sigma_{xy}^{(1)} \approx \frac{e^2 B}{c} \int_{m - \Delta/2}^{m + \Delta/2} d\epsilon \frac{d\epsilon}{\epsilon} \left[ -f_T''(\epsilon) + f_T''(-\epsilon) \right]
\end{equation}

Similar expressions can also be obtained for $\sigma_{xx}^{(1)}$ and $\sigma_{xx}^{(2)}$. However, we find that $\sigma_{xx}^{(2)} \ll \sigma_{xx}^{(1)}$ and $\sigma_{xy}^{(2)} \ll \sigma_{xy}^{(1)}$ in the temperature of our interests. Then, conductivities in (B17) dominate. In particular, it is easy to see that $\sigma_{xy}^{(1)} = 0$ when $\mu = 0$ (which follows the particle-hole symmetry of the Dirac fermion), which indicates a sign reverse of $R_H$ when $\mu$ crosses zero.

To compute the Seebeck coefficients $S_{xx, y}$, we make use of the generalized Mott formula obtained in Ref. [28] for non-interaction fermion: $\hat{S} = \hat{\rho} \hat{\epsilon}$, where

\begin{equation}
\varepsilon_{ij} = -\frac{1}{eT} \int_{-\infty}^{\infty} d\epsilon \frac{d\epsilon}{\epsilon} \left[ f_T''(\epsilon) - f_T''(-\epsilon) \right] \sigma_{ij}(0, \epsilon)
\end{equation}

where $\sigma_{ij}(0, \epsilon)$ is the conductivity at $T = 0$ and chemical potential $\mu = \epsilon$. We will only compute the zero-field Seebeck coefficient $S_{xx} = \rho_{xx} \varepsilon_{xx}$. With the expressions of $\sigma_{xx}^{(1)}$ and $\sigma_{xx}^{(2)}$, the conductivity $\sigma_{xx}(0, \epsilon)$ can be easily evaluated, from which we obtain

\begin{equation}
\varepsilon_{xx} \approx -\frac{e^2}{3\lambda B} \int_{m - \Delta/2}^{m + \Delta/2} d\epsilon \frac{d\epsilon}{\epsilon} \left[ f_T''(\epsilon) - f_T''(-\epsilon) \right] - \frac{2e\hbar c_0}{3T \lambda B^2 m^*} \int_{\Delta}^{\infty} d\epsilon \frac{d\epsilon}{\epsilon} \left[ f_T''(\epsilon) - f_T''(-\epsilon) \right]
\end{equation}

In the second line which originates from $\sigma_{xx}^{(2)}$, we have assumed $\Gamma_2 \ll T$, which is not quite true. However, $\sigma_{xx}^{(1)}$ is much smaller than $\sigma_{xx}^{(1)}$, so this approximation does not matter too much. If the second line is neglected, we see that $\varepsilon_{xx} = 0$ when $\mu = 0$. Accordingly, a sign reverse is expected when $\mu$ crosses zero, similarly to $R_H$.

3. Transport with finite $B$

Now we consider magnetotransport in a uniform magnetic field $B$ along the $\hat{z}$ direction. The magnetic field is included by the minimal coupling $p \rightarrow p + eA/c$ in the Hamiltonians. We work in the Landau gauge $A = (0, Bx, 0)$. The eigenstates (Landau level states) are well known for both Dirac and quadratic fermions, and can be denoted by $|Nk_y, k_z, \lambda\rangle$ and $|Nk_y, k_z, \lambda\rangle$ respectively, where $N$ is the Landau level index, $k_y$ and $k_z$ are canonical momenta along $y$ and $z$ directions, $\lambda = \pm 1$ denotes spin, and $\lambda = \pm 1$ denotes the positive/negative energy states of the Dirac fermion. One may consult Refs. 23 and 24 for Landau levels of Dirac fermions, and we do not discuss the details here. After a long yet straightforward calculation of the velocity matrix elements in the Landau level states, we obtain the following expressions for the longitudinal conductivities

\begin{equation}
\sigma_{xx}^{(1)} = \frac{e^2}{h} v_y^2 \int \frac{dk_z}{2\pi} \sum_{N \geq 0} \sum_{\lambda'} M_{\lambda\lambda'}(N, k_z) \mathcal{P}(\lambda E_N k_z - \mu, \lambda' E_{(N+1)k_z} - \mu)
\end{equation}

\begin{equation}
\sigma_{xx}^{(2)} = \frac{2\kappa e^2}{h} \sqrt{\frac{m_0^2}{m^*_c}} \int \frac{dk_z}{2\pi} \sum_{N \geq 0} (N + 1) \mathcal{P}(E_N k_z - \mu, E_{(N+1)k_z} - \mu)
\end{equation}
where $\sigma^{(1)}_{xx}$ and $\sigma^{(2)}_{xx}$ are contributions from the Dirac and quadratic fermions respectively, and

$$M_{\lambda\lambda'}(N, k_z) = \frac{1}{2} - \frac{\lambda\lambda'}{2} \frac{\hbar^2 v_z k_z^2 + m^2}{E_{(N+1)k_z} - E_{Nk_z}},$$

$$E_{Nk_z} = \sqrt{m^2 + \hbar^2 \omega^2 c_1 N + \hbar^2 v_z^2 k_z^2},$$

$$E'_{Nk_z} = \hbar \omega c_2 (N + 1/2) + \hbar^2 k_z^2 / 2m^*_z + \Delta$$

(B22)

The conductivities $\sigma^{(i)}_{yy}$ can be obtained by swapping the indices $x$ and $y$ in the above expressions. Calculations of the Hall conductivities $\sigma^{(1)}_{xy}$ and $\sigma^{(2)}_{xy}$ are very similar, which give rise to the following expressions

$$\sigma^{(1)}_{xy} = \frac{e^2}{h} \frac{\hbar^2 \omega^2 c_1}{2\pi} \int \frac{dk_z}{2\pi} \sum_{N \geq 0} \sum_{\lambda\lambda'} M_{\lambda\lambda'}(N, k_z) Q(\lambda E_{Nk_z} - \mu, \lambda' E_{(N+1)k_z} - \mu)$$

(B23)

$$\sigma^{(2)}_{xy} = \frac{2\kappa e^2}{h} \frac{\hbar^2 \omega^2 c_2}{2\pi} \int \frac{dk_z}{2\pi} \sum_{N \geq 0} (N + 1) Q(E'_{Nk_z} - \mu, E'_{(N+1)k_z} - \mu)$$

(B24)

Note that the function $Q(E_a, E_b)$ is antisymmetric in $E_a$ and $E_b$, so the Hall conductivities are zero when $B = 0$. With these expressions, we then compute the resistivity tensor $\hat{\rho} = \hat{\sigma}^{-1}$ numerically, with the chemical potential $\mu(B, T)$ determined in Eq. (3) in the main text. The numerical results are shown in Fig. 4. One can check that in the zero-field limit $B \rightarrow 0$, Eqs. (B20), (B21), (B23) and (B24) reduce to the zero-field expressions (B12), (B13), (B15) and (B16).