Dirac Polarons and Resistivity Anomaly in ZrTe$_5$ and HfTe$_5$

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Resistivity anomaly, a sharp peak of resistivity at finite temperatures, in the transition-metal pentatellurides ZrTe$_5$ and HfTe$_5$ was observed four decades ago, and more exotic and anomalous behaviors of electric and thermoelectric transport were revealed recent years. Here we present a theory of Dirac polarons, composed by massive Dirac electrons and holes in an encircling cloud of lattice displacements or phonons at finite temperatures. The chemical potential of Dirac polarons sweeps the band gap of the topological band structure by increasing the temperature, leading to the resistivity anomaly. Formation of a nearly neutral state of Dirac polarons accounts for the anomalous behaviors of the electric and thermoelectric resistivity.

Introduction  Resistivity in the transition-metal pentatellurides ZrTe$_5$ and HfTe$_5$ exhibits a sharp peak at a finite temperature $T_p$. The peak occurs approximately at a large range of temperatures from 50 to 200K, but the exact value varies from sample to sample. The effect was observed forty years ago [1,2], but has yet to be understood very well. At the beginning, it was thought as a structural phase transition, or occurrence of charge density wave. The idea was soon negated as no substantial evidence is found to support the picture [3-6]. The measurements of the Hall and Seebeck coefficients showed that the type of charge carriers dominating the electrical transport changes its sign around the peak, which indicates the chemical potential of the charge carriers sweeps band gap around the transition temperature $T_p$ [7-10]. Thus the anomaly is believed to originate in the strong temperature dependence of the chemical potential and carrier mobility. Recent years the advent of topological insulators revives extensive interests to explore the physical properties of ZrTe$_5$ and HfTe$_5$. The first principles calculation suggested that the band structures of ZrTe$_5$ and HfTe$_5$ are topologically nontrivial or very close to the topological transition points [11]. An infrared transmission study provides spectroscopic evidence of the band inversion of the conduction bands and valence bands [12], and the angle-resolved photoemission spectroscopy (ARPES) measurement also suggested it is a strong topological insulator [13]. Further studies uncover more exotic physics in these compounds [14-24], such as the chiral magnetic effect and three-dimensional quantum Hall effect. Other possible causes have been advanced much recently [25-27], but the physical origin of the resistivity anomaly is still unclear. For example, it was suggested that a topological quantum phase transition might occur, and the gap closing and reopening give rise to the resistivity anomaly [27]. However it contradicts with the observation of the ARPES measurement [28,29].

Strong temperature dependence of the band structure [28] implies that the interaction between the Bloch electrons and the lattice vibrations, i.e., electron-phonon interaction (EPI), is an indispensable ingredient to understand the anomaly [30]. In this Letter, we consider the topologically nontrivial band structure and EPI in ZrTe$_5$ and HfTe$_5$, and propose a theory of Dirac polarons for the resistivity anomaly at finite temperatures. The Dirac polarons are mixtures of massive Dirac electrons and holes encircling a cloud of phonons, and are the effective charge carriers in the compounds. Increasing temperature will change the overlapping of the Dirac polarons drastically. The chemical potential of Dirac polarons sweeping the band gap from conduction bands to valence bands with increasing the temperature. Consequently, when the chemical potential of Dirac polarons locates around the middle of the band gap, the resistivity is enhanced drastically to form a pronounced peak at a finite temperature. The carriers dominated the charge transport change the sign around the transition. The formation of a nearly neutral state of Dirac polarons accounts for anomalous electric and magneto transport properties in the compounds.

Finite temperature spectral function and quasiparticle properties  The charge carriers in the conduction and valence bands of the bulk ZrTe$_5$ and HfTe$_5$ are strongly coupled together due to spin-orbit interaction and behave like massive Dirac fermions with nontrivial band topology instead of conventional electrons in semiconductors and metals [13,31,32]. In the following, we only focus on ZrTe$_5$ for comparison with experimental measurements and theoretical calculations with loss of generality. When the electrons (or holes) are moving through the ionic lattices, the surrounding lattice will be displaced from the original equilibrium positions; consequently, the electrons (or holes) will be encircled by the lattice distortions, or phonons. At finite temperatures the quasiparticles for the coupled electron-lattice systems are composed of both massive Dirac electrons and holes in a cloud of phonons due to the thermal activation when the chemical potential is located around the band edges as illustrated in Fig.1(A). The Hamiltonian describing the EPI in Dirac materials has the form [32], $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{Dirac}} + \mathcal{H}_{\text{ph}} + \mathcal{H}_{\text{ep}}$. Here the electron system is described by the modified massive Dirac Hamiltonian $\mathcal{H}_{\text{Dirac}}$, the phonon part $\mathcal{H}_{\text{ph}}$ is in the harmonic approximation, and the EPI part $\mathcal{H}_{\text{ep}}$ is dominantly contributed by longitudinal acoustic
Figure 1. (a) A comparison of the renormalized energy spectrums according to the theory (the solid lines) and the temperature-dependent band structures from ARPES measurement adopted from Fig. 2(b) in Ref. [28]. (b) The renormalized Dirac mass \( m \) due to the EPI and (c) the temperature dependent chemical potential \( \mu \), the experiment data are extracted from Fig.2(d) and (f) in Ref. [28]. The model parameters are set to be \( v = 4 \times 10^5 \text{m/s}, b = 350 \text{meVnm}^2, \)
d = -310 \text{meVnm}^2, and \( m = 15.0 \text{meV} \) for all the figures if there is no further claiming. The carrier density used here is \( n = 1.3 \times 10^{11} \text{cm}^{-3} \).

The low-energy physics of the electronic states of ZrTe_5 and HfTe_5 near the \( \Gamma \) point can be well described by the Hamiltonian,

\[
\mathcal{H}_{\text{Dirac}} = \sum_p \psi_p \left[ dp^2 - \mu + i
\psi_p \psi_p^\dagger \left( m - bp^2 \right) \right],
\]

where \( p = (p_x, p_y, p_z) \) is the momentum in the vicinity of \( \Gamma \) point, \( \psi_p \) and \( \psi_p^\dagger \) are the four-component fermionic field operators, \( v \) is the effective velocity, \( \mu \) is the chemical potential. \( dp^2 \) breaks the particle-hole symmetry, and plays essential role in the Dirac polaron physics. \( m - bp^2 \) is the momentum dependent Dirac mass, where the sign of \( mb \) determines the topological properties of the system [34]. The Dirac matrices are chosen to be \( \alpha = \sigma_x \otimes (\sigma_x, \sigma_y, \sigma_z) \) and \( \beta = \tau_z \otimes \sigma_0 \), where \( \sigma \) and \( \tau \) are the Pauli matrices acting on spin and orbital space, respectively. The quantitative information about these physical properties, such as the Dirac velocity, the Dirac mass or the energy gap can be extracted from the ARPES data [28, 35, 36]. To explore the EPI effect, we treat \( \mathcal{H}_{\text{ep}} \) as a perturbation to either electrons or phonons in the Migdal approximation [37] that the self-energy arises from the virtual exchange of a phonon at temperature \( T \). Due to the spinor nature of Dirac electrons, the retarded self-energy can be recast in a matrix form as [38]

\[
\Sigma_{ep}(p, \epsilon) = \Sigma_f(p, \epsilon) + \lambda_\alpha(p, \epsilon) \hbar v_p \cdot \alpha + \Sigma_\beta(p, \epsilon) \beta,
\]

where \( \Sigma_f(p, \epsilon) \) is the renormalization to the chemical potential, \( \lambda_\alpha(p, \epsilon) \) is the velocity dressing function and \( \Sigma_\beta(p, \epsilon) \) is the renormalization to the Dirac mass \( m \).

The quasiparticle properties can be obtained by solving the poles of the retarded Green’s function \( G_R(p, \epsilon) = (\epsilon - \mathcal{H}_{\text{Dirac}}(p) - \Sigma_R(p, \epsilon))^{-1} \), which is in the complex plane with its real part gives the spectrum of the quasiparticle and the imaginary part gives its lifetime. The self-energy \( \Sigma_R(p, \epsilon) = \Sigma_{ep}(p, \epsilon) + \Sigma_{\text{imp}}(p, \epsilon) \) includes the contribution from the impurities scattering. The spectral function of the quasiparticle properties, i.e., Dirac polarons, is given by the imaginary part of \( G_R(p, \epsilon) \),

\[
A_\zeta(p, \epsilon) = -\frac{1}{\pi} (\zeta sp \text{Im} G_R(p, \epsilon) |\zeta sp|),
\]

where \( |\zeta sp| \) are the band states with the band indices \( \zeta = \pm \) for the conduction band and valence band and spin indices \( s = \pm \). In the absence of disorder and EPI, the spectral function \( A_\zeta(p, \epsilon) \) is a \( \delta \) function reflecting that the wave vector \( p \) is a good quantum number and all its weight ratio is precisely at \( \epsilon = \xi_p \). In the presence of disorder and EPI, at low temperatures, \( A_\zeta(p, \epsilon) \) exhibits a sharp peak of the Lorentzian type due to a long lifetime. As temperature increases, \( A_\zeta(p, \epsilon) \) maintains the Lorentzian line shape but becomes broader due to the increasing of the scattering rate, and the peak position moves to the positive energy due to the renormalization of the energy level. The trajectories of the peaks of the spectral function give us the renormalized dispersion \( \xi_\zeta(p) \). As shown in Fig. 1(a), we plot the derived energy dispersions \( \xi_\zeta(p) \) for different temperatures with the black and red lines corresponding the conduction and valence band respectively. The ARPES data extracted from Ref. [28] are also presented as the background for a comparison. The excellent agreement can be found between our theoretical calculations and the experiment data. The overall band structure shifts up to higher energy with increasing temperature. The peak structure of the spectral function can be clearly observed in the temperature range considered, which suggests that a quasiparticle picture is still appropriate at low energy and the EPI largely preserving the weakly perturbed Fermi-liquid behavior.

The renormalized Dirac mass \( m \) is given by the difference between two energy levels \( \xi_+(0) \) and \( \xi_-(0) \) for the states at the band edge (\( p = 0 \)): \( \tilde{m} = \frac{1}{2} [\xi_+(0) - \xi_-(0)] \).

At higher temperature, the effective mass varies with the temperature as \( \tilde{m} \approx m + g_m T \) shown in Fig. 1(b). The coefficient \( g_m \) are determined by the band structure of massive Dirac fermions and the EPI strength (see the details in Ref. [38]). For Dirac materials, the renormalization of the energy levels is attributed to the contributions from both intra-band and inter-band scatterings. With increasing the temperature, 

the more phonon modes with high momenta are active, the larger the renormalization is. The chemical potential is determined by the total number of charge carriers $n = \int_{[0,\bar{n}]} d\omega [\bar{\nu}_+(\omega)n_F(\omega - \mu) - \bar{\nu}_-(\omega)n_F(\omega + \mu)]$ where $n_F(x) = [\exp(x/k_BT) + 1]^{-1}$ is the Fermi distribution function and $\bar{\nu}_\pm(\omega)$ are the renormalized density of states for the conduction and valence band respectively. In the band structure of ZrTe$_5$, the particle-hole symmetry is broken and the valence band is narrower than the conduction band. At the fixed carrier density $n$, the temperature dependence $\mu(T)$ are plotted in Fig. 1(c). The calculated results demonstrate that the chemical potential sweeps over the energy band gap of the massive Dirac particles with increasing the temperature. At low temperature, the chemical potential $\mu(T) \approx \mu(0) - \frac{e^2}{\hbar} (k_BT)^2 \frac{d^2\bar{\nu}_+(\omega)/d\omega}{\bar{\nu}_+(\omega)} |_{\omega=\mu(0)}$ shows a quadratic temperature dependence by means of the Sommerfeld expansion. $\mu(T) = 0$ means the chemical potential is located at the mid-gap, which approximately defines the transition temperature $t_p$ around. At high temperatures, due to the strong particle-hole asymmetry and the relatively low electron concentration, the chemical potential shifts into the valence band in a relatively linear fashion with increasing the temperature.

The resistivity anomaly With the phonon-induced self-energy in hand, we are ready to present the electrical resistivity as a function of temperature by means of the linear response theory [33, 38]. At finite temperatures, the conductivities and the thermoelectric coefficients are contributed from both the electron-like bands and hole-like bands after the phonon-induced renormalization. The two contributions are weighted by the negative energy derivative of the Fermi-Dirac function, whose value is nearly zero except for energies within a narrow window of $k_BT$ near the chemical potential $\mu$. Figure 2(a) reproduces the resistivity peak at several initial chemical potentials $\mu(T = 0)$, or equivalently carrier densities at $T = 0$. For the initial chemical potential locating in the conduction band $[\mu(T = 0) > 0]$, as it moves down to the valance band with increasing temperature, it will inevitably sweep over the band gap. When $T = T_p$, the effective chemical potential lies around the middle of the effective band gap $\mu(T = T_p) \approx 0$ and the resistivity reaches the maximum. As the $n$-type carrier concentration is decreased, the resistivity peak will move to the lower temperature with the higher magnitude. The peak temperature as a function of the carrier density is plotted in Fig. 2(b). For a lower carrier concentration, the chemical potential reaches the middle of the band gap with a lower temperature. The height of the resistivity peak is determined by the ratio $\bar{m}(T_p)/(kB T_p)$. With increasing the ratio, the peak height increases drastically, and becomes divergent if $\bar{m}(T_p) \gg kB T_p$. It explains why in some experiments with extreme low carrier concentration no resistivity peak is observed [19, 45], which can be regarded as the situation of $T_p \sim 0$. Thus the sweeping chemical potential over the band gap of Dirac fermions gives rise to the resistivity anomaly at finite temperatures. We use the model parameters in Fig. 1 to calculate the resistivity, which is in a good agreement with the experimental data as shown in Fig. 2(c). The slight deviation at the high temperature might be caused by neglecting the contributions from the optical modes of phonons.

Sign change of the Hall and Seebeck coefficients The resistivity anomaly is always accompanied with the sign change of the Hall and Seebeck coefficients around the transition temperature [3, 22, 41, 46, 47, 50], which can be reproduced in the present theory. As shown in Fig. 3(a), for a positive $\mu(T = 0)$ with carrier concentration being $n$-type, with increasing the temperature, the Hall coefficient $(R_H = \partial \rho_{xy}/\partial B|_{B=0})$ first maintains its value $(1/\bar{n})$ at low temperature then decreases down until reaching the minimum. By further increasing the temperature, $R_H$ changes from the negative to positive sign at some temperature and then continues to decrease.

![Figure 2](image1.png)  
(a) The zero-field resistivity $\rho$ as a function of temperature for several carrier density $n$. (b) The peak temperature $T_p$ as a function of the carrier density. (c) The comparison of the experimental data and theoretical prediction by using the same parameters as Fig. 1. The experimental data are extracted from Fig. 1(d) in Ref. [28]. Both resistivity curves have been normalized to their maximum values $\rho_{peak}$.

![Figure 3](image2.png)  
(a) The Hall coefficient $R_H$ and (b) the Seebeck coefficient $S$ as functions of temperature several carrier density $n$. 

\[ \mu(T) = 0 \approx \mu(0) - \frac{e^2}{\hbar} (k_BT)^2 \frac{d^2\bar{\nu}_+(\omega)/d\omega}{\bar{\nu}_+(\omega)} |_{\omega=\mu(0)} \]
down to nearly zero at high temperature. The sign change of $R_H$ indicates the electron-dominated transport is transformed into the hole-dominated as the chemical potential moves from the conduction band to valence band. As the carrier concentration decreases, the Hall coefficient crosses 0 at a lower temperature with its maximum being larger. As shown in Fig. 3(b), the Seebeck coefficient $S_{xx}$ also reveals a systematic shift in temperature as the carrier density increases. For each curve with fixed carrier density as the temperature increases from zero to room temperature, $S_{xx}$ displays similar nonmonotonic temperature dependence as $R_H$, except that $S_{xx}$ starts from absolute zero and exhibits a relative large positive ($p$-type) Seebeck coefficient at high temperature. At low temperature, the chemical potential lies deep in the bulk band, the Mott formula relates the thermoelectric conductivity with the derivative of the electrical conductivity for the thermopower $S_{xx} = \frac{e^2 k_B T}{\sigma(\omega)} \frac{d\sigma(\omega)}{d\omega}|_{\omega=E_F}$ with $\sigma(\omega)$ is the energy-dependent conductivity. The conductivity $\sigma(\omega)$ is proportional to the square of the group velocity. Hence, as chemical potential locates in conduction band, $S_{xx}$ is negative ($n$-type) and decreases with increasing temperature. $S_{xx}$ attains its largest value when $n$ is tiny but nonvanishing, and varies rapidly with the temperature around $T_p$. $T_p$ decreases with the reduction of the $n$-type carrier concentration at zero temperature qualitatively agrees with previous measurements for single crystals with different carrier concentrations [49]. Near $T = T_p$ and if the band gap $\tilde{m}(T_p)$ is comparably smaller than the thermal energy $k_BT_p$, either $R_H$ or $S_{xx}$ is linear in temperature and the system enters a nearly neutral state of Dirac polarons due to the strong thermal activation.

**Magnetotransport in nearly neutral state of Dirac polarons** The presence of an external magnetic field reveals the exotic behaviors of magnetoresistivity near the transition temperature [10, 14, 22, 25, 47, 51]. Without loss of generality we assume the magnetic field is along the $z$ direction. As shown in Fig. 4(a), the transverse magnetoresistivity $\rho_{xx}(B)$ displays significantly different behaviors for temperature above and below $T_p$. Below 120K, a narrow dip is observed around zero magnetic field and above 200K, $\rho_{xx}$ shows a quadratic field dependence. As approaching the peak temperature, $\rho_{xx}$ becomes large and nonsaturating. To see the effect more clear, we plot the resistivity as a function of temperature for different magnetic fields. As shown in Fig. 4(b), $\rho_{xx}(B)$ displays striking resistivity peaks when the temperature crosses the region of the neutral state of Dirac polarons. The peak is strongly enhanced with increasing magnetic field, and even becomes nonsaturated. Its position is observed to shift slightly to a higher temperature with the field increasing, i.e. $T_p$ is a function of magnetic field. This effect has been reported experimentally in Ref. [11, 22]. The appearance of giant and nonsaturated transverse magnetoresistivity can be viewed as the electrical signature of the neutral state of Dirac polarons. As shown in Fig. 4(c), the slope of the Hall resistivity $\rho_{xy}$ is negative, indicating a electron-dominated charge transport. As the temperature increases, the nonlinearity of $\rho_{xy}$ becomes more apparent. In the intermediate temperature (120 ~ 180K) around $T_p$, due to the formation of the nearly neutral state of Dirac polarons, the slope of the Hall resistivity changes from positive (hole type) at low magnetic field to negative (electron type) at high field, showing a zigzag shaped profile. At high temperature (above 200K), the hole carrier dominates the charge transport thus the slope of $\rho_{xy}$ become positive. The effect of an applied magnetic field on $\rho_{xy}$ as a function of temperature is shown in Fig. 4(d). There is a systematic shift to the higher temperatures with increasing field. The calculated $\rho_{xx}$ and $\rho_{xy}$ as functions of either temperature $T$ or magnetic field $B$ are in an excellent agreement with the experimental measurements in $ZrTe_5$ and $HfTe_5$ [22, 23, 47, 51]. Lastly, we want to point out the differences between the present theory and the two-band model for magnetoresistance [52]. The two-band model commonly requires that the Fermi surface is composed of both electron and hole pockets and predicts a quadratical magnetoresistance, while the present theory only involves a single Dirac band and the multi-carrier transport is activated through thermal excitation and gives a sublinear magnetoresistance over a wide range of temperature.

**Discussion** From an experimental standpoint, a temperature-dependent effective carrier density can be deduced from the Hall measurement. The shift of the chemical potential or effective carrier density with the variation of temperature is the key issue to the resistivity anomaly. With no absorption or desorption process through extrinsic doping, the temperature dependent variation of the density of charge carriers or even sign change of charge carriers seems to violate the conservation law of the total charge. However, the relative contribution from each carrier to the total Hall effect also
depends on its ability to respond to the applied magnetic field such as velocity and mobility. In Dirac materials with extreme low carrier density and tiny band gap, the strong particle-hole asymmetry will induce a significant temperature variation of the chemical potential, even shifts from conduction band to valence band. The effective carrier density also displays strong temperature dependence. This is a striking feature of the massive Dirac materials with low carrier density at finite temperatures.

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[1] S. Okada, T. Sambongi, M. Ido, Giant resistivity anomaly in ZrTe$_5$, J. Phys. Soc. Jpn. 49, 839-840 (1980).
[2] M. Izumi, K. Uchinokura, E. Matsuura, Anomalous electrical resistivity in HfTe$_5$. Solid State Commun. 37, 641-642 (1981).
[3] F. DiSalvo, R. Fleming, J. Waszczak, Possible phase transition in the quasi-one-dimensional materials ZrTe$_5$ or HfTe$_5$. Phys. Rev. B 24, 2935 (1981).
[4] S. Okada, T. Sambongi, M. Ido, Y. Tazuke, R. Aoki, O. Fujita. Negative evidences for charge/spin density wave in ZrTe$_5$. J. Phys. Soc. Jpn. 51, 460-467 (1982).
[5] D. Bullet, Absence of a phase transition in ZrTe$_5$. Solid State Commun. 42, 691-693 (1982).
[6] H. Fjellvag, A. Kjekshus, Structural properties of ZrTe$_5$ and HfTe$_5$ as seen by powder diffraction. Solid State Commun. 60, 91-93 (1986).
[7] M. Izumi, K. Uchinokura, E. Matsuura, S. Harada, Hall effect and transverse magnetoresistance in a low-dimensional. Solid State Commun. 42, 773-778 (1982).
[8] T. Jones, W. Fuller, T. Wieting, F. Levy, Thermoelectric power of HfTe$_5$ and ZrTe$_5$. Solid State Commun. 42, 793-798 (1982).
[9] R. T. Littleton Iv, T. M. Tritt, J. W. Kolis, and D. Ketchum, Transition-metal pentatellurides as potential low-temperature thermoelectric refrigeration materials. Phys. Rev. B 60, 19453 (1999).
[10] T. M. Tritt, N. D. Lowhorn, R. T. Littleton I, A. Pope, C. R. Feger, and J. W. Kolis, Large enhancement of the resistive anomaly in the pentatelluride materials HfTe$_5$ and ZrTe$_5$ with applied magnetic field. Phys. Rev. B 60, 7816 (1999).
[11] H. Weng, X. Dai, Z. Fang, Transition-metal pentatelluride ZrTe$_5$ and HfTe$_5$: a paradigm for large-gap quantum spin Hall insulators. Phys. Rev. X 4, 011002 (2014).
[12] Z.-G. Chen, R. Chen, R. Zhong, J. Schneeloch, C. Zhang, Y. Huang, F. Qu, R. Yu, Q. Li, G. Gu, N. Wang, Spectroscopic evidence for bulk-band inversion and three-dimensional massive Dirac fermions in ZrTe$_5$. Proc. Natl. Acad. Sci. U.S.A. 114, 816-821 (2017).
[13] G. Manzoni, L. Gragnaniello, G. Autât, T. Kuhn, A. Sterzi, F. Cilento, M. Zacchigna, V. Enenkel, I. Vobornik, L. Barba, F. Bisti, P. Bugnon, A. Magrez, V. N. Strocov, H. Berger, O.-V. Yazyev, M. Fonin, F. Parmigiani, A. Crepaldi, Evidence for a strong topological insulator phase in ZrTe$_5$. Phys. Rev. Lett. 117, 237601 (2016).
[14] Q. Li, D. E. Kharzeev, C. Zhang, Y. Huang, I. Pletikosic, A. Fedorov, R. Zhong, J. Schneeloch, G. Gu, T. Valla, Chiral magnetic effect in ZrTe$_5$. Nat. Phys. 12, 550-554 (2016).
[15] Y. Zhou, J. Wu, W. Ning, N. Li, Y. Du, X. Chen, R. Zhang, Z. Chi, X. Wang, X. Zhu, P. O. Lu, C. Ji, X. Wan, Z. Yang, J. Sun, W. Yang, M. Tian, Y. Zhang, and H.-k. Mao, Pressure-induced superconductivity in a three-dimensional topological material ZrTe$_5$. Proc. Nat. Acad. Sci. USA, 113, 2904 (2016).
[16] P. Li, C. H. Zhang, J. W. Zhang, Y. Wen, and X. X. Zhang, Giant planar Hall effect in the Dirac semimetal ZrTe$_5$. Phys. Rev. B 98, 121108(R) (2018).
[17] H. Wang, H. Liu, Y. Li, Y. Liu, J. Wang, J. Liu, J.-Y. Dai, Y. Wang, L. Li, J. Yan, D. Mandrus, X. C. Xie and J. Wang. Discovery of log-periodic oscillations in ultraquantum topological materials. Sci. Adv. 4, eaau5096 (2018).
[18] H. Wang, Y. Liu, Y. Liu, C. Xi, J. Wang, J. Liu, Y. Wang, L. Li, S. P. Lau, M. Tian, J. Yan, D. Mandrus, J. Y. Dai, H. Liu, X. C. Xie, J. Wang, Log-periodic quantum magneto-oscillations and discrete-scale invariance in topological material HfTe5. Natl. Sci. Rev. 6, 914-920 (2019).
[19] T. Liang, J. Lin, Q. Gibson, S. Kushwaha, M. Liu, W. Wang, H. Xiong, J. A. Sobota, M. Hashimoto, P. S. Kirchmann, Z. Shen, R. J. Cava, N. P. Ong, Anomalous Hall effect in ZrTe$_5$. Nat. Phys. 14, 451-455 (2018).
[20] J. L. Zhang, C. M. Wang, C. Y. Guo, X. D. Zhu, Y. Zhang, J. Y. Yang, Y. Q. Wang, Z. Qu, L. Pi, H.-Z. Lu, and M. L. Tian, Anomalous thermoelectric effects of ZrTe$_5$ in and beyond the quantum limit. Phys. Rev. Lett. 123, 196602 (2019).
[21] J. Hu, M. Caputo, E. B. Guedes, S. Tu, E. Martino, A. Magrez, H. Berger, J. H. Dil, H. Yu, J.-P. Ansermet, Large magnetothermopower and anomalous Nernst effect in ZrTe$_5$. Phys. Rev. B 100, 115201 (2019).
[22] F. Tang, Y. Ren, P. Wang, R. Zhong, J. Schneeloch, S. A. Yang, K. Yang, P. A. Lee, G. Gu, Z. Qiao, L. Zhang, Three-dimensional quantum Hall effect and metal-insulator transition in ZrTe$_5$. Nature 569, 537-541 (2019).
[23] P. Wang, Y. Ren, F. Tang, P. Wang, T. Hou, H. Zeng, L. Zhang, Z. Qiao, Approaching three-dimensional quantum Hall effect in bulk HfTe$_5$. Phys. Rev. B 101, 161201 (2020).
[24] R. Y. Chen, S. J. Zhang, J. A. Schneeloch, C. Zhang, Q. Li, G. D. Gu, and N. L. Wang, Optical spectroscopy study of the three-dimensional Dirac semimetal ZrTe$_5$. Phys. Rev. B 92, 075107 (2015).
[25] L.-X. Zhao, X.-C. Huang, Y.-J. Long, D. Chen, H. Liang, Z.-H. Yang, M.-Q. Xue, Z.-A. Ren, H.-M. Weng, Z. Fang, X. Dai, G.-F. Chen, Anomalous Magneto-Transport Behavior in Transition Metal Pentatelluride HfTe$_5$, Chin. Phys. Lett. 34, 037102 (2017).
[26] P. Shahi, D. J. Singh, J. P. Sun, L. X. Zhao, G. F. Chen, Y. Y. Lv, J. Li, J.-Q. Yan, D. G. Mandrus, J.-G. Cheng, Bipolar conduction as the possible origin of the electronic transition in pentatellurides: metallic vs semiconducting materials. J. Phys. Soc. Jpn. 86, 053701 (2017).
behavior. *Phys. Rev. X* **8**, 021055 (2018).

[27] B. Xu, L. Zhao, P. Marsik, E. Sheveleva, F. Lyzwa, Y. Dai, G. Chen, X. Qiu, C. Bernhard, Temperature-driven topological phase transition and intermediate Dirac semimetal phase in ZrTe$_5$. *Phys. Rev. Lett.* **121**, 187401 (2018).

[28] Y. Zhang, C. Wang, L. Yu, G. Liu, A. Liang, J. Huang, S. Nie, X. Sun, Y. Zhang, B. Shen, J. Liu, H. Weng, L. Zhao, G. Chen, X. Jia, C. Hu, Y. Ding, W. Zhao, Q. Gao, C. Li, S. He, L. Zhao, F. Zhang, S. Zhang, F. Yang, Z. Wang, Q. Peng, X. Dai, Z. Fung, Z. Xu, C. Chen, X. Zhou, Electronic evidence of temperature-induced Lifshitz transition and topological nature in ZrTe$_5$. *Nat. Commun.* **8**, 15512 (2017).

[29] Y. Zhang, C. Wang, G. Liu, A. Liang, L. Zhao, J. Huang, Q. Gao, B. Shen, J. Liu, C. Hu, W. Zhao, G. Chen , X. Jia, L. Yu, L. Zhao, , S. He, F. Zhang, S. Zhang, F. Yang, Z. Wang, Q. Peng, Z. Xu, C. Chen, X. Zhou, Temperature-induced Lifshitz transition in topological insulator candidate HfTe$_5$. *Sci. Bull.* **62**, 950-956 (2017).

[30] M. Rubinstein, HfTe$_5$ and ZrTe$_5$: Possible polaronic conductors. *Phys. Rev. B* **60**, 1627 (1999).

[31] R. Wu, J.-Z. Ma, S.-M. Nie, L.-X. Zhao, X. Huang, J.-X. Yin, B.-B. Fu, P. Richard, G.-F. Chen, Z. Fang, X. Dai, H.-M. Teng, T. Qian, H. Ding, S. H. Pan, Evidence for topological edge states in a large energy gap near the step edges on the surface of ZrTe$_5$. *Phys. Rev. X* **6**, 021017 (2016).

[32] X.-B. Li, W.-K. Huang, Y.-Y. Lv, K.-W. Zhang, C.-L. Yang, B.-B. Zhang, Y. B. Chen, S.-H. Yao, J. Zhou, M.-H. Lu, L. Sheng, S.-C. Li, J.-F. Jia, Q.-K. Xue, Y.-F. Chen, D.-Y. Xing, Experimental observation of topological edge states at the surface step edge of the topological insulator ZrTe$_5$. *Phys. Rev. Lett.* **116**, 176803 (2016).

[33] G. D. Mahan, *Many-Body Physics* (Plenum Press, New York, ed.2,1990).

[34] S. Q. Shen, *Topological Insulators* (Springer, Singapore, ed. 2, 2017), vol. 187 of *Springer Series in Solid-State Sciences*.

[35] L. Moreschini, J. C. Johanssen, H. Berger, J. Denlinger, C. Jozwiack, E. Rotenberg, K. S. Kim, A. Bostwick, and M. Grioni, Nature and topological of the low-energy states in ZrTe$_5$. *Phys. Rev. B* **94**, 081101(R) (2016).

[36] G. Manzoni, A. Sterzi, A. Crepaldi, M. Diego, F. Cilento, M. Zacchigna, Ph. Bugnon, H. Berger, A. Magrez, M. Grioni, and F. Parmigiani, Ultrafast Optical Control of the Electronic Properties of ZrTe$_5$, *Phys. Rev. Lett.* **115**, 207402 (2015).

[37] A. B. Migdal, Interaction between electrons and lattice vibrations in a normal metal. *Sov. Phys. JETP* **34**, 996-1001 (1958).

[38] See Supplemental Material at [URL to be added by publisher] for details of (Sec. SI) the model for electron-phonon interaction, (Sec. SII) the phonon-induced self-energy, (Sec. SIII) the renormalization of the energy level of Dirac polaron, and (Sec. SIV) finite temperature conductivity, which includes Refs. **23, 33, 37, 40–43, 52, 54, 57, 38, 44**.

[39] J. Zhu, T. Feng, S. Mills, P. Wang, X. Wu, L. Zhang, S. T. Pantelides, X. Du, X. Wang, Record-low and anisotropic thermal conductivity of a quasi-one-dimensional bulk ZrTe$_5$ single crystal. *ACS Appl. Mater. Interfaces* **10**, 40740 (2018).

[40] N. Aryal, X. Jia, Q. Li, A. M. Tsvelik, and W. Yin, Topological phase transition and phonon-space Dirac topology surfaces. in ZrTe$_5$, https://arxiv.org/pdf/2004.13326.pdf

[41] W. Zhang, P. Wang, B. Skinner, R. Bi, V. Koziì, C.-W. Cho, R. Zhong, J. Schnedoòl, D. Yu, G. Gu, L. Fu, X. Wu, L. Zhang, Observation of a thermoelectric Hall plateau in the extreme quantum limit, *Nat. Commun.* **11**, 1046 (2020).

[42] P. Streda, Quantised Hall effect in a two-dimensional periodical potential. *J. Phys. C: Solid State Phys.* **15**, L1299 (1982).

[43] H. W. Wang, B. Fu, and S. Q. Shen, Intrinsic magnetoresistance in three-dimensional Dirac materials with low carrier density. Phys. Rev. B **98**, 081202(R) (2018).

[44] E. Akkermans, and G. Montambaux. *Mesoscopic physics of electrons and photons* (Cambridge university press, England, 2007).

[45] J. Mutch, W.-C. Chen, P. Went, T. Qian, I. Z. Wilson, A. Andreev, C.-C. Chen, J.-H. Chu, Evidence for a strain-tuned topological phase transition in ZrTe$_5$. *Sci. Adv.* **5**, eaax9771 (2019).

[46] S. A. Miller, I. Witting, U. Aydemir, L. Peng, A. J. E. Rettie, P. Gorai, D. Y. Chung, M. G. Kanatzidis, M. Grayson, V. Stevanovic, E. S. Toherer, and G. J. Snyder, Polycrystalline ZrTe$_5$ Parametrized as a Narrow-Band-Gap Semiconductor for Thermoelectric Performance, *Phys. Rev. Appl.* **9**, 014025 (2018).

[47] A. C. Niemann, J. Gooth, Y. Sun, F. Thiel, A. Thomas, C. Shekhar, V. Suš, C. Felser, and K. Nielsch, Magnetothermoelectric characterization of a HfTe$_5$ micro-ribbon, *Appl. Phys. Lett.* **115**, 072109 (2019).

[48] M. Cutler, N. F. Mott, Observation of Anderson Localization in an Electron Gas, *Phys. Rev.* **181**, 1336 (1969).

[49] G. S. Nolas, J. Sharp, H. J. Godsmid, *Thermoelectrics: Basic Principles and New materials Developments*. (Springer, Heidelberg, 2007) vol. 45 of Springer Series in material science.

[50] H. Chi, C. Zhang, G. Gu, D. E. Kharzeev, X. Dai, Q. Li, Lifshitz transition mediated electronic transport anomaly in bulk ZrTe$_5$. *New J. Phys.* **19**, 015005 (2017).

[51] Y.-Y. Lv, X. Li, L. Cao, D. Lin, S.-H. Yao, S.-S. Chen, S.-T. Dong, J. Zhou, Y. B. Chen, and Y.-F. Chen, Tunable Resistance or Magnetoresistance Cusp and Extremely Large Magnetoresistance in Defect-Engineered HfTe$_{5-\delta}$ Single Crystals, *Phys. Rev. Appl.* **9**, 054049 (2018).

[52] A. B. Pippard, *Magnetoresistance in Metals* (Cambridge University Press, New York, 1989).