Anomalous temperature evolution of the Dirac band in ZrTe$_5$ across topological phase transition

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Characteristic features of topological phase transition (TPT) in solid-state materials usually compose of a non-monotonic band gap evolution across the parameter space and a gap closure at the transition point. Here, using semiconducting zirconium pentatelluride (ZrTe$_5$) and magneto-infrared spectroscopy, we identify a TPT from a strong topological insulator (TI) to a weak TI with increasing temperatures, but the band gap exhibits different behavior. Specifically, we find that the band gap in ZrTe$_5$ does not fully close at the TPT, and it becomes temperature independent at lower temperatures. Our observations can be explained by considering the effect of conduction-valence band mixing and band inversion in the strong TI phase of ZrTe$_5$ at low temperatures.

In single-electron band theory, a topological phase transition (TPT) from a topological insulator (TI) to a normal insulator (NI) is accompanied by a band gap evolution from an inverted gap to a zero gap and then a normal gap [1]. Consequently, a non-monotonic band gap behavior (Figure 1b) is often used as evidence for a TPT. However, when considering a more realistic band structure and interactions between the bands, one may find the above criterion no longer holds. Here, we showcase an unusual band evolution of a thermal expansion driven TPT in zirconium pentatelluride (ZrTe5) using magneto-infrared (magneto-IR) spectroscopy.

ZrTe$_5$ is a van der Waals material with the layer stacking direction along the b-axis of the crystal (Figure 1). The recent interest in ZrTe$_5$ originates from the theoretical prediction of a room-temperature quantum spin Hall insulator phase in its monolayer limit and a three-dimensional TI phase in its bulk form [2]. The prediction has sparked intensive experimental investigations into both the electronic and topological properties of ZrTe$_5$ [3,21]. However, different topological phases, i.e., weak/strong TIs (WTI/STI) and Dirac/Weyl semimetals, have all been reported in ZrTe$_5$ from different experiments [3,4,13,21]. Such discrepancy may result from the sensitive dependence of the topological phase on the lattice constants [2,22], inviting controllable measurements across the TPT to reconcile the experimental observations.

While several different techniques exist to manipulate the lattice constants in materials (such as using strain [23] or ultrafast laser [24, 25]), temperature remains the most convenient method, and it has been used to explore the topological phases in ZrTe$_5$ [16, 26, 27]. Unfortunately, in these experiments, the band gap behavior across the TPT remains elusive. For example, high-resolution angle-resolved photoemission spectroscopy measurements find that the band gap never closes in the temperature range of $2 < T < 255$ K [20, 26, 28, 30], while a zero-field IR optical conductivity measurement reveals gap closure at an intermediate temperature. Additionally, as many temperature-dependent measurements are performed on ZrTe$_5$ samples grown by the chemical vapor transport method, they are known to exhibit an anomalous resistance peak in $R(T)$ at a critical temperature $T^*_1$ [31]. This peak has been attributed to a Lifshitz transition, where the Fermi level shifts from the conduction band to the valence band with increasing temperature [29,32]. However, the relationship between the resistance anomaly and the TPT is still under debate [27,33].

In this work, we examine the band structure evolution in temperature of the molten Te-flux grown ZrTe$_5$ single crystals using magneto-IR spectroscopy. The flux growth method is known to effectively minimize the amount of impurities in samples and eliminate the effect of resistance anomaly [13,34]. More importantly, magneto-IR spectroscopy can directly probe the band structures of different carriers with high accuracy by tracing their Landau level (LL) transitions. It helps alleviate the complications caused by Fermi level shifting and other thermally excited carriers. Surprisingly, by tracing the Dirac band in ZrTe$_5$ up to 175 K, we identify a TPT at around 60 K but without a gap closure expected from theory. In addition, the band gap remains a constant below the transition temperature. We argue that this behavior is caused by the band inversion and the associated orbital mixing effect. Our work sheds light on the importance of the conduction-valence band mixing in describing the TPT.

The Te-flux growth of ZrTe$_5$ single crystals is described in our previous work [35]. Figure 1 shows the normalized temperature-dependent resistance, $R(T)/R(300K)$, of our sample, where no visible anomalous resistance peak is observed except at very low temperatures. X-ray powder diffraction measurements also find that the
FIG. 1. (a) Crystal structure of ZrTe$_5$ in the b-c plane. (b) Conventional theoretical prediction of the evolution of the topological phases across TPT and the associated low-energy band structure around Γ point. Here, 2∆ is the band gap. The WTI phase is expected to have a normal band gap in the bulk, similar to that of NI. The red and blue colors denote the conduction and valence band characters in different energy bands. (c) Temperature dependence of the lattice constants along different crystallographic directions, determined by x-ray powder diffraction measurements. (d) Temperature-dependent resistance for the Te-flux grown ZrTe$_5$. The curve is normalized to the resistance value at 300 K.

thermal expansion of the lattice is smooth in the temperature range of 40 < T < 300 K (Figure 1c). No structure change is spotted. For magneto-IR measurements, we repeatedly exfoliate a bulk crystal over an IR-transparent Scotch tape to achieve maximum coverage of the tape. The sample/tape composite is then placed on a metal aperture with a heater wrapped around it and a temperature sensor on the backside. After loading the sample into the magnet (in Faraday geometry), the transmission spectra are taken with a Fourier transform IR spectrometer, where the transmitted IR intensity from a Globar light source is detected by a Si bolometer shortly behind the sample. The temperature range of the sample is varied from 6 K to 175 K.

Figure 2a shows the magnetic field dependence of the normalized magneto-transmission spectra (i.e., $T(B)/T(0T)$) of ZrTe$_5$ at the lowest temperature of 6 K. A series of strong dips can be observed once the magnetic field is applied, which blueshifts with increasing the field. It has been well established that these absorption dips arise from the optical transitions between the LLs in ZrTe$_5$ [17, 18, 35–37], and one can employ the LL index $n$ to label the allowed interband transitions $L_{-n(n-1)} \rightarrow L_{n+1(n)}$. Between these strong transitions, we also observe a series of weak transitions indicated by the asterisk symbol (*). In fact, the presence of two sets of LL transitions indicates the STI phase in ZrTe$_5$ [35]. Other prominent features in Figure 2a include the sharp dips between 20-40 meV, originating from the IR-active phonon modes [13, 27]. The energies of these modes do not change as a function of magnetic field, and they do not contribute to the electronic structure of ZrTe$_5$ studied in this work.

Figure 2b shows a typical temperature evolution of the normalized magneto-transmission spectra, $T(B)/T(0T)$, at 1.5 T and from 6 K to 175 K. Here, the transmission spectra are normalized to the zero-field spectra at each temperature to avoid background complications from the temperature change. As temperature increases, the LL transitions start to smear out or weaken due to the thermal broadening effect. At the highest temperature (175 K), only the $n \leq 1$ LL transitions remain visible, and the weaker set of transitions labeled by the * symbol is visible up to around 65 K. The temperature evolution of the LL transitions exhibits different behavior for different modes. With increasing temperature, the $n = 0$ mode shifts toward higher energy, while the $n \geq 1$ modes shift toward lower energy within the measurement range. In addition, a new mode emerges at elevated temperatures and forms a well-defined dip at $\sim$17 meV at the highest temperature. Based on the energy of this mode, one can attribute it to the cyclotron resonance (CR) mode $L_{-1} \rightarrow L_{0-}$, given that the sample is hole-doped in the measurement temperature range [31]. In Figure 2c, we present the false color map of the temperature dependence of the normalized transmission at 3 T, where the CR and $n = 0$ modes are more prominent. One can clearly see that these two modes separate from each other at around 60 K.

From the magneto-IR spectroscopy data (Figure 2), one can also extract information about the mobility ($\mu$) and carrier density in our samples. The formation of distinct LLs requires the semiclassical condition $\mu B > 1$, which sets the lower bound in mobility estimation [38]. For all the temperatures studied in this work, the LL transitions can be identified at as low as 1 T. Hence, $\mu > 10,000$ cm$^2$V$^{-1}$s$^{-1}$ up to $T = 175$ K. Furthermore, even though the emergence of the CR mode implies an increase in carrier density at elevated temperatures, the observation of the $n = 0$ transition in Figure 2 suggests that our samples enter the quantum limits at $B < 1$ T for the entire temperature range and sets the upper limit for the carrier density. Therefore, we can deduce that the sample remains a very low carrier density or Fermi energy within the measurement temperature range. Our observation is in contrast to the density extracted from the reported temperature-dependent Hall measurements, which increases about two orders of magnitudes with increasing temperature [31]. Since electronic transport measurement probes the contributions from all bands crossing the Fermi level, whereas magneto-IR measurement focuses on a specific band, the discrepancy in carrier density suggests that the dominant contribution in thermally activated carriers in the Hall mea-
FIG. 2. (a) Magnetic field dependence of normalized magneto-transmission spectra, $T(B)/T(0T)$, of ZrTe$_5$ measured at 6 K from 1 T to 4.5 T. (b) Temperature-dependent magneto-transmission spectra, $T(B)/T(0T)$, of ZrTe$_5$ from 6 K to 175 K at 1.5 T. The integer index $n$ labels the interband LL transitions $L_{-n} \rightarrow L_{n+1}$. The asterisk symbol (*) indicates the second set of LL transitions, a hallmark of the STI phase in ZrTe$_5$ at low temperatures [35]. A CR mode emerges at elevated temperatures, which can be attributed to the $L_{-1} \rightarrow L_0$ transition. (c) False color map of the temperature evolution of the normalized magneto-transmission spectra, $T(B)/T(0T)$, of ZrTe$_5$ measured at 3 T. The symbols and lines denote the CR (red symbol) and interband $n = 0$ (orange symbol) transition energies calculated from the band parameters extracted from the model fitting of the interband LL transitions. All measurements are performed with $B \parallel b$-axis. The spectra are offset vertically for clarity in (a) and (b).

Measurements is from other trivial bands in ZrTe$_5$, while the Dirac electrons retain its high mobility and low density up to 175 K. We note that our work is the first to show a clear LL formation at such elevated temperatures in ZrTe$_5$ using magneto-optics. As a comparison, magneto-transport measurement can only probe LLs up to around 20 K [31, 39]. These results suggest that ZrTe$_5$ holds great promise in optoelectronics applications with Dirac electrons and could be further manipulated by magnetic fields.

Next, we turn to a quantitative analysis of the band structure evolution in ZrTe$_5$ as a function of temperature. We first investigate the strong interband LL transitions labeled by integer $n$ in Figure 2a,b. It has been well established that at low temperatures, these transitions can be described by a simple massive Dirac fermion model [18, 35–37], and the LL energies read

$$E_n = \alpha \sqrt{2e \hbar v_F n B + \Delta^2}, \quad (1)$$

with $\alpha = \pm 1$ is the band index, $e$ the electron charge, $\hbar$ the reduced Planck’s constant, and $\Delta$ the Dirac mass. The allowed LL transitions satisfy the conventional selection rule $\Delta n = \pm 1$, and their transition energies can be calculated accordingly. From eq. (1), one can see that the change in band gap ($2\Delta$) mostly impacts the energy of the $n = 0$ LL transition, and the effect quickly becomes unnoticeable for a higher $n$ as the dominant energy scale for higher LL transitions is determined by $v_F$.

Therefore, we will consider the temperature dependence of both $\Delta(T)$ and $v_F(T)$ to understand the different temperature evolution observed in Figure 2a,c for different modes. Specifically, we reveal that the blueshift of the $n = 0$ mode with increasing temperature is dominated by $\Delta(T)$, while the redshift of the $n > 1$ modes is due to $v_F(T)$. The temperature dependence of the $n = 1$ mode reflects the competition between the two effects.

We then extract the energies of interband LL transitions at selected magnetic fields and plot the magnetic field dependence of each mode at specific temperatures. Figure 3a-c shows the extracted data (symbols) at three different temperatures as well as the fits (solid lines) using eq. (1). Excellent agreement between the experiment and model calculation is achieved throughout the measured temperature range. Figure 3d illustrates the calculated Landau fan diagram at $T = 175$ K and the corresponding LL transitions following the color code in Figure 3a-c. For simplicity, we only label out the $\Delta n = +1$ transitions.

Figure 4 summarizes the temperature dependence of the extracted band gaps and Fermi velocities. We find that $2|\Delta|$ remains almost unchanged up to around 60 K, and further increase in temperature leads to an increase in $2|\Delta|$ and an almost concurrent decrease in $v_F$. Using these parameters, we can confirm that the origin of the additional energy mode labeled by “CR” in Figure 2b is indeed the cyclotron resonance mode $L_{-1} \rightarrow L_0$. 


FIG. 3. Magnetic field dependence of LL transitions at selected temperatures of (a) \( T = 6 \) K, (b) \( T = 105 \) K, and (c) \( T = 175 \) K. The black squares are the experimentally extracted transition energies, and the size of the squares is larger than the uncertainty of the transition energies. The solid lines are the best fits to the data using the massive Dirac fermion model. (d) Representative Landau fan diagram for \( T = 175 \) K. The LLs are labeled by the index \( n = 0, 1, 2, \ldots \), and their corresponding LL transitions \( L_{n+1(n)} \rightarrow L_{n+1(n)} \) are color-coded consistent with those in (a)-(c). Due to the electron-hole symmetry at low fields, the \( \Delta n = \pm 1 \) transitions degenerate. For simplicity, we only label out the \( \Delta n = +1 \) transitions.

From eq. (1), the energy difference between the interband \( n = 0 \) transition and the CR should be equal to the band gap. At low temperatures, the band gap is small, and the CR and interband \( n = 0 \) transition merge together. As the band gap increases at elevated temperatures, the distance between the two modes starts to increase, and therefore the CR mode is observed. We note that although it is difficult to accurately extract the CR energy due to the lineshape distortion caused by nearby phonon modes, one can instead calculate the CR and \( n = 0 \) transition energies at \( B = 3 \) T, using the extracted band parameters from the model fitting of the interband LL transitions. The calculation results are shown as symbols in Figure 2. As one can see, the calculated energy positions correctly capture the trend of the optical weight change as a function of temperature, further confirming the origin of the CR mode and the temperature evolution of the band gap and Fermi velocity.

Having firmly established the temperature dependence of the band parameters in ZrTe\(_5\), we can now discuss its implication in TPT. For the band gap, theory predicts that as temperature increases, the volume expansion may lead to two possible scenarios: (1) the band gap magnitude \( 2|\Delta| \) first decreases to zero and then increases across a TPT from the STI to WTI phase; and (2) a monotonic increase in \( 2|\Delta| \) if the initial low-temperature phase is a WTI. Both cases are consistent with our data in the \( T > 60 \) K regime (Figure 4a), where \( 2|\Delta| \) in the WTI phase increases with temperature. However, in the temperature range of 6-60 K, \( 2|\Delta| \) exhibits a nearly temperature-independent behavior in our experiment, making the topological state assignment ambiguous. As discussed earlier, the presence of the second set of LL transitions indicates band inversion and a STI phase in our samples at low temperatures; this persists up to around 65 K (Figure 2b). Therefore, a TPT is expected, but we do not observe any sign of band gap closure during the transition, in contrast to a recent zero-field temperature-dependent IR measurement.

In fact, it has been previously shown that the band gap closure does not necessarily occur during the TPT driven by temperature or magnetic field.

Anticrossing gap can exist in the system due to the orbital mixing between the conduction and valence bands, hence preventing the band gap closure. Together with our recent discovery of a second band gap in the vicinity of \( \Gamma \) point in the STI phase of ZrTe\(_5\), we propose the following scenario to explain the anomalous temper-

FIG. 4. (a) Temperature dependence of the extracted Fermi velocities and band gaps. The error bars are determined from the LL transition energy uncertainties. (b) Schematic drawing of the band structure evolution as a function of temperature from our experiment.
ature dependence of the band gap in our experiment. In Figure 4b, we schematically depict the temperature evolution of the band structure across the TPT. At the elevated temperature above the TPT, the system is in the WTI phase, and the band structure takes the form of a conventional massive Dirac electron with only one extremum at Γ point. The incident IR light thus probes the band gap $2\Delta$ at Γ point. Once the temperature drops to the TPT temperature at around 60 K, the conduction and valence bands come close enough so that the orbital mixing effect starts to play a role and leads to an anticrossing gap of finite size [40, 41]. When the temperature is further reduced, the system is in the STI phase. Due to the competition between the band inversion and the linear dispersion component, the band structure develops a second band gap in the vicinity of Γ point along the layer stacking direction (b direction) [31, 35]. Such a band structure resembles that in a gapped Weyl node system, and the size of the second band gap is determined by the strength of hybridization between the conduction and valence bands in an inverted band structure [42].

Our previous calculation shows that the joint density of states across the second band gap could dominate that at Γ point [35]. Therefore, the incident IR light no longer probes the band gap at Γ point but the hybridization gap at its vicinity. In this situation, the temperature-independent $2\Delta$ observed in our experiment reflects the size of the hybridization gap, which remains a constant below the TPT. Our result does not violate the theoretical prediction about the increasing gap at Γ point as lowering the temperature.

In conclusion, we have performed a magneto-IR spectroscopy study of the LL transitions in Te-flux grown ZrTe$_5$ samples in the temperature range of 6 K to 175 K and observed distinct temperature dependence for different low-energy modes. Using a massive Dirac fermion model, we extract the band gaps and Fermi velocities from the observed LL transitions and find that as temperature decreases, the band gap (Fermi velocity) first decreases (increases) and then saturates at low temperatures. We explain such a temperature dependence as a TPT from the WTI to STI phase at around 60 K. We attribute the finite band gap at TPT and the saturation at low temperatures to the formation of the second band gap (due to band inversion) and the associated orbital mixing effect.

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