Temperature-induced Lifshitz transition and possible excitonic instability in ZrSiSe

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The nodal-line semimetals have attracted immense interest due to the unique electronic structures such as the linear dispersion and the vanishing density of states as the Fermi energy approaches the nodes. Here, we report temperature-dependent transport and scanning tunneling microscopy(spectroscopy)[STM(S)] measurements on nodal-line semimetal ZrSiSe. Our experimental results and theoretical analyses consistently demonstrate that the temperature induces Lifshitz transitions at 80 K and 106 K in ZrSiSe, which results in the transport anomalies at the same temperatures. More strikingly, we observe a V-shape dip structure around Fermi energy from the STS spectrum at low temperature, which can be attributed to co-effect of the spin-orbit coupling and excitonic instability. Our observations indicate the correlation interaction may play an important role in ZrSiSe, which owns the quasi-two-dimensional electronic structures.

Lifshitz transition, which is characterized by the change of the Fermi surface topology[1], can happen among various materials through changing some external parameters such as chemical doping, pressure or magnetic field[2–7]. Recently, a new type of temperature-driven Lifshitz transition has been observed in Dirac and Weyl semimetals, in which the transition usually happens as the Fermi energy crosses the Dirac and Weyl nodes[8–10]. Near these nodes, the carriers have high mobility and can switch from n-type to p-type as the Fermi energy decreases (increases) to cross the nodes[10]. As a consequence, a Lifshitz transition usually has a close relationship with the transport anomalies at low temperature in Dirac and Weyl semimetals[11–14]. However, no such transition has been observed in nodal-line semimetal. In terms of materials, the experimentally confirmed compounds include PbTaSe2, PtSn4 and ZrSiM (M=S, Se Te) family[15–21]. Among them, ZrSiM attracts much attention due to the quite large energy window of the linear band dispersion in some region of the Brillouin zone. As the element M changes from S to Te, the electronic structures between ZrSiM show some subtle but important differences. In ZrSiSe and ZrSiTe, some new tiny trivial bands could cross the Fermi energy. This feature implies the electronic structures of these two compounds are in the vicinity of a Lifshitz transition, which could be achieved by tuning some external parameters, such as temperature. Furthermore, the first-principles calculations predict a spin-orbit coupling (SOC) gap (20–60 meV), which can destroy the nodal-line structure[15, 18, 21]. When the correlation interaction is taken into account, the nodal-line structure can further become instable and various correlation-driven nodal-line instabilities could emerge such as mass enhanced effect, excitonic insulator, charge/spin density wave etc[22–24]. These destructive instabilities could break down and obscure the topological physics based on the nodal-line structures in ZrSiM. However, the experimentally testing and verifying the destructive instabilities is still lacking.

In this work, we synthesize the high-quality single crystal ZrSiSe, and perform the detailed transport and scanning tunneling microscopy(spectroscopy) [STM(S)] measurements. The technical details are present in Supplemental Materials (SMs)[25]. The transport measurements show that ZrSiSe is a p-type metal above a critical temperature $T_c = 106 K$, whereas a portion of n-type carriers suddenly arise accompanying with the mobility sharply dropping when the temperature decreases below 106 K. As temperature further decreases, the mobility of n-type carriers suddenly ascends at another critical temperature $T = 80 K$. In combined with the first-
principles calculations, these transport anomalies can be interpreted by the change of the topology of the Fermi surface induced by Fermi level shift as temperature changes. Furthermore, our STM/S measurements demonstrate the carrier density ratio between $n$-type and $p$-type develops from 0.7 at $T=77$ K to 0.95 at $T=4.5$ K. The charge neutrality from imbalance to balance as temperature decreases further proves the change of the topology of the Fermi surface. These self-consistent interpretations to the independent transport and STM/S measurements strongly indicate the temperature-dependent Lifshitz transition in ZrSiSe. Through investigating the average differential conductance spectra from STS measurements, we observe a V-shape dip structure around Fermi energy. Our theoretical model and analyses indicate that the dip formation in ZrSiSe is referable to the co-effect of SOC and the destructive correlation effect, which gives rise to the excitonic instability. Thus, ZrSiSe is a promising candidate for studying the destructive effect from correlation effect and SOC to Dirac nodal-line physics.

The crystal structure of ZrSiSe is shown in Fig. 1(a). ZrSiSe has a PbFCl-type crystal structure with space group $P4/nmm$. The band structure along some momentum lines are plotted in Fig. 1(b). When the Fermi level is at 0 eV (intrinsic case) in Fig. 1(b), a series of Dirac-type bands with linear dispersion form the nodal-line structure in the $(k_x, k_y)$-plane around $k_z=0$, which is similar to the bands in ZrSiS[22–24]. As $k_z$ approaching $\pi$, however, along Z-R line, a new Fermi surface emerges as the band across the Fermi energy as shown in Fig. 1 (b).

Figure 2 (a) and (b) display representative $\rho_{xy}$-$H$ and $\rho_{xx}$-$H$ curves at selected temperatures. Detailed information is given in SMs[25]. As seen in Fig. 2(a), the $\rho_{xy}(H)$ curves exhibit three remarkable features. First, the nonlinearity for $\rho_{xy}(H)$ develops as the temperature decreases at low magnetic field. This feature indicates the carriers from multiband are involved in the transport as temperature decreases[12, 14]. Second, the $\rho_{xy}(H)$ curves have positive slope for $T> 40$ K, which indicates the majority of carriers are $p$-type at high temperature. Third, for $T< 40$ K, the initial positive slope of $\rho_{xy}(H)$ curves tends to change sign as $H$ increases from 0 T to 9 T, which indicates the compensated semimetal behavior with balance of $n$-type and $p$-type carriers at low temperature[12, 14]. In Fig. S2, temperature-dependent Hall coefficient, $R_H(T) = d\rho_{xy}(T)/dH$ at zero field limit shows a hump structure at $T \sim 106$ K, which indicates the minimum value of the total carrier density as temperature crosses 106 K[25]. To further verifying the deductions, we analyze the Hall conductivity $\sigma_{xy}=\rho_{xy}/(\rho_{xx}^2+\rho_{yy}^2)$ and use the two-component model to extract the intrinsic carrier densities and carrier mobilities at various temperatures[9, 24].

$$\sigma_{xy} = \frac{\mu_1^2}{1 + u_1^2 B^2} + \frac{\mu_2^2}{1 + u_2^2 B^2} eB. \quad (1)$$

Here, $n_1(n_2)$, $\mu_1(\mu_2)$ denote the carrier density [negative(positive)]for electrons[holes] and relevant in-plane mobility, respectively. In Fig. 2(c) and (d), the open symbols and the solid lines label the experiment data and the fitting results, respectively. The model fits well for the experimental data at all fixed temperatures. Figure 2 (e) and (f) show the temperature-dependent fitting parameters. At the lowest temperature $T=5$ K, the magnitude of $n_1$ and $n_2$ is nearly balanced. As temperature increases, $n_1$ and $\mu_1$ decrease smoothly. In contrast, $\mu_2$ shows two sharp jumps at $T=80$ K and 106 K labeled by the left dashed red and right dashed green lines in Fig. 2 (f), respectively. $n_2$ sharply decreases and becomes positive above $T=106$ K with negligible value in comparison with $n_1$.

Now, we elaborate the temperature-induced Lifshitz transition can give a natural interpretation to these transport anomalies. The Hall analyses in Fig. 2 clarify that the compensated electrons and holes at low temperature and the majority of $p$-type carriers at high temperature. In combined with Fig. 1, these behaviors imply that ZrSiSe should have zero Fermi level $E_F=0$ eV at low temperature and the Fermi level should descend at high temperature. Such Fermi level shift driven by temperature can be induced by the change of the lattice constants [10] supported by our powder X-ray diffraction (XRD) measurements (See Fig. S6 and Fig. S7 in SMs for details)[25], the localization or delocalization induced by
As temperature further increases, the second jump of \( \mu_2 \) emerges at \( T = 106 \) K. This process corresponds to shifting the Fermi level from the position labeled by the dotted red line to the Dirac point labeled by the long dashed green line in Fig. 1(b), because the carriers at Dirac point have the largest mobility. Above 106 K, the Fermi level descends below the Dirac point. The \( n \)-type Fermi pockets disappear (the blue band is not occupied in Fig. 1(b)), and only the \( p \)-type Fermi pockets survive (only the red band is occupied in Fig. 1(b)). It means that the \( n \)-type component (\( n_2 \), \( \mu_2 \)) undergoes the second Lifshitz transition at 106 K. Note that it seems that two \( p \)-type components still exist from Fig. 2(e) and (f), though only one band survives. In the whole temperature regime, two-component model is adopted to fit the experimental results. It is natural for each component is not zero. However, above 106 K, the weight of one component should be very small. It is explicit that \( n_2 \) is insignificantly small in comparison to \( n_1 \). Meanwhile, the \( \mu_1 \) and \( \mu_2 \) have the same trend. Thus, above 106 K, we argue that the \( n_1 \) and \( n_2 \) may be from the same band (red band in Fig. 1(b)), and the small value of \( n_2 \) may be from the anisotropy of the magenta Fermi pockets in Fig. 1(e).

STM/S can help to understand the picture extracted from and or beyond the transport measurements\[40-45\]. Figure 3 (b) shows the topography of a Se cleaved surface and the corresponding fast Fourier transform (FFT) image at \( T = 4.5 \) K. Figure 3 (c) and (d) show the zoom-in view of the topography at \( T = 4.5 \) K and \( T = 77 \) K, in which the two interleaved lattices (Zr and Se) and the Si square net can be well identified. We next present in the Fig. 3 (e) and Fig. S9 the line-cut averaged \( dI/dV \) spectra (proportional to the density of states (DOS)) measured at \( T = 4.5 \) K (black curve) and \( T = 77 \) K (red curve) along different scanning paths. The spectra in Fig. 3(e) and Fig. S9 are averaged by taking several spectra along a Zr-Se-Zr line, and Se-Si-Se line, respectively. The remarkable difference between two spectra appears at near zero bias. A broad V-shape dip emerges at \( T = 4.5 \) K and disappears at \( T = 77 \) K. To estimate the temperature-driven change of carriers density, we present the line-cut map crossing four unit cells (UCs) along Zr-Se-Zr line at \( T = 4.5 \) K in Fig. 3 (f). The original \( dI/dV \) spectra were shown in Fig. S8 in SMs\[25\]. The position-dependent STS spectrum\[46\] and angle-resolved photoemission spectroscopy\[15, 21\] have proven that Zr and Se in ZrSiSe dominate the holes channel and electron channel, respectively, which is similar with some semiconductor materials, such as GaAs\[47\]. Thus, the imbalance between electron extraction at negative bias and electron injection at positive bias, i.e., the ratio of \( e/h \) asymmetric \( R(r) \), could be directly obtained through the following equation\[43-45\],

\[
R(r) = \frac{\int_{-E_F}^{E_F} N(r, E) \, dE}{\int_{-E_F}^{E_F} N(r, E) \, dE}.
\]

By integrating the filled and empty states in the vicinity of the \( E_F \) from -100 mV to 100 mV, the result was shown in Fig. 3g. The \( e/h \) ratio varies between 0.88 and 1.02 within a unit cell, while the overall ratio takes the value \( e/h = 0.95 \), indicating the nearly perfect compensated band structure. At \( T = 77 \) K, as shown in Fig. 3(h) and (i), the orbital texture changes obviously comparing
FIG. 3: (a) Top view of crystal structure of ZrSiSe. (b) Atomically resolved STM topographic image of the cleaved ZrSiSe surface at \(T = 4.5\) K with \(V_t = 600\) mV and \(I_t = 200\) pA. The inset shows the fast Fourier transform (FFT) image. (c)-(d) Zoom-in views of the cleaved surface at \(T = 4.5\) K (\(V_t = 600\) mV and \(I_t = 500\) pA) and \(T = 77\) K (\(V_t = 600\) mV and \(I_t = 200\) pA). (e) Line-cut averaged \(dI/dV\) spectrum acquired in ZrSiSe at \(T = 4.5\) K (black curve) and \(T = 77\) K (red curve) along the Zr-Se-Zr direction. All spectra are normalized at \(V = 200\) mV. The black-solid arrow labels the V-shape dip structure. The red-solid arrow in Fig. 3(c) labels the line-cut direction. (f) and (h) The STS line-cut map along the Zr-Se-Zr direction at \(T = 4.5\) K and 77 K, respectively. (g) and (i) The calculated ratio of \(c/h\) asymmetry based on the spectra measurement in (f) and (h), respectively.

with the case at \(T = 4.5\) K. The overall \(c/h\) ratio equals 0.7. Note that the choice of integration limits [-100 meV, 100 meV] guarantees that evolution of the \(n\)-type band is smooth and undergoes a Lifshitz transition from the Fermi levels of 4.5 K and 77 K to -100 meV, respectively. In comparison with the calculated results shown in Fig. 1 (b), (c), (d) and the two-component model fitting results shown in Fig. 2 (e), the temperature-induced carriers density evolution obtained from STM/S measurement follows the same tendency and supports the temperature induced Lifshitz transitions. The balanced \(c/h\) ratio also provides a straightforward explanation of the non-saturated magnetoresistance (MR) at \(T = 5\) K (See Fig. S10 for details)[25, 48, 49].

Now, we turn to understand the V-shape dip of \(dI/dV\) at temperature \(T = 4.5\) K. Besides SOC, there exists several possible mechanism to induce the V-shape dip. Since our sample is very clean with the mobility as high as \(10^4\) cm\(^2\)V\(^{-1}\)S\(^{-1}\), which excludes the possible disorder effect, such as the well-known zero-bias anomaly[50-57]. The correlated interaction can induce some long-range order, such as superconducting and excitonic orders. The superconducting order can be easily excluded, because the V-shape dip structure is robust against the strong magnetic field in our measurement. Recall that a quite strong Coulomb interaction can open an excitonic gap to the Dirac nodes in two-dimensional graphene and the mass enhancement has been recently observed in ZrSIS[58-61]. It is naturally to think that the Dirac nodal-line structure can be gapped by the similar excitonic order, which results in the V-shape dip. To verify such a deduction and figure out the relation between SOC, excitonic instability and the V-shape dip structure. We construct a simplified model to do a simulation. Let’s reconsider the Hall analyses in Fig. 2 and the electronic structure in Fig. 1 (b) and (c). The minimal model should includes two parts at least. One part captures the Dirac nodal-line bands, while another part describes the trivial quadratic band. Note that the effect of surface bands can merge into the trivial quadratic band, because surface bands only contribute a large trivial electron pockets centered at \(M\) point and four small hole pockets around \(X\) point in surface Brillouin zone[62, 63]. Furthermore, both bulk DOS and surface DOS are calculated (See Fig. S3 in SMs for details)[25]. Without considering the excitonic instability, none of them can produce the V-shape dip feature.

The detailed theoretical modeling is presented in the SMs[25], and we only list the results here. Figure 4(a) and (b) simulates Dirac nodal-line structure and Fermi surface from the trivial quadratic band. Figure 4 (c) gives several calculated DOS curves with different SOC \(\lambda_{soc}\) and excitonic order parameter \(\Delta_{ex}\). The curve 1 indicates nonzero \(\lambda_{soc}\) can open a gap to the Dirac nodal lines. The
curve 3 indicates the coexistence of both $\lambda_{soc}$ and $\Delta_{ex}$ can suppress the nodal-line gap opened by $\lambda_{soc}$. The blue color curve gives the DOS of the trivial quadratic band from Fig. 4 (b). The curve 8 is the sum from the curve 1 and the blue color one, which is not similar to the 4.5 K experimental result shown in Fig. 3 (e). It indicates that the sole SOC $\lambda_{soc}$ can not explain the experimental result. However, by taking into account both SOC $\lambda_{soc}$ and the excitonic order parameter $\Delta_{ex}$, the curve 10 give similar result in Fig. 3 (e) at 4.5 K. Furthermore, the thermal broadening effect of $dI/dV$ is proportional to $\int d\omega [-f'(\omega - eV)N(\omega)]$ with $f$ and $N(\omega)$ the Fermi function and zero-temperature DOS, respectively. The missing V-shape dip structure of the $dI/dV$ curve at 77 K shown in Fig. 3 (e) is well captured by Fig. 4 (d). To see the effect of both $\lambda_{soc}$ and $\Delta_{ex}$ clearer, the zoom-in parts of Fig. 4 (c) are shown in Fig. 4 (e) and (f), where more curves with different values of $\Delta_{ex}$ are plotted besides the ones in Fig. 4 (c). As $\Delta_{ex}$ increases from zero, the curves 5, 6, 7 show the visible two dip structures labeled by the red-dashed arrow in Fig. 4 (e). Then, the dip structures of relevant curves 12, 13, 14 become to deviate from the V-shape labeled by the red-dashed arrow in Fig. 4 (f). According to our simulation, the optimal value of $\Delta_{ex}$ to obtain the V-shape dip structure is $\Delta_{ex} \sim 1/3\lambda_{soc}$, which can strongly suppress the SOC gap without induce visible two-dip structure.

In conclusion, our transport, STM/S measurements and theoretical analyses consistently demonstrate that the temperature induces Lifshitz transitions in ZrSiSe. We also observed a V-shape dip structure around Fermi energy from the STS spectrum at low temperature. Our theoretical modeling simulation clarifies the V-shape dip structure of relevant curves 12, 13, 14 become to deviate from the V-shape labeled by the red-dashed arrow in Fig. 4 (f). According to our simulation, the optimal value of $\Delta_{ex}$ to obtain the V-shape dip structure is $\Delta_{ex} \sim 1/3\lambda_{soc}$, which can strongly suppress the SOC gap without induce visible two-dip structure.

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See Supplemental Material at [url] for details on the sample preparation, sample characterization, band structure calculations and the theoretical modeling of the STS spectra, which includes Refs. [19–26 – 37].

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