Quantum transport evidence of topological band structures of kagome superconductor 
CsV$_3$Sb$_5$

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We report the transport properties of kagome superconductor CsV$_3$Sb$_5$ single crystals at magnetic field up to 32 T. The Shubnikov de Haas (SdH) oscillations emerge at low temperature and four frequencies of $F_\alpha = 27$ T, $F_\beta = 73$ T, $F_\gamma = 727$ T, and $F_\eta = 786$ T with relatively small cyclotron masses are observed. For $F_\beta$ and $F_\eta$, the Berry phases are close to $\pi$, providing a clear evidence of nontrivial topological band structures of CsV$_3$Sb$_5$. Furthermore, the consistence between theoretical calculations and experimental results implies that these frequencies can be assigned to the Fermi surfaces locating near the boundary of Brillouin zone and confirms that the structure with an inverse Star of David distortion could be the most stable structure at charge density wave state. These results will shed light on the nature of correlated topological physics in kagome material CsV$_3$Sb$_5$.

Because of special lattice geometry and multiple sublattices in a unit cell, materials with a kagome lattice exhibit many of novel physical properties. For example, insulating magnetic kagome materials with strongly geometrical frustration are very promising systems to realize quantum spin liquid state with fractionalized excitations [1]. In contrast, kagome metals exhibit nontrivial topological electronic structures, like Dirac or Weyl nodal points and flat bands [2,3]. When combined with long-range magnetism, many of exotic phenomena appear in the magnetic kagome metals, such as large anomalous Hall effect (AHE) [2,4,5], negative magnetism of flat band [6], and large magnetic-field tunability [7,8]. Thus, kagome metals have become an important platform to study novel physics of correlated topological materials.

Recently, the coexistence of charge density wave (CDW) state and superconductivity has been discovered in AV$_3$Sb$_5$ ($A$ = K, Rb and Cs) with the kagome lattice of V atoms, which also have a nonzero $Z_2$ topological invariant [11,13]. Further studies indicate that there is a three-dimensional (3D) 2×2×2 superlattice at CDW state [13,16], which could lead to an inverse Star of David (ISD) distortion in kagome lattice and a possible chiral charge order accompanying with large anomalous Hall conductivity even the long-range magnetic order is absent [17,23]. It could be closely related to the saddlepoint singularity and the nesting of Fermi surface (FS) near van Hove filling [24,25]. Interestingly, the formation of superlattice in AV$_3$Sb$_5$ below CDW transition temperature $T_{CDW} \sim 80$ K - 110 K [13,14] results in the appearance of charge gap observed in optical spectroscopy but the softening of acoustic phonon is absent near the CDW vector [16,24,28]. In addition, another 4$a_0$ unidirectional superlattice has also been observed at low temperature [29,30]. On the other hand, superconductivity in these materials also exhibits some intricate relationship with the CDW state and the nature of superconductivity in these materials is still under debate [13,20,33]. For example, the $T_{CDW}$ decreases with pressure when the superconducting transition temperature $T_c$ shows an unusual multiple-dome feature with a significant enhancement to about 8 K at 2 GPa [31,34,36].

In comparison to the intensive studies on the CDW state and superconductivity of AV$_3$Sb$_5$, the experimental investigations of topological features of these materials are still scarce. In this work, we present a detailed study on transport properties of CsV$_3$Sb$_5$ single crystals in a magnetic field up to 32 T. The analysis of Shubnikov-de Haas (SdH) oscillations of $ab$-plane resistivity $\rho_{xx}$ and the results of theoretical calculations using the structure with in-plane ISD distortion reveal the existence of several extremal orbits of FSs with relatively small cyclotron masses $m^*$s and nonzero Berry phases, providing a direct evidence for the existence of nontrivial topological electronic structures in CsV$_3$Sb$_5$ at CDW state.

CsV$_3$Sb$_5$ single crystals were grown by the self-flux method. The detailed methods of experimental characterizations and theoretical calculations are shown in Supplemental Material (SM) [37]. The $\rho_{xx}(T)$ of CsV$_3$Sb$_5$ single crystal exhibits a metallic behavior with a kink at $T_{CDW} \sim 92$ K due to the CDW transition (Fig. 1(a)) [12], which also leads to a sharp drop of magnetic susceptibility $\chi(T)$ at the same temperature (Fig. 1(b)). The nearly overlapped zero-field-cooling (ZFC) and field-cooling (FC) $\chi(T)$ curves suggest that this anomaly should be ascribed to the charge ordering transition.
low temperature, superconductivity appears at $T_c \sim 2.5$ K, leading to the zero-resistance and diamagnetic transitions (insets of Figs. 1(a) and 1(b)), similar to previous result [12]. At $T = 1.8$ K, the superconducting volume fraction (SVF) estimated from the ZFC $4\pi\chi(T)$ curve for $H\parallel ab$ below 3.5 K, indicating a bulk superconductivity of CsV$_3$Sb$_5$ single crystal. The small SVF obtained from the FC $4\pi\chi(T)$ curve implies the relatively strong flux pinning effect in CsV$_3$Sb$_5$. Figure 1(c) shows the field dependence of $\rho_{xx}(\mu_0 H)$ up to 32 T for $H\parallel c$ at various temperatures. At 1.8 K, there is a fast increase of $\rho_{xx}(\mu_0 H)$ at low-field region due to the suppression of superconductivity under field. At higher fields, all of $\rho_{xx}(\mu_0 H)$ curves exhibit a positive magnetoresistance without saturation up to 32 T. The most prominent feature of $\rho_{xx}(\mu_0 H)$ curves is the appearance of SdH oscillations at high-field region, which decays with increasing temperature. After subtracting a smooth background, the oscillatory parts of $\Delta \rho_{xx}(\mu_0 H) = \rho_{xx} - \rho_{xx}(\mu_0 H)$) as a function of $1/\mu_0 H$ exhibit complex periodic behaviors (Fig. 1(d)), indicating the contributions of several frequency components. The low-frequency SdH oscillations are still observable at 30 K, while the high-frequency ones disappear at 15 K.

As shown in Fig. 2(a) and its inset, the fast Fourier transform (FFT) spectra of SdH oscillations between 4 T and 32 T for $H\parallel c$ reveal several frequencies at $F_{\alpha} = 27$ T, $F_{\beta} = 73$ T, $F_\epsilon = 727$ T and $F_\eta = 786$ T. The two low-frequency peaks are close to previously reported results [22]. The peak at 5 T is excluded for the further analysis because of its limited number of periods in the field range from 4 T to 32 T. According to the Onsager relation $F = (h/2\pi\epsilon)A_F$ where $A_F$ is the area of extremal orbit of FS [48], the determined $A_F$s are 0.00258, 0.00697, 0.06940 and 0.07503 Å$^{-2}$ for $F_{\alpha}$, $F_{\beta}$, $F_\epsilon$, and $F_\eta$, respectively. The $A_{F_{\alpha}}$ and $A_{F_\eta}$ are very small, taking only about 0.17 % and 0.46 % of the whole area of BZ in the $k_x-k_y$ plane when taking $a = 5.50552$ Å (Fig. S1 of SM) [37]. In contrast, $A_{F_{\beta}}$ and $A_{F_\epsilon}$ take about 4.61 % and 4.99 % of the Brillouin zone (BZ) area.

In general, the SdH oscillations with several frequencies can be described by linear superposition of the multifrequency Lifshitz-Kosevich (L-K) formula, and each of which can be expressed as [48, 49],

$$\Delta \rho_{xx}^i \propto \frac{\mu_0 H}{2F} R_T R_D R_S \cos[2\pi(F/\mu_0 H + \gamma - \delta + \varphi)],$$

where for the $i$th SdH oscillation component, $F$ is frequency, $R_T = (\lambda m^* T/\mu_0 H)/\sinh(\lambda m^* T/\mu_0 H)$, $R_D = \exp(-\lambda m^* T_D/\mu_0 H)$, $R_S = \cos(\pi n^* g^*)$, $m^*$ is cyclotron mass in unit of free electron mass $m_e$, $T_D$ is the Dingle temperature, $g^*$ is the effective g factor, and constant $\lambda = 2e^2 k_B m_e/eh \approx 14.7$ T/K. The phase factor $\gamma - \delta + \varphi$ contains $\gamma = 1/2 - \phi_B/2\pi$ where $\phi_B$ is Berry phase, $\delta$ is determined by the dimensionality of FS ($\delta = 0$ and $\pm 1/8$ for the respective two-dimensional (2D) and
the $\varphi = 0.332(3)$ and $(B_{\text{avg}} = 1.8 \text{ K})$, the high-frequency components of SdH oscillations have damped completely at this temperature. For $|\rho_{xx}|/|\rho_{yx}| \sim 5$ for $\mu_0 H < 14 \text{ T}$ (Fig. S2 of SM) and $\Delta \rho_{xx}/\rho_{xx} < 0.04$, the longitudinal conductivity $\sigma_{xx}(\omega = \omega_{\text{avg}})$ is $1.076(4)$, perfectly consistent with above value obtained from above analysis and setting $\varphi = 0$, $\varphi = 1/8$, $2 \varphi$, $4 \varphi$, and $\varphi = 0$ represent the frequencies calculated from the cross sections of unfolded FSs for $\theta = 0$ and $\theta = 50^\circ$, respectively. The fitted oscillation frequencies at $1.8 \text{ K}$ can be fitted using the formula $\Delta \rho_{xx}/\rho_{xx} = (1 - 0.44(7)) \eta_\beta + 0.04\eta_\alpha$, and $\eta_\beta$ and $\eta_\alpha$ are out of phase with relatively small $|\Delta \rho_{xx}/\rho_{xx}|$ and $\eta_\beta$ is close to $20^\circ$, probably because of the quasi-2D nature of the Fermi surface forming the 3D limit. The angular dependence of the FFT amplitudes to the high-frequency oscillations is constructed from the SdH oscillations for $H < 15 \text{ K}$ (Fig. 2(c)) because the high-frequency oscillations are out of phase with those in the $p_{xx}$. Correspondingly, the LL integer $n$ should be assigned to the oscillatory maxima of $\rho_{xx}$ while the LL half-integer index $n+1/2$ is assigned to the oscillatory minimum of $p_{xx}$. From the linear fit of the $n$ as a function of $1/\mu_0 H$, the intercept on the LL index axis is $0.44(7)$ in between $3/8$ and $5/8$, indicating a nontrivial $\varphi_3 = \left(1 - \frac{0.44(7)}{2\pi}\right) \times 2\pi = 1.1(1)\pi$ for $F_3$ as expected in a Dirac system. This value also implies that the $\delta$ deviates from the 3D limit $|\delta| = 1/8$, probably because of the quasi-2D nature of the Fermi surface forming the 3D limit. The blue dashed line is calculated from the formula $F_\beta(\theta) = F_\beta(0^\circ)/\cos \theta$. The solid symbols at $\theta = 0$ represent the frequencies calculated from the cross sections of unfolded FSs in pristine BZ shown in Figs. 4(b) and 4(c). The error bars originate from the uncertainties when evaluating the areas of cross sections of unfolded FSs. The red solid line is obtained from theoretical calculations using the FS in the reconstructed BZ.

FIG. 3. (a) Field dependence of FFT amplitudes of SdH oscillations at various field directions ($\theta$) when $T = 1.8 \text{ K}$. The data at different field directions have been shifted for clarity. (b) Angular dependence of oscillation frequencies $F_\alpha$, $F_\beta$, and $F_\gamma$ with $\varphi = 0$ and $\varphi = 1/8$. Inset in (b) shows the definition of $\theta$. Error bars are defined as the half width at the half-height of FFT peaks and the angle uncertainty of measurement ($\sim 3^\circ$). The blue dashed line is calculated from the formula $F_\beta(\theta) = F_\beta(0^\circ)/\cos \theta$. The solid symbols at $\theta = 0$ represent the frequencies calculated from the cross sections of unfolded FSs. The red solid line is obtained from theoretical calculations using the FS in the reconstructed BZ.
It is similar to the previous report [18]. The unfolded band calculation for simplicity of analysis. The unfolded band structure in CDW state with the ISD distortion along c-axis is unchanged, especially for those bands originating from the Sb orbitals which have been confirmed by the APRES measurements. Due to the weak interlayer interaction, only the in-plane distortion, i.e., 2×2×1 superlattice, is considered during theoretical calculation for simplicity of analysis. The unfolded band structure in CDW state with the ISD distortion along the high-symmetry paths in the pristine BZ is shown in Fig. 4(a) and it is similar to the previous report [18]. It is noted that the $E_F$ is shifted down slightly by 33.3 meV in order to match the experimental results of SdH oscillation. When compared with the pristine phase without structural distortion (Fig. S5 of SM) [37], the general feature of band structure at CDW state is unchanged, especially for those bands originating from the Sb orbitals such as the band near $\Gamma$ point. Moreover, the Dirac cones at $K$ and $H$ points of BZ below $E_F$ are also almost intact, which have been confirmed by the APRES measurements [34]. However, the bands near the BZ boundary such as $M$ and $L$ points mainly contributed from the V orbitals are modified obviously, which is reasonable because the 2×2 ISD distortion appears in the V-kagome lattice.

Figures 4(b) and 4(c) show the cross sections of unfolded FSs at $k_z = 0$ and $\pi/c$ planes in the pristine BZ. There are a tiny oval cross section of FSs (labelled as $F_1$) in the $\Gamma - K$ line and a small circular-shaped one (labelled as $F_2$) appearing around the $L$ point. In contrast, two FSs at $K$ and $H$ points show a rounded triangular shape (labelled as $F_3$ and $F_4$). On the other hand, the cross sections of FSs locating at the center of BZ ($\Gamma$ and $A$ points) have circular shapes with different radii. Moreover, there is a large hexagonal-shaped cross section of FS around the $A$ point and it becomes a discontinued hexagon when moving to the $k_z = 0$ plane. Above results are consistent with the angle-resolved photoemission spectroscopy (ARPES) results in principle [12, 54, 55]. Assuming the extremal orbits contributed from these cross sections of FSs, the corresponding frequencies below 1000 T are calculated and shown in Fig. 3(b). It is found that the experimental $F_\alpha - F_\eta$ could be assigned to the calculated FS sections of $F_1 - F_4$ (Figs. 4(b) and 4(c)). Taking $F_3$ as an example, the validity of assignment is further confirmed by calculating angular dependence of frequencies using the FS in the reconstructed BZ (Fig. S6 of SM) [37]. As shown in Fig. 3(b), the theoretical curve (red solid line) can describe the trend of experimental result very well. Because the FS related to $F_3$ is a prolate ellipsoid in shape centering at $L$ point (see the red pocket in Fig. S6 of SM) [37], this explains the similar trend of theoretical curve and that calculated using the formula $F_3(\theta) = F_3(0^\circ)/\cos \theta$ when $\theta < 50^\circ$. In addition, the calculated $m^*$ is 0.145 $m_e$, which is also in good agreement with the experimental value of $F_3 (0.142(4) m_e)$. Such small $m^*$ reflects the linear dispersion of this electronic pocket at $L$ point. Importantly, according to previous theoretical calculations [38], the ISD phase in the CDW state has a topologically nontrivial band structure with nonzero $Z_2$ topological invariants for the bands near $E_F$. Thus, it will lead to a π Berry phase accumulated along the cyclotron orbit, consistent with present experimental value of $\phi_B$. On the other hand, the differences between $F_\alpha (F_\eta)$ and the calculated value for $F_3 (F_4)$ may be due to the influence of lattice distortion along the c-direction at CDW state with 3D 2×2×2 superlattice [12, 14]. In that case, the band folding also happens along the $k_z$ direction and the $F_3$ and $F_4$ will overlap each other, possibly leading to the modifications of both cross sections of FSs, i.e., the changes of corresponding frequencies. Further study is needed in order to clarify this issue.

It is worth mentioning that another study [56] on the SdH oscillation of CsV$_3$Sb$_5$ with the field up to 14 T reported in very recent shows similar results about the Fermiology of CsV$_3$Sb$_5$ to present work. Although the calculated frequencies of extremal orbits are different slightly, the qualitative consistence between experiments and theoretical calculations in these two studies suggests that the structure with an ISD distortion could be the most stable structure at CDW state.
low temperature indicate that there are several SdH oscillation frequencies with relatively small m’s for CsV₃Sb₅. Theoretical calculations using the structure with an ISD distortion at CDW state suggest that the frequencies of SdH oscillations could be related to the extremal orbits of FSs near the high-symmetry points at BZ boundary. Importantly, the $\phi_B$ of FSs related to the frequencies of $F_\beta$ and $F_\gamma$ are close to $\pi$, confirming the predicted nontrivial topological properties of CsV₃Sb₅ at CDW state. Thus, the kagome metals AV₃Sb₅ pave a new way to study the correlation effects on topological electronic structures.

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See Supplemental Material at for the detailed methods of crystal growth, experimental characterizations and theoretical calculations, powder x-ray diffractions, Hall resistivity measurements, the SdH quantum oscillation as a function of $1/\mu_0 H$ at 15 K with the fit using the two-frequency L-K formula, $\Delta \rho_{xx}$ as a function of $1/\mu_0 H$ at 1.8 K with various field directions, band structure of pristine phase, and FSs in reconstructed BZ of CsV$_3$Sb$_5$ which includes Refs. [38–47].

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