

**Electronic structure of the kagome metal YbTi<sub>3</sub>Bi<sub>4</sub> studied using torque magnetometry**Kyryl Shtefienko<sup>1,\*</sup>, Cole Phillips<sup>1,\*</sup>, Brenden R. Ortiz<sup>2</sup>, David E. Graf<sup>3,4</sup> and Keshav Shrestha<sup>1,†</sup><sup>1</sup>*Department of Chemistry and Physics, West Texas A&M University, Canyon, Texas 79016, USA*<sup>2</sup>*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*<sup>3</sup>*Department of Physics, Florida State University, Tallahassee, Florida 32306, USA*<sup>4</sup>*National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA*

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This study investigates the electronic structure of the kagome metal YbTi<sub>3</sub>Bi<sub>4</sub> using high-field torque magnetometry. The torque signal measured at a maximum field of 41.5 T reveals clear de Haas–van Alphen (dHvA) oscillations with a major frequency peak at  $F_\delta \sim 130$  T. By rotating the sample at various tilt angles  $\theta$ , we observed that  $F_\delta$  exhibits a nearly  $1/\cos\theta$  dependence, indicating the presence of a quasi-two-dimensional (2D) Fermi surface (FS) in YbTi<sub>3</sub>Bi<sub>4</sub>. This argument is further supported by the detection of a forward-leaning, sawtoothlike waveform in the dHvA effect, a hallmark of 2D FS characteristics. Notably, we identified two high-frequency peaks near  $F_\chi \sim 1900$  T and  $F_\lambda \sim 5600$  T; however, these peaks quickly disappear at  $\theta$  greater than  $21^\circ$ . To better understand experimental observations, we computed the electronic band structure and FS using *ab initio* density-functional theory (DFT). The electronic bands reveal the presence of several Dirac points, flat bands, and van Hove singularities near the Fermi level. Five bands cross the Fermi level and contribute to the FS of this material. The FS comprises cylindrical sheets, with theoretical frequencies from the FS pockets aligning well with the experimental dHvA frequencies. Several FS parameters characterizing  $F_\delta$  were determined by analyzing the temperature and field dependence of the dHvA oscillations using the Lifshitz-Kosevich theory. The detailed electronic properties presented in this work provide critical insights into the electronic structure of YbTi<sub>3</sub>Bi<sub>4</sub> and other titanium-based kagome compounds.

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Kagome materials have attracted significant research interest due to their intriguing physical and electronic structures, which include features such as charge-density wave (CDW) phenomena, nontrivial topology, Dirac points, saddle points, flat bands, and more [1–3]. These materials feature a quasi-two-dimensional (2D) lattice structure resembling a traditional Japanese basket-weaving pattern [4]. One notable example is the vanadium-based family AV<sub>3</sub>Sb<sub>5</sub> ( $A = \text{K, Rb, and Cs}$ ), also known as the 135 family, which forms a hexagonal lattice of V atoms coordinated by Sb atoms [5–7]. This family exhibits a range of exotic quantum phenomena, including superconductivity with critical temperatures ( $T_c$ ) ranging from 0.3 to 3 K, CDW order near  $T_{\text{CDW}} \sim 80$ –110 K, nontrivial topology, a van Hove singularity and more [8–12]. The coexistence of nontrivial topology and superconductivity in AV<sub>3</sub>Sb<sub>5</sub> makes these materials potential candidates for exploring topological superconductivity and Majorana fermions. Our group, along with others, has performed quantum oscillation studies to map the Fermi surface (FS) of AV<sub>3</sub>Sb<sub>5</sub> [13–23].

Additionally, another vanadium-based family, RV<sub>6</sub>Sn<sub>6</sub> ( $R = \text{Rare earth}$ ), known as the 166 compounds, has been discovered [24–31]. Among these, GdV<sub>6</sub>Sn<sub>6</sub>, HoV<sub>6</sub>Sn<sub>6</sub>, and

YV<sub>6</sub>Sn<sub>6</sub> have been found to exhibit topological properties [26,32]. ScV<sub>6</sub>Sn<sub>6</sub> is the only member of the 166 family to display CDW order below  $T_{\text{CDW}} = 92$  K [31,33], although no superconductivity has been observed in ScV<sub>6</sub>Sn<sub>6</sub> under ambient conditions or pressures up to 11 GPa [34]. It is important to note that a density wavelike transition has been recently reported in LuNb<sub>6</sub>Sn<sub>6</sub> [35]. A different class of Ti-based kagome systems, ATi<sub>3</sub>Bi<sub>5</sub> (where  $A = \text{Cs, Rb}$ ) [36–38], crystallizes in the same structure as AV<sub>3</sub>Sb<sub>5</sub>, but with Ti atoms forming the kagome net instead of V, and Bi substituting for Sb. Unlike AV<sub>3</sub>Sb<sub>5</sub>, the ATi<sub>3</sub>Bi<sub>5</sub> system shows no evidence of the CDW order or superconductivity (SC). Another recently synthesized Ti-based kagome system, LnTi<sub>3</sub>Bi<sub>4</sub> ( $Ln = \text{Lanthanides}$ ) [39,40], adopts an orthorhombic structure with the  $Fmmm$  space group (No. 69). The unit cell has four kagome layers of the Ti sublattice, as shown in Figs. 1(a) and 1(b). Unlike the previously studied AV<sub>3</sub>Sb<sub>5</sub> and ATi<sub>3</sub>Bi<sub>5</sub> compounds, LnTi<sub>3</sub>Bi<sub>4</sub> features slightly distorted kagome lattices and zigzag Ln chains within Ln-Bi bilayers. The density-functional theory (DFT) and angle-resolved photoemission spectroscopy (ARPES) studies [41–45] find the presence of van Hove singularities and Dirac points near the Fermi level of this material. Due to the presence of magnetism in rare earth elements in LnTi<sub>3</sub>Bi<sub>4</sub>, it is a suitable system for tuning magnetism by rare-earth engineering. Electrical transport and magnetic properties of this family have recently been reported, both at ambient conditions and under pressure [46–48]. Among this family, YbTi<sub>3</sub>Bi<sub>4</sub>

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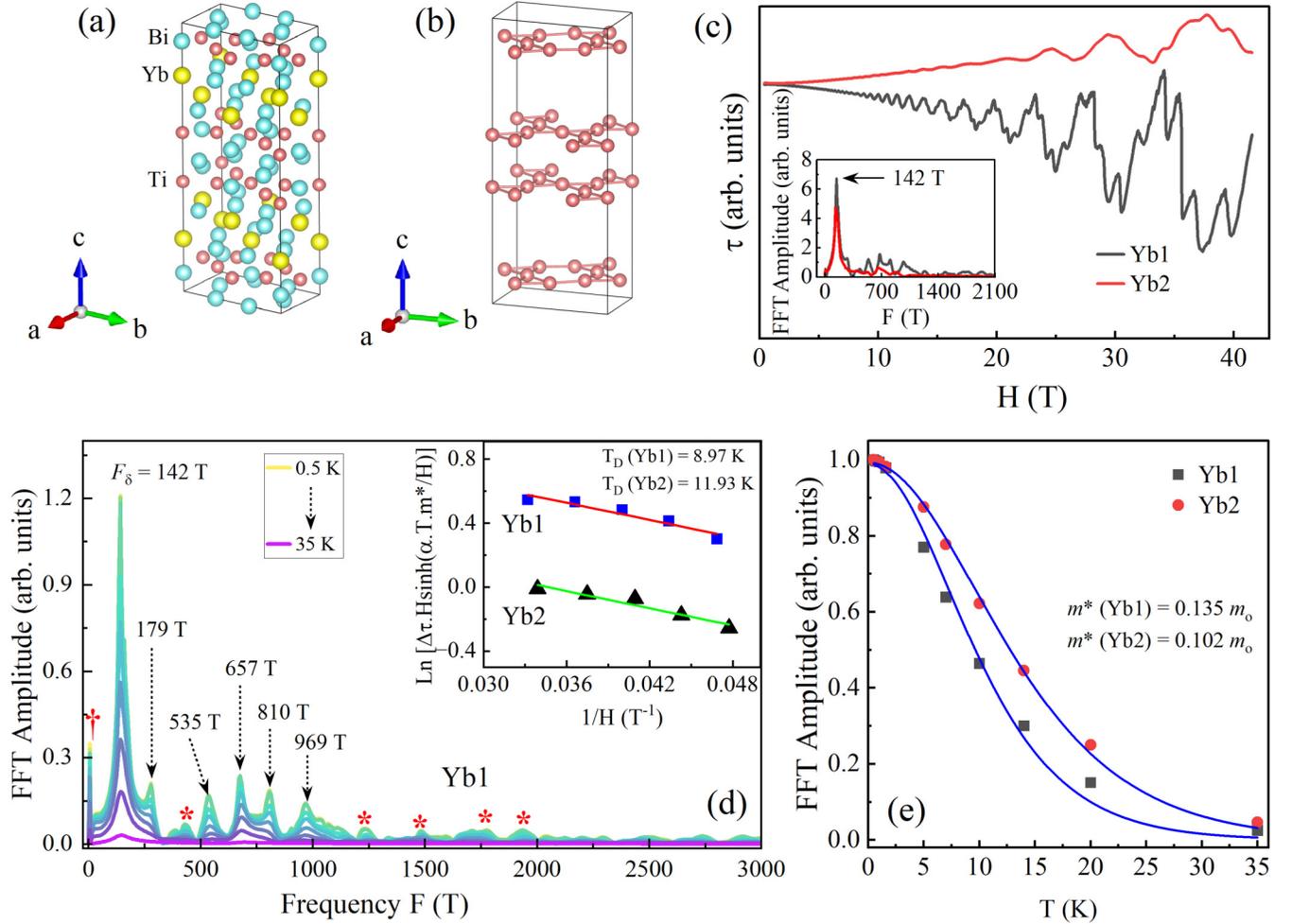


FIG. 1. (a) Unit cell of  $\text{YbTi}_3\text{Bi}_4$ . (b) Kagome layers of the Ti lattice within the unit cell. (c) Torque  $\tau$  signal for two  $\text{YbTi}_3\text{Bi}_4$  single crystals (Yb1 and Yb2) up to 41.5 T at  $\theta = 28^\circ$  and  $T = 0.5$  K, showing clear dHvA oscillations above 4 T. Inset: Frequency spectra of the dHvA oscillations for Yb1 and Yb2, displaying similar spectra with a major frequency peak at  $F_\delta = 142$  T. (d) Temperature dependence of the frequency spectrum for Yb1, revealing six well-defined frequency peaks. Inset: Dingle temperature analysis for Yb1 and Yb2, where scattered data are experimental data and the solid lines are the best fits. (e) Lifshitz-Kosevich analysis of the temperature-dependent frequency data for Yb1 and Yb2.

and  $\text{LaTi}_3\text{Bi}_4$ , along with  $\text{CaTi}_3\text{Bi}_4$ , are the only members known to exhibit nonmagnetic properties. This is due to the valence states of  $\text{Yb}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{La}^{3+}$ . No superconducting, structural, or electronic instabilities are observed down to 60 mK in  $\text{LnTi}_3\text{Bi}_4$  [39,42].

A detailed understanding of the FS is essential for grasping the electronic properties of  $\text{LnTi}_3\text{Bi}_4$ . Despite several ARPES and DFT studies, quantum oscillation studies to map the FS properties of  $\text{LnTi}_3\text{Bi}_4$  have not been reported. In this study, we conducted torque magnetometry measurements with applied fields up to 41.5 T to map the electronic structure of  $\text{YbTi}_3\text{Bi}_4$ . We observed a major peak at  $F_\delta \sim 130$  T in the de Haas-van Alphen (dHvA) oscillations. By rotating the sample in the magnetic field, we successfully mapped the FS of  $F_\delta$ . Interestingly, the dHvA oscillations exhibit a forward-leaning sawtoothlike wave form, clearly indicating the presence of a 2D FS in  $\text{YbTi}_3\text{Bi}_4$ . To support the experimental observations, we computed the electronic bands and FS using DFT. Our DFT calculations reveal several Dirac points, flat bands, and

van Hove singularities near the Fermi level, along with quasi-2D FS sheets, consistent with the experimentally observed nearly  $1/\cos\theta$  dependence of  $F_\delta$ .

## II. EXPERIMENTAL AND COMPUTATIONAL DETAILS

$\text{YbTi}_3\text{Bi}_4$  single crystals are grown through a bismuth self-flux. Yb metal (Ames) (Alfa 99.5%), Ti powder (Alfa 99.9%), and Bi shot (Alfa 99.999% low-oxide) were placed into a  $\sim 5$  mL Canfield crucible fitted with a catch crucible and a porous frit [49] at a ratio of  $2:3:20 = \text{Yb}:\text{Ti}:\text{Bi}$ . The crucibles were sealed under approximately  $\sim 0.7$  atm of argon gas in fused silica ampoules. Samples were heated to  $1100^\circ\text{C}$  at a rate of  $200^\circ\text{C}/\text{hr}$  and thermalized at  $1100^\circ\text{C}$  for 12 h. The growth proceeded with a cooling rate of  $2^\circ\text{C}/\text{hr}$  to  $600^\circ\text{C}$ . Excess bismuth was removed through centrifugation at  $600^\circ\text{C}$ . Resulting crystals are pseudohexagonal plates with typical dimensions ranging from  $1 \times 1 \times 0.2$  mm<sup>3</sup> to  $5 \times 5 \times 1$  mm<sup>3</sup>. Crystals have a

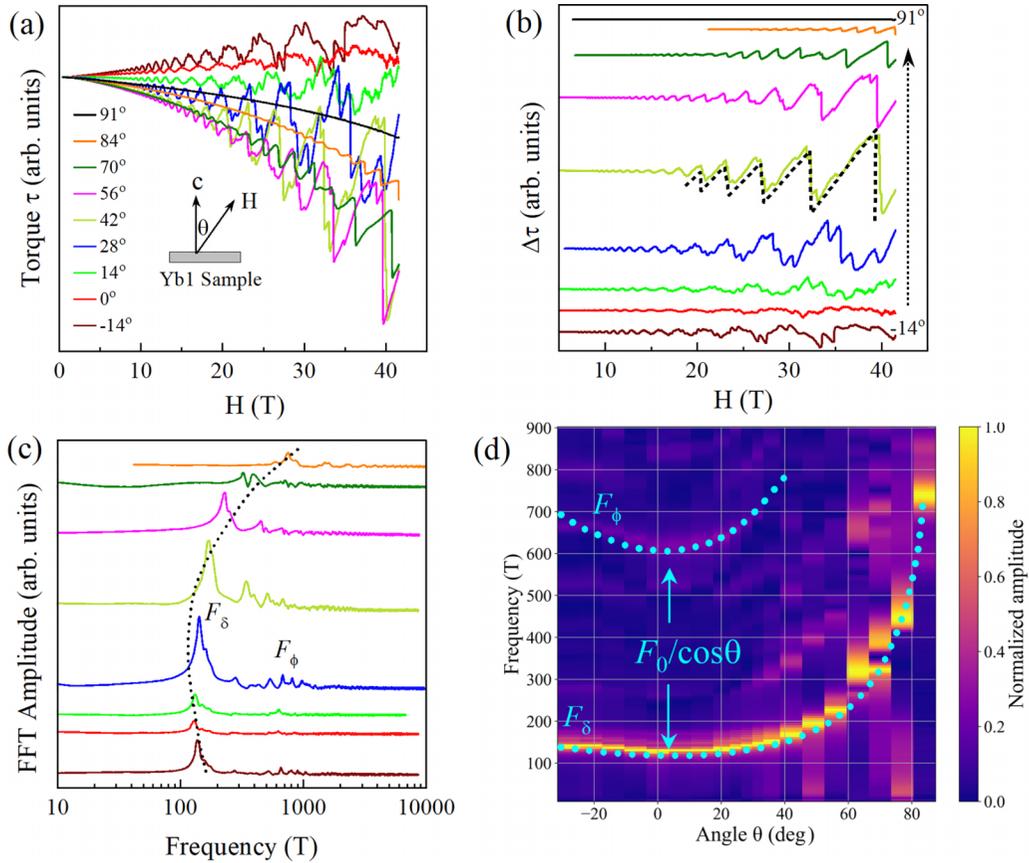


FIG. 2. (a) Angular dependence of dHvA oscillations for the  $\text{YbTi}_3\text{Bi}_4$  (Yb1 sample) measured at  $T = 0.5$  K. The tilt angle  $\theta$  is defined as the angle between the magnetic field and the  $c$  axis. (b) Background-subtracted torque data showing how the amplitude and period of quantum oscillations change with  $\theta$ . The dHvA oscillations exhibit a forward-leaning sawtooth pattern, as illustrated by the dashed wave form. (c) Frequency spectrum of dHvA oscillations at different  $\theta$  values. A major frequency of 140 T is observed at  $\theta = 0^\circ$ , which shifts to higher values at larger  $\theta$ , as indicated by the dashed curve. The curves in (b) and (c) are offset, with (c) displayed on a logarithmic scale for clarity. (d) Color plot showing the angular dependence of Yb1.  $F_\delta$  and  $F_\phi$  nearly follow an  $F_0/\cos\theta$  dependence, where  $F_0$  is frequency at  $\theta = 0^\circ$ , as indicated by the dotted curves.

brilliant metallic luster and are easily exfoliated. We noted mild sensitivity of the samples to air and water. The detailed information about the sample synthesis and studies of the electrical and magnetic properties of  $\text{YbTi}_3\text{Bi}_4$  have been reported in separate publications [39,42]. We used single crystals of this material from the same batch of the sample growth.

Torque measurements were performed using a miniature piezoresistive cantilever to observe dHvA oscillations. A selected single crystal of  $\text{YbTi}_3\text{Bi}_4$  was attached to the cantilever arm using vacuum grease and then mounted on a rotating platform. The probe was slowly cooled to a base temperature of 0.5 K. Two resistive elements on the cantilever, along with two room-temperature resistors, formed a Wheatstone bridge that was balanced at the base temperature before sweeping the magnetic field. The sample was rotated *in situ* in applied fields at various tilt angles  $\theta$ , where  $\theta$  is the angle between the magnetic field and the  $c$  axis of the sample [inset in Fig. 2(a)]. Magnetic fields were swept at each fixed temperature at a rate of 1.5 T/min.

Electronic band and FS calculations were performed by using an open-source code Quantum Espresso (QE) [50], which is programmed based on the density-function theory (DFT)

formalism [51,52]. The unit-cell structure was relaxed without implementing constraints under vc-relax mode. To ensure the convergence of structural parameters and cell energies during structural optimization, the wave functions' kinetic energy and charge-density cutoffs were set to 70 and 750 Ry, respectively. The self-consistent iterative process was set to be  $10^{-8}$  Ry to achieve the minimum total-energy difference convergence criteria.

### III. RESULTS AND DISCUSSION

Figure 1(c) shows the torque  $\tau$  for two  $\text{YbTi}_3\text{Bi}_4$  single crystals (Yb1 and Yb2) with applied fields  $H$  up to 41.5 T at 0.5 K. The  $\tau$  signal varies almost linearly with  $H$  and shows clear dHvA oscillations above 4 T. The dHvA oscillations are observed in both Yb1 and Yb2 samples. The oscillation signal is more pronounced in Yb1 than in Yb2 although both signals have the comparable frequency spectrum, as shown in the inset. It is important to note that the frequency spectra of Yb1 and Yb2 look similar, with both showing a major peak at  $F_\delta = 142$  T. However, there are slight differences, especially in the frequencies near 700 T. This indicates that the Fermi levels of the two samples are slightly different. Therefore, we have

presented detailed temperature- and angular-dependence data for Yb1 in the main text. To get frequency spectrum, we carried out background subtraction by fitting a smooth polynomial background and finally performed the fast Fourier transform (FFT). Figure 1(d) shows the frequency spectrum of Yb1 at different temperatures measured at  $\theta = 28^\circ$ . As shown in the graph, there is a dominant peak at  $F_\delta = 142$  T, along with five other distinct peaks at 179 T, 535 T, 657 T, 810 T, and 969 T. Several smaller peaks, indicated by stars, are less pronounced and disappear quickly at temperatures above 2 K. Therefore, we have not taken them into consideration here. Furthermore, with careful analysis of the background subtraction, we resolved two high-frequency peaks near  $F_\chi \sim 1900$  T and  $F_\lambda \sim 5600$  T. We will discuss this in detail later. The amplitude of the dHvA oscillations decreases at higher temperatures and this behavior can be described by the Lifshitz-Kosevich (LK) theory [53]. The LK formula enables estimating the effective mass  $m^*$  of the charge carriers. According to this theory, the temperature dependence of dHvA oscillations is given by

$$\Delta\tau(T, H) \propto e^{-\lambda_D} \frac{\lambda(T/H)}{\sinh[\lambda(T/H)]}, \quad (1)$$

with  $\lambda_D(H) = \frac{2\pi^2 k_B m^* T_D}{\hbar e}$  and  $\lambda(T/H) = \frac{2\pi^2 k_B m^* T}{\hbar e}$ . Here,  $T_D$ ,  $\hbar$ , and  $k_B$  represent the Dingle temperature, the reduced Planck's constant, and Boltzmann's constant, respectively. The first term is the Dingle factor, which describes the attenuation of the oscillations with decreasing field  $H$ . The second term explains the weakening of the oscillations at higher temperatures.

We have carried our LK analyses only for the major peak  $F_\delta$ . Figure 1(e) shows the temperature dependence of the normalized FFT amplitudes of  $F_\delta$  for Yb1 and Yb2 samples. The scattered data are experimental data while the solid curves are the best fits using the LK formula [Eq. (1)]. As seen in the figure, the LK theory fits temperature dependence of frequency data very well. From the best fitting, we have estimated  $m^* = 0.135m_o$  and  $0.102m_o$ , where  $m_o$  is the free mass of electron, for Yb1 and Yb2, respectively. The  $m^*$  values for Yb1 and Yb2 are in good agreement with each other and are also comparable with the effective masses of other kagome compounds [30,38,54].

To determine other physical parameters of charge carriers, we have also conducted the Dingle temperature analyses for  $F_\delta$  peak of both Yb1 and Yb2, as illustrated in the inset of Fig. 1(d). From the best fit curve, it is found that  $T_D = (8.97 \pm 1.58)$  K and  $(11.93 \pm 1.84)$  K, for Yb1 and Yb2, respectively. Using the value of  $T_D$  and  $m^*$ , we have estimated several parameters characterizing the Fermi pocket of  $F_\delta$ . Taking Yb1 as an example, we used Onsager's relation [53], the frequency  $f = \hbar/(2e)k_F^2$ , and estimated the Fermi momentum corresponds to  $k_F = 0.065\text{\AA}^{-1}$ . Using the linear dispersion relation for the surface state  $v_F = \hbar k_F/m^*$ , we have estimated the Fermi velocity  $v_F = 5.612 \times 10^5$  m s $^{-1}$ . With the value of  $T_D = 8.97$  K, the surface carrier life time  $\tau = \hbar/2\pi k_B T_D$  is estimated to be  $\tau = 0.135 \times 10^{-12}$  s. Similarly, other physical parameters like the mean-free path  $\ell_{2D} = v_F \tau$  and mobility  $\mu = e\tau/m^*$  are estimated to be 7.57 nm and  $0.176m^2$  V $^{-1}$  s $^{-1}$ ,

respectively. The estimated FS parameters for both Yb1 and Yb2 are presented in Table I. As shown in the table, the parameters for Yb1 and Yb2 are in good agreement and comparable to those of other kagome and topological compounds [55–57].

According to Onsager's relation [53,58], the frequency of quantum oscillation is directly proportional to the cross section of the FS. Therefore, it is possible to map the FS by rotating the sample in the magnetic field. For this, we rotated the sample *in situ* magnetic field at different  $\theta$  values. Angular dependence of torque data at selected  $\theta$  values for Yb1 is shown in Fig. 2(a). While increasing angle, we can clearly see that the amplitude of oscillation changes. The oscillation is completely absent when the magnetic field is aligned along the *ab* plane, as shown in Figs. 2(a) and 2(b) ( $\theta = 91^\circ$ ). The same feature is also observed in another sample, Yb1, as presented in Fig. S1 of the Supplemental Material (SM) [59]. The absence of dHvA oscillations at  $\theta = 91^\circ$  strongly suggests the presence of a quasi-2D Fermi surface [60,61] in YbTi $_3$ Bi $_4$ .

It is noteworthy that dHvA oscillations [Fig. 2(b)] display a forward-leaning, sawtoothlike pattern at higher magnetic fields (above 20 T), with this feature becoming more pronounced at tilt angles ( $\theta$ ) greater than  $28^\circ$ , as indicated by the dashed line. A similar forward-leaning, sawtoothlike feature has also been observed in the Yb2 sample, as shown in Fig. S1(b) of SM [59]. This behavior is characteristic of ideal two-dimensional metals [62–64]. The forward-leaning sawtooth wave form arises from jumps in the chemical potential between discrete filled and empty Landau levels as the magnetic field is swept [63–65]. This sawtooth wave-form feature has recently been observed in torque measurements of underdoped cuprates [66] in pseudogap region, providing the evidence of a 2D Fermi pocket. Therefore, observation of such feature strongly suggests the presence of the 2D Fermi surface in YbTi $_3$ Bi $_4$ .

Figure 2(c) shows the frequency spectrum of YbTi $_3$ Bi $_4$  at different  $\theta$  values. As seen in the graph, the major frequency peak near 140 T at  $\theta = 0^\circ$  gradually increases at higher angles, as indicated by the dashed curve. Due to the presence of multiple peaks in the frequency spectrum, we used a color plot to visualize the angle-dependent data [Fig. 2(d)]. The bright, intense color represents  $F_\delta$ , which increases at higher angles. It appears that both  $F_\delta$  and the frequency near  $F_\phi = 620$  T exhibit an  $F_0/\cos\theta$  dependence, where  $F_0$  is the frequency value at  $\theta = 0^\circ$ , as indicated by the dotted curves. The dHvA oscillations observed in a second sample, Yb2, exhibit similar angular-dependence characteristics. A comprehensive analysis of the angular dependence for Yb2 is provided in Figures S1 and S2 of SM [59]. This  $1/\cos\theta$  behavior strongly suggests the presence of cylindrical Fermi sheets in YbTi $_3$ Bi $_4$ .

To better understand the electronic properties of YbTi $_3$ Bi $_4$  and explain experimental observation, we performed electronic band structure and FS calculations using *ab initio* DFT. Figure 3 displays the electronic band structure of YbTi $_3$ Bi $_4$  along the high-symmetry direction shown in the inset. Our electronic bands look similar to previous reports [42,43,67] on LnTi $_3$ Bi $_4$ . The band structure reveals intriguing features, such as dispersionless flat bands at **A** and **X**, located around

TABLE I. Physical parameters of Yb1 and Yb2: the frequency ( $F$ ), FS area ( $S_F$ ), Fermi wave vector ( $k_F$ ), effective mass ( $m^*$ ), Fermi velocity ( $v_F$ ), Dingle temperature  $T_D$ , quantum relaxation time ( $\tau_s$ ), mean-free path ( $\ell_{2D}$ ), and quantum mobility ( $\mu$ ), characterizing the dHvA oscillations of YbTi<sub>3</sub>Bi<sub>4</sub>.

Sample	$F$ (T)	$k_F$ ( $\text{\AA}^{-1}$ )	$S_F$ ( $\text{\AA}^{-2}$ )	$m^*/m_o$	$v_F$ ( $10^5 \text{ ms}^{-1}$ )	$T_D$ (K)	$\tau_s$ ( $10^{-12} \text{ s}$ )	$\ell_{2D}$ (nm)	$\mu$ ( $\text{m}^2\text{V}^{-1}\text{s}^{-1}$ )
Yb1	142	0.065	1.354	0.135	5.612	8.97	0.135	7.57	0.176
Yb2	145	0.066	1.383	0.102	7.506	11.93	0.101	7.61	0.175

0.36 eV and 0.6 eV below the Fermi level, as highlighted by dashed arrows. Additionally, van Hove singularities (VHS) are present near **Y**, as indicated by arrows. Dirac-like crossings are observed near **A** and **X**, marked by dotted circles. Several bands cross the Fermi level, confirming the metallic nature of YbTi<sub>3</sub>Bi<sub>4</sub>.

There are five bands that cross the Fermi level and contribute to the FS. Figure 4 shows the band-resolved FS of YbTi<sub>3</sub>Bi<sub>4</sub>. The FS consists of five sheets originating from Bands 7, 8, 9, 10, and 11. The FSs of Bands 7, 8, and 9 are located at the corners of the Brillouin zone, while that of Band 10 is at the  $\Gamma$  point, and all of them appear cylindrical. Band 11 has two concavelike sheets facing upward and downward. These FS pockets resemble those in other V-based AV<sub>3</sub>Sb<sub>5</sub> ( $A = \text{Cs, K, Rb}$ ) and Ti-based CsTi<sub>3</sub>Bi<sub>5</sub> Kagome systems [68,69]. The nearly two-dimensional nature of the FS indicates strong in-plane bonding and weak interlayer coupling in this material.

Figure 5(a) shows the Fermi surface of Band 7, Band 8, and Band 9 that are present at the Brillouin zone boundary. The presence of cylindrical FS sheets is consistent with the nearly  $1/\cos\theta$  dependence of the frequency peaks in Fig. 2(d). We computed theoretical frequencies using the Onsager relationship [58]. We used the SKEAF code [70] to extract the theoretical frequencies from the FS cross-sectional area. Figures 5(b) and 5(c) present the frequencies derived from all FS sheets of YbTi<sub>3</sub>Bi<sub>4</sub>.

As shown in the graph, the FS of Band 7 contributes smaller frequencies of 150 T and 300 T compared to other

bands; thus, it is plotted separately in Fig. 5(b). Additionally, the FS of Band 7 contributes the smallest frequency, approximately 170 T, which is also plotted separately in Fig. 5(b). As illustrated in Fig. 4, Band 10 exhibits a large cylindrical FS, resulting in a high frequency of 20 000 T. Similarly, the FSs of Bands 8 and 9 are cylindrical near the Brillouin zone boundary [Fig. 5(a)], contributing frequencies of approximately 2000 T and 5500 T, respectively, as shown in Fig. 5(c). The frequency associated with the FS of Band 11 is around 2000 T and decreases at higher  $\theta$  values. Theoretical frequencies (except for Band 11) increase nearly parabolically with  $\theta$ , consistent with expectations for cylindrical FSs.

For comparison with theoretical frequencies, we also included experimental frequencies derived from dHvA oscillations. In our dHvA data, we observed a major peak near  $F_\delta \sim 130$  T. As shown in Fig. 5(b),  $F_\delta$  and another peak near  $F_\epsilon \sim 300$  T are consistent with the theoretical frequencies derived from the Fermi pocket of Band 7. Furthermore,  $F_\delta$  and  $F_\epsilon$  values extracted from Yb1 and Yb2 are comparable to the frequencies derived from Band 7, and they exhibit nearly the same angular dependence. To identify potential high-frequency signals in YbTi<sub>3</sub>Bi<sub>4</sub>, as predicted by theoretical calculations, we performed careful background subtraction and detected faint high-frequency signals near  $F_\chi \sim 1900$  T and  $F_\lambda \sim 5600$  T, as shown in Fig. S3 in SM [59]. These high frequencies were observed in both Yb1 and Yb2, confirming their intrinsic nature. As illustrated in Fig. 5(c), the values of  $F_\chi$  and  $F_\lambda$  are comparable to the theoretical frequencies derived from Band 8 (or Band 11) and Band 9,

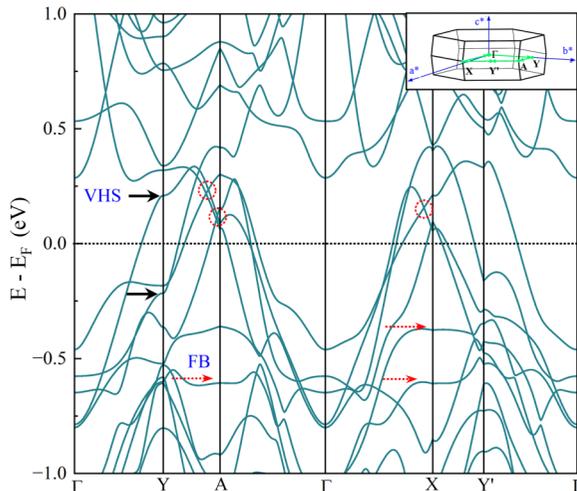


FIG. 3. Electronic band structure of YbTi<sub>3</sub>Bi<sub>4</sub>. The flat band, van-Hove singularity (VHS), and Dirac point near the Fermi level are denoted by the dashed-arrows, solid arrows, and dotted circles, respectively. Inset: Brillouin zone with high-symmetry  $k$  path.

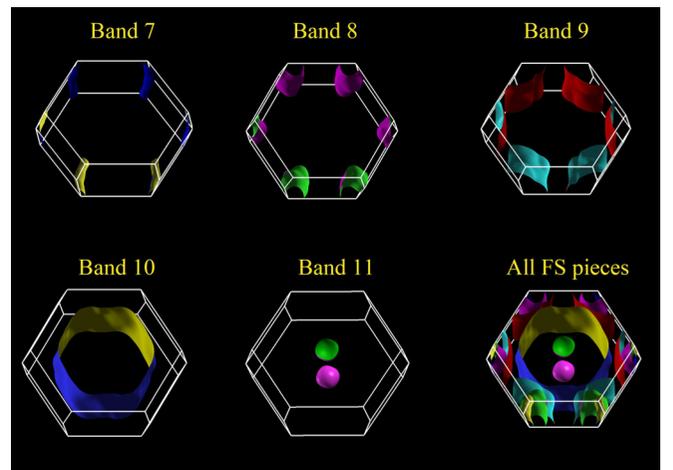


FIG. 4. Band-resolved Fermi surface (FS) pockets of YbTi<sub>3</sub>Bi<sub>4</sub>. There are five bands: Band 7, Band 8, Band 9, Band 10, and Band 11 contribute to the FS of YbTi<sub>3</sub>Bi<sub>4</sub>. The last graph is the combined FS contributions from all bands.

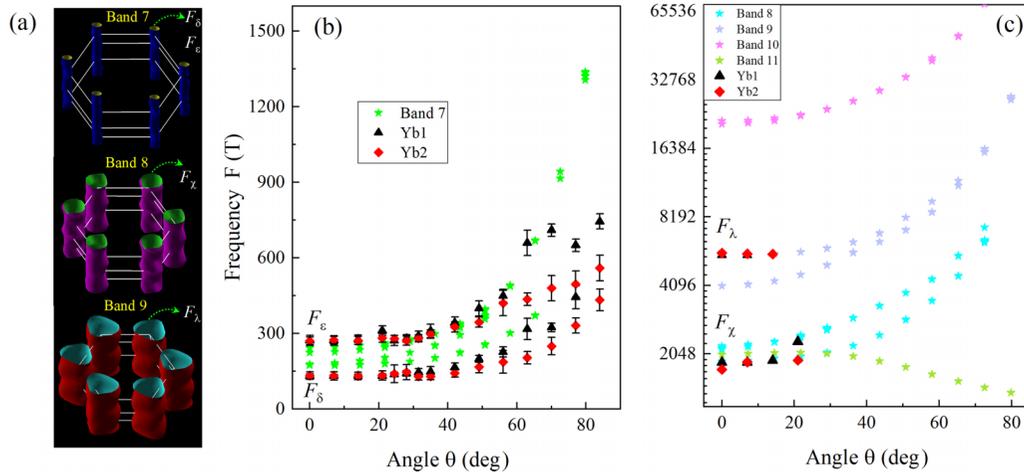


FIG. 5. (a) Fermi pockets for Bands 7, 8, and 9, showing their overall appearance. These pockets appear as deformed cylindrical shapes. (b) Comparison of experimental frequencies from dHvA oscillations with theoretical frequencies derived from the Fermi surface (FS) pocket of Band 7 for  $\text{YbTi}_3\text{Bi}_4$ . Solid circles and open triangles represent theoretical and experimental frequencies, respectively. (c) Frequencies calculated from the FS sheets of Bands 8, 9, 10, and 11 for  $\text{YbTi}_3\text{Bi}_4$ . The frequencies increase nearly parabolically, as expected for cylindrical FSs, except for Band 11, where the frequency decreases at higher angles. The y axis is presented on a logarithmic scale for better data visibility.

respectively.  $F_\chi$  and  $F_\lambda$  are tiny signals and they are overshadowed by  $F_\delta$ ; therefore, we could not resolve them above  $\theta = 21^\circ$ . Increasing the magnetic field strength could improve the signal-to-noise ratio, potentially allowing for clearer resolution of these high-frequency peaks.

#### IV. SUMMARY

To summarize, we performed high-field torque magnetometry on the newly discovered Ti-based kagome material  $\text{YbTi}_3\text{Bi}_4$ . The torque signal exhibited well-defined de Haas–van Alphen (dHvA) oscillations, with a prominent peak  $F_\delta$  around 140 T. By analyzing both angular and temperature-dependent dHvA oscillations, we extracted several key physical parameters that characterize the Fermi surface (FS) of  $F_\delta$ . The observation of the characteristic forward-leaning sawtoothlike dHvA oscillations, combined with the  $1/\cos\theta$  dependence of the dHvA signal, provides conclusive evidence for the presence of two-dimensional Fermi pockets in  $\text{YbTi}_3\text{Bi}_4$ .

In addition, we employed *ab initio* density-functional theory (DFT) calculations to explore the electronic band structure and FS of  $\text{YbTi}_3\text{Bi}_4$ . The electronic band structure revealed several intriguing features, including multiple Dirac points, van Hove singularities, and flat bands near the Fermi level. Five electronic bands intersect the Fermi level, contributing to a FS composed of quasi-2D cylindrical Fermi sheets. Theoretical frequencies derived from the Fermi surface of Band 7 are comparable to  $F_\delta$  and exhibit a similar angular dependence. However, the frequencies derived from the Fermi surfaces of other bands are much higher, of the order of several kilo teslas. With the careful background subtraction in the dHvA oscillation, we could detect the additional frequency peaks near 1900 T and 5600 T, which are present in both measured samples Yb1 and Yb2, and are consistent with the theoretical frequencies derived from the Fermi pocket of 8 (or Band 11) and Band 9, respectively. These high-frequency peaks are very

tiny and these signals quickly disappeared at higher tilt angles above  $21^\circ$ .

We noticed that  $F_\delta$  splits at higher tilt angles ( $\theta$ ) above  $60^\circ$  [Fig. 2(c)] and this splitting is clearly visible in the color plot [Fig. 2(d)]. A similar splitting is also seen in another sample, Yb2, as shown in Fig. S2 SM [59]. This splitting is likely due to the contribution of different extremal orbits to the dHvA oscillations. In contrast to other kagome systems, such as  $\text{AV}_3\text{Sb}_5$  and  $\text{ATi}_3\text{Bi}_5$ , the kagome lattice formed by Ti atoms in  $\text{YbTi}_3\text{Bi}_4$  exhibits slight buckling. The Fermi pockets in this system also show a deformed, cylindrical-like shape with varying cross-sectional areas [see Fig. 4 and Fig. 5(a)]. As the tilt angle  $\theta$  increases, the cyclotron orbit changes, leading to slightly different frequencies corresponding to the varying orientations of the Fermi surface.

Interestingly, our torque measurements reveal a forward-leaning triangular sawtoothlike wave-form pattern, strongly suggesting the presence of a quasi-2D Fermi surface. The angular dependence of  $F_\delta$  follows a  $1/\cos\theta$  dependence, which further supports the quasi-2D nature of the Fermi surface in  $\text{YbTi}_3\text{Bi}_4$ . These experimental findings are reinforced by the observation of cylindrical Fermi pockets and, importantly, the excellent agreement between the theoretical frequencies calculated from density-functional theory (DFT) and the experimental dHvA frequencies. The combined experimental and computational results for  $\text{YbTi}_3\text{Bi}_4$  provide valuable insights into its electronic properties and will be crucial for understanding similar systems, including other members of the  $\text{LnTi}_3\text{Bi}_4$  ( $\text{Ln} = \text{Lanthanide}$ ) and other titanium- and vanadium-based kagome compounds.

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