

de Haas–van Alphen study of the Dirac nodal-line semimetal candidate TaPtTe₅Maximilian Daschner^{1,2,*} and F. Malte Grosche^{1,†}¹*Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom*²*Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany*

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We report a quantum oscillation study in the Dirac nodal-line semimetal candidate TaPtTe₅. The Fermi surface is probed via magnetic torque measurements with the magnetic field applied in the crystallographic *a-b* and *b-c* planes. The experimentally determined de Haas–van Alphen frequencies are consistent with results from band-structure calculations. This study serves as an extension to the scarce quantum oscillation data on TaPtTe₅ currently present in the literature.

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I. INTRODUCTION

Ever since the classification of topological phases according to the tenfold way [1], the dimensionality of a system has become a central aspect in its study. Albeit being gapless phases, Dirac and Weyl semimetals fall into the field of topological materials, and have proven to show intriguing physics such as the chiral anomaly [2,3] or Fermi arcs [4]. Candidates for Dirac and Weyl semimetals are, e.g., layered transition metal tellurides such as the family XYTe₄ (*X* = Nb, Ta; *Y* = Ir, Rh) [5–11].

More recently, so-called nodal-line semimetals (NLSMs) have gained attention as well. Such NLSMs form band crossings along a line instead of just single points in reciprocal space. The most prominent family hosting Dirac nodal lines, ZrXY (*X* = Si, Ge; *Y* = S, Se, Te) [12–21], has shown experimental signatures not present in conventional nodal-point Dirac/Weyl semimetals such as butterfly-shaped magnetoresistance [21] or unconventional mass enhancement [17]. The structural similarities and intricate topological properties present in ternary transition metal tellurides motivate further investigations of such systems. A fairly novel candidate that falls into that category is the quasi-one-dimensional nonmagnetic family of compounds TaXTe₅ (*X* = Ni, Pd, Pt) [22–39], whose low dimensionality was investigated in transport and spectroscopy measurements.

In this work, we examine one representative of this family, TaPtTe₅. The de Haas–van Alphen (dHvA) oscillations in TaPtTe₅ have been previously reported for fields along the crystallographic *b* axis [39], but a more comprehensive determination of its electronic structure has been lacking. Here, we

report a full rotation study of dHvA oscillations in TaPtTe₅ for fields in the *a-b* and *b-c* planes. Our electronic structure calculations within density functional theory (DFT) suggest fourfold degenerate nodal lines in the *k_z* = ± π /*c* plane of the Brillouin zone. We compare the dHvA oscillation frequencies extracted from the numerically predicted electronic structure to experimentally determined dHvA frequencies. Our findings suggest that the Fermi surface of TaPtTe₅ includes a small cylindrical pocket that encloses a nodal line in the *k_z* = ± π /*c* plane.

II. METHODS

Single crystals of TaPtTe₅ were grown via the self-flux growth method using Te as flux following Xiao *et al.* [38]. Ta powder (Alfa Aesar: 99.95%), Pt fragments cut off from an ingot (Produits Artistiques Métaux Précieux: 99.95%), and Te lumps (Alfa Aesar: 99.999%) were mixed together at a molar ratio of Ta:Pt:Te = 1:1:10 inside an Ar-filled glove box. The mixture is placed inside an alumina crucible which is then put inside an evacuated quartz ampoule. It is then heated in a muffle furnace with the temperature profile described in Refs. [38,39], after which crystals are extracted mechanically. The energy-dispersive x-ray spectrum (EDS) and a scanning electron microscope (SEM) image of a typical crystal are shown in Appendix A.

Among the crystals in each growth, the majority are alien phases such as TaTe₂, TaTe₄, TaPt₂, PtTe₂, or Te as reported in the literature [37], where only a small fraction (~1%) of the crystals in the batch turned out to be TaPtTe₅. EDS was used to distinguish the latter from other phases, however, the shape was often enough to visually filter out most unwanted crystals. The obtained TaPtTe₅ crystals are air stable and grow in shiny gray flattened needlelike shapes. The residual resistance ratio (RRR) resulted in $\rho(298\text{ K})/\rho(1.6\text{ K}) \approx 13$ which is close to the value of RRR ≈ 15 reported before [39].

Magnetic torque measurements were conducted with homemade piezoresistive cantilevers read out through a Wheatstone bridge via a lock-in amplifier. Cryogenic temperatures were reached using a custom-designed cryostat by

*Contact author: md867@cam.ac.uk,
maximilian.daschner@lmu.de

†Contact author: fmg12@cam.ac.uk

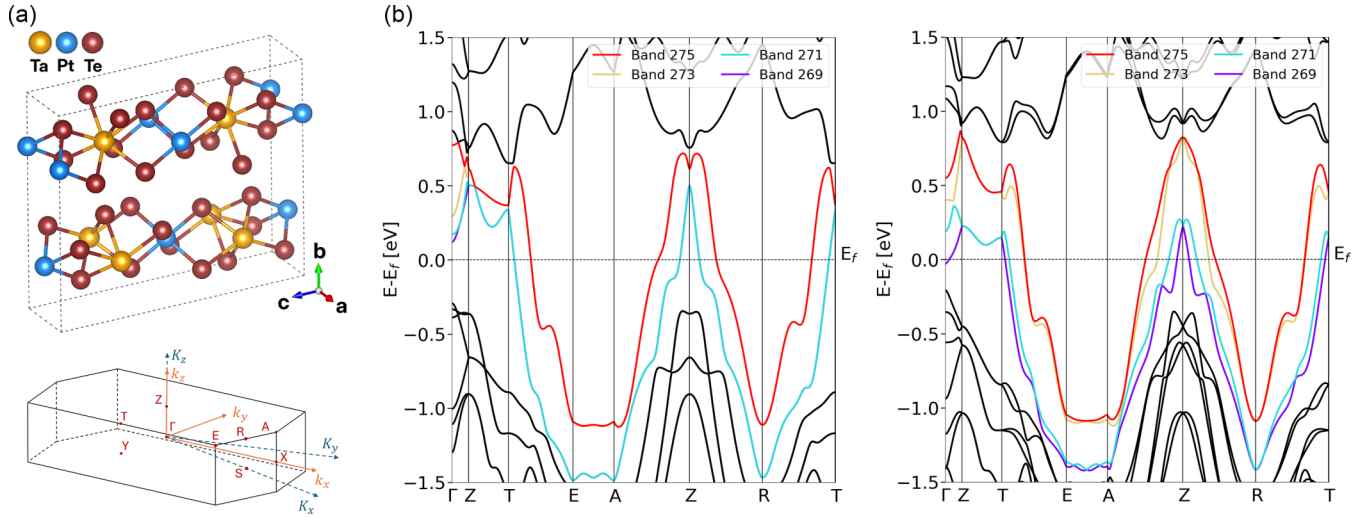


FIG. 1. (a) Crystal structure of TaPtTe₅ where the unit cell is indicated by dashed lines, and the corresponding Brillouin zone. Lowercase k_n ($n = x, y, z$) point in conventional unit cell vector directions, while uppercase K_n are the reciprocal lattice vectors that represent the periodicity of the Brillouin zone. (b) Band structure without (left) and with (right) spin-orbit coupling in TaPtTe₅ with all high-symmetry points chosen in the plane at which $k_z = \pm\pi/c$ (except Γ). Spin-degenerate partners for each band are labeled with even numbers (not shown here). When SOC is excluded, all bands show fourfold degeneracy, and the $k_z = \pm\pi/c$ plane can thus be viewed as a nodal surface. Upon including SOC, the degeneracy is lifted (spin degeneracy remains) in most of the $k_z = \pm\pi/c$ plane, but remains along the Z-T high-symmetry line and in the high-symmetry point R. The observations are independent of the energy, i.e., nodal lines and nodal points form at all energies in these high-symmetry regions.

Oxford Instruments with fields of up to 15 T. All measurements were performed at the base temperature of 1.6(1) K.

To gain insights into the electronic structure of TaPtTe₅, we performed DFT calculations using WIEN2K [40] with the same parameters as chosen in Ref. [23]. The generalized gradient approximation (GGA) based on the Perdew-Burke-Ernzerhof (PBE) exchange-correlation potential [41] was used. The atomic sphere radii (muffin-tin radii) were chosen as $R_{\text{mt}} = 2.5$ a.u. for Ta and Pt atoms and $R_{\text{mt}} = 2.43$ for all Te atoms. The plane-wave cutoff parameter was chosen as $R_{\text{mt}}K_{\text{max}} = 8$, where R_{mt} is the smallest atomic sphere radius in the unit cell and K_{max} is the magnitude of the largest k vector. Calculations were performed on a $59 \times 59 \times 13$ k -point mesh in the full Brillouin zone for the band-structure calculations shown here. The dHvA frequencies were extracted using the supercell K-space extremal area finder (SKEAF) [42,43], while Fermi-surface plots were generated with PY_FS [44].

III. AB INITIO CALCULATIONS

TaPtTe₅ crystallizes in an orthorhombic layered structure with space-group $Cmcm$ (No. 63), with lattice constants $a = 3.729(4)$ Å, $b = 13.231(11)$ Å, and $c = 15.452(10)$ Å as shown in Fig. 1(a), and was reported to exhibit Pauli paramagnetism [37]. The unit cell consists of two TaPtTe₅ layers, where each layer can be described as a series of bi-capped trigonal prismatic TaTe₅ chains stuck together with Pt atoms. The TaPtTe₅ layers are stacked by shifting them along the a axis by half a lattice vector with respect to each other.

The numerical analysis here follows [38], and will be used to interpret experimental results from quantum oscillation measurements. Figure 1(b) illustrates the resulting band structure without and with spin-orbit coupling (SOC) with all high-symmetry points chosen in the plane at which $k_z = \pm\pi/c$ (except Γ). In the case without spin-orbit coupling, one can clearly see two-band degeneracies (fourfold if spin for each band is included) whose degeneracy is only lifted away from the $k_z = \pm\pi/c$ plane as illustrated on the Γ -Z high-symmetry line. The $k_z = \pm\pi/c$ plane can therefore be referred to as a nodal surface. Here, the labels only include one band since their spin-degenerate partners are identical due to the presence of $\mathcal{PT}$ symmetry across the whole Brillouin zone. When SOC is included, the two-band degeneracies in this plane are mostly lifted (spin degeneracy still remains) except at the high-symmetry line Z-T and in the high-symmetry point R. To get a better overview of all the nodal lines away from the high-symmetry regions, we visualize the four bands that cross the Fermi energy and hence contribute Fermi pockets to dHvA oscillations in Appendix B for the whole $k_z = \pm\pi/c$ plane (including spin-orbit coupling). The energetic difference between those bands clearly shows the presence of band crossings. The nodal line along Z-T is protected from spin-orbit coupling by the crystal symmetries, which was shown theoretically for this and other materials in the same symmetry group ($Cmcm$) (see e.g. TaNiTe₅ [33], TaPtTe₅ [38], LaNiGa₂ [45], and Th₂BC₂ [46]).

IV. RESULTS AND DISCUSSION

Quantum oscillation measurements in the magnetic torque τ in an external field $\mathbf{B}$ can be captured via the relation

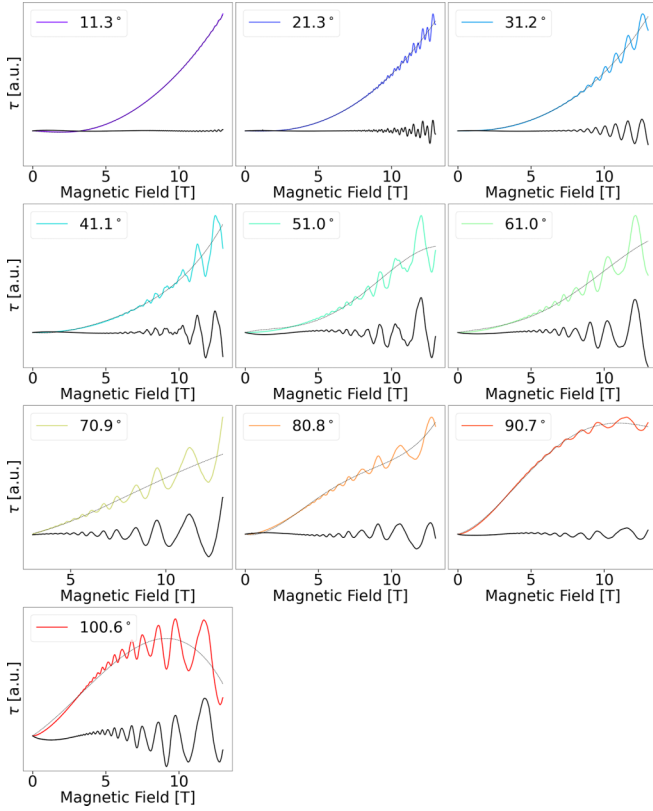


FIG. 2. Magnetic torque of a TaPtTe₅ sample rotated in the b - c plane measured up to 13 T. The whole dataset was fitted with a fourth-degree polynomial (dashed black line), and the background-subtracted data are given as a solid black line. 0° corresponds to the magnetic field being aligned with the c axis.

[47]

$$\tau = CB^{3/2} \sum_i \frac{dF_i}{d\theta} \left| \frac{\partial^2 A_i}{\partial k_{\parallel}^2} \right|^{-1/2} \sum_{p=1}^{\infty} p^{-3/2} R_D R_T R_S \times \sin \left[2\pi p \left(\frac{F_i}{B} - \gamma \right) \pm \delta \right], \quad (1)$$

where C is a field-independent constant, θ is the angle between the extremal area A and the magnetic field, while $k_{\parallel}$ is the wave vector parallel to $\mathbf{B}$. The indices i and p range over all orbits and higher harmonics, respectively. R_D , R_T , and R_S are various damping terms arising from finite electron lifetime, finite temperature, and spin splitting, respectively. The phase shift γ arises from the topological properties of the semimetal and is often approximated with $\gamma = \frac{1}{2} - \frac{\phi_B}{2\pi}$ with Berry phase ϕ_B , while δ depends on the dimensionality of the Fermi sheet. To find the frequency F one can use the Onsager relation

$$F = \left(\frac{\hbar}{2\pi e} \right) A, \quad (2)$$

where A is the extremal area of an orbit, while $\hbar$ and e are the reduced Planck constant and the electron charge, respectively.

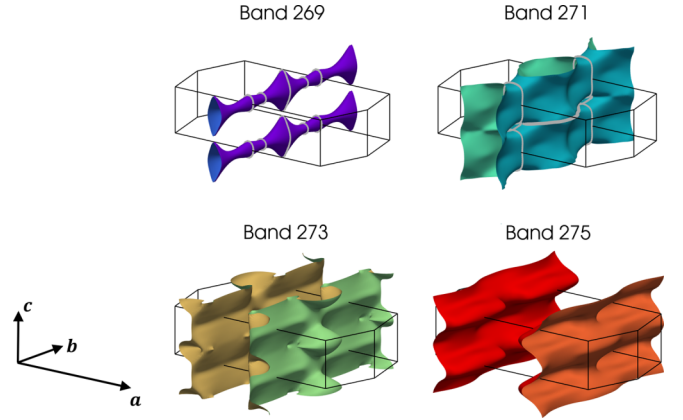


FIG. 3. Fermi sheets for TaPtTe₅ with the Fermi level shifted to lower energies by 20.4 meV. Extremal orbits are shown for the magnetic field along a , b , and c as gray lines in the first Brillouin zone.

A. dHvA frequencies

The dHvA oscillations in the magnetization were investigated by Jiao *et al.* [39] up to 7 T with the magnetic field along the crystallographic b axis. The authors performed a mass study and found two fundamental frequencies at $F = 63.5$ T and $F = 95.2$ T with light effective masses of $m = 0.108m_e$ and $m = 0.119m_e$, respectively. Although DFT calculations were also performed, the dHvA data consisting of only two frequencies along one crystallographic axis are not sufficient to verify such calculations with high accuracy, and thus a more thorough investigation to higher fields, and along multiple crystallographic axes is required.

An overview of magnetic torque measurements performed here with the external magnetic field $\mathbf{B}$ applied in the b - c plane is shown in Fig. 2. The nonlinear background, mostly induced by the inhomogeneity of the piezoresistive cantilever, is corrected by subtracting a fourth-degree polynomial. In Appendix C, additional data obtained on a different cantilever with the magnetic field of up to 15 T are provided together with respective fast Fourier transforms (FFTs). The raw data for field sweeps with $\mathbf{B}$ in the a - b plane and its respective FFT spectrum are also included.

Due to the lack of data at temperatures above the base temperatures of the cryostat, no effective masses or Dingle temperatures could be extracted reliably. The angles were determined from the torque caused by the weight of the sample in zero field. The extracted frequency peaks are shown in Fig. 4. Note that quantum oscillations in the a - b and b - c planes were measured separately. In each plane, frequencies measured at angles below 0° and above 90° were folded back into the 0°–90° range due to the periodicity of the crystal.

To compare these experimental findings with results obtained from DFT calculations, the band structure can be used to extract the Fermi surface as shown in Fig. 3. Extremal areas with respect to the magnetic field direction are indicated by gray lines and allow one to find the frequency expected from dHvA oscillations via the Onsager relation. Only two

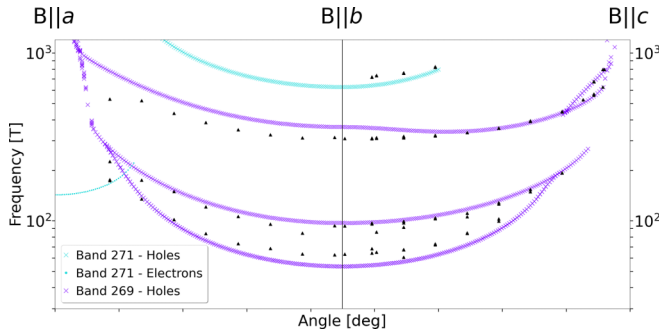


FIG. 4. de Haas–van Alphen frequencies in the magnetic torque as a function of angle in the a - b and b - c planes for a TaPtTe₅ sample (black triangles). Results from DFT calculations are included as colored points (electronlike orbit) and crosses (holelike orbit). Ticks on the x axis correspond to steps of 20°.

bands (band 269 and 271) possess closed orbits and contribute dHvA frequencies. A good match between calculated and observed dHvA frequencies was obtained by moving the band edges of band 269 and 271 by 20.4 meV. The other two bands (273 and 275) may shift in the opposite direction for overall charge neutrality, or slight off-stoichiometry could cause a change in band filling. The extracted frequencies as a function of angle are included in Fig. 4 and show consistency with the experimental values. Band 269 contributes multiple holelike frequencies due to its irregular shape, which diverge as the magnetic field deviates from the b axis in line with the behavior expected from quasicylindrical Fermi surfaces. This Fermi sheet is particularly interesting because it wraps around the nodal line Z - T in the $k_z = \pm\pi/c$ plane. Band 271 shows an electronlike frequency branch with its center on the a axis, and a holelike frequency branch with its center on the b axis.

Overall, the dHvA oscillations seem to agree well with the DFT calculations, which confirms the numerical results that form the basis for Appendix B and provides indirect evidence for the existence of such Dirac nodal lines.

B. Phase analysis

The phase shift measured in quantum oscillations can in principle allow one to obtain information about the topological properties of a material [48], if it can be extracted reliably and other nontopological contributions can be ruled out.

Regarding the phase shifts in TaPtTe₅, we expect to obtain a nonzero Berry phase for the Fermi surface arising from band 269 as it surrounds the nodal line along Z - T [49]. All three branches from band 269 shown in Fig. 4 should in principle return such a nontrivial phase shift when the magnetic field is aligned with the b axis. Jiao *et al.* [39] did indeed find nonzero Berry phase shifts for the lowest two hole branches of band 269. The accuracy of these results is, however, questionable, since the magnetic fields used to measure dHvA oscillations did not exceed 7 T and are thus far below the quantum limit even for the lowest frequency at 63.5 T. The quantum limit is reached when the external magnetic field approaches the

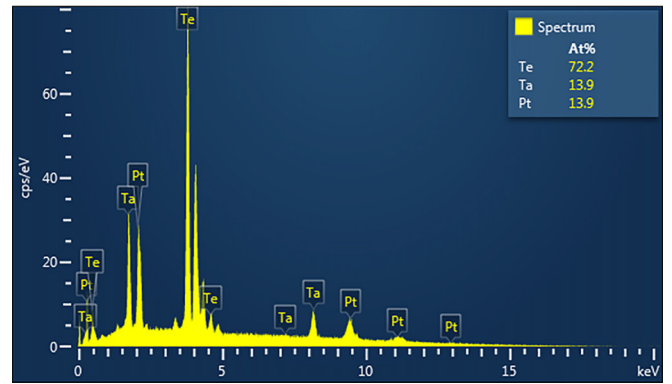
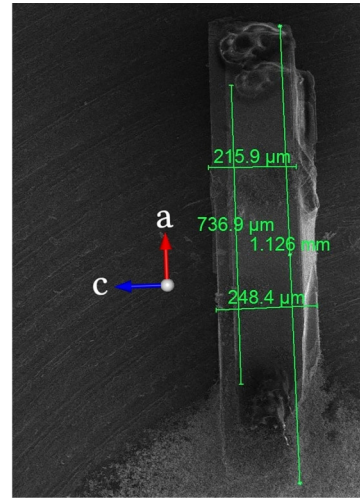


FIG. 5. Top: Close-up scan in a SEM of a TaPtTe₅ sample. The sample is attached to a metallic pin with conductive silver epoxy at the bottom such that no charging effects occur during SEM operation. Furthermore, small dots of silver epoxy can be seen on the sample where gold wires were attached for transport measurements (not shown in this work). Bottom: EDS results for a TaPtTe₅ sample. The spectrum confirms that the atomic ratio is close to Ta:Pt:Te = 1:1:5.

frequency of a cyclotron orbit. The uncertainty regarding the phase shift is evident in the fact that direct fits of the quantum oscillation amplitude and evaluation of Berry phase shifts using Landau fan diagrams are inconsistent with each other in the study performed by these authors.

Furthermore, Ref. [39] find different phase shifts for the two frequency branches, despite the fact that both encircle the same nodal line and arise from the same band. Besides that, Berry phases are difficult to interpret as other, nontopological, effects can also lead to a phase shift of π (see, e.g., spin splitting [50] and other effects [51]).

Attempts to extract the phase shift from the data presented in this work show similar uncertainty. Besides the low magnetic fields used in the measurements, the multioscillation nature of TaPtTe₅ introduces additional difficulty when extracting such phases. To determine the topological nature of this material, higher magnetic fields are therefore necessary.

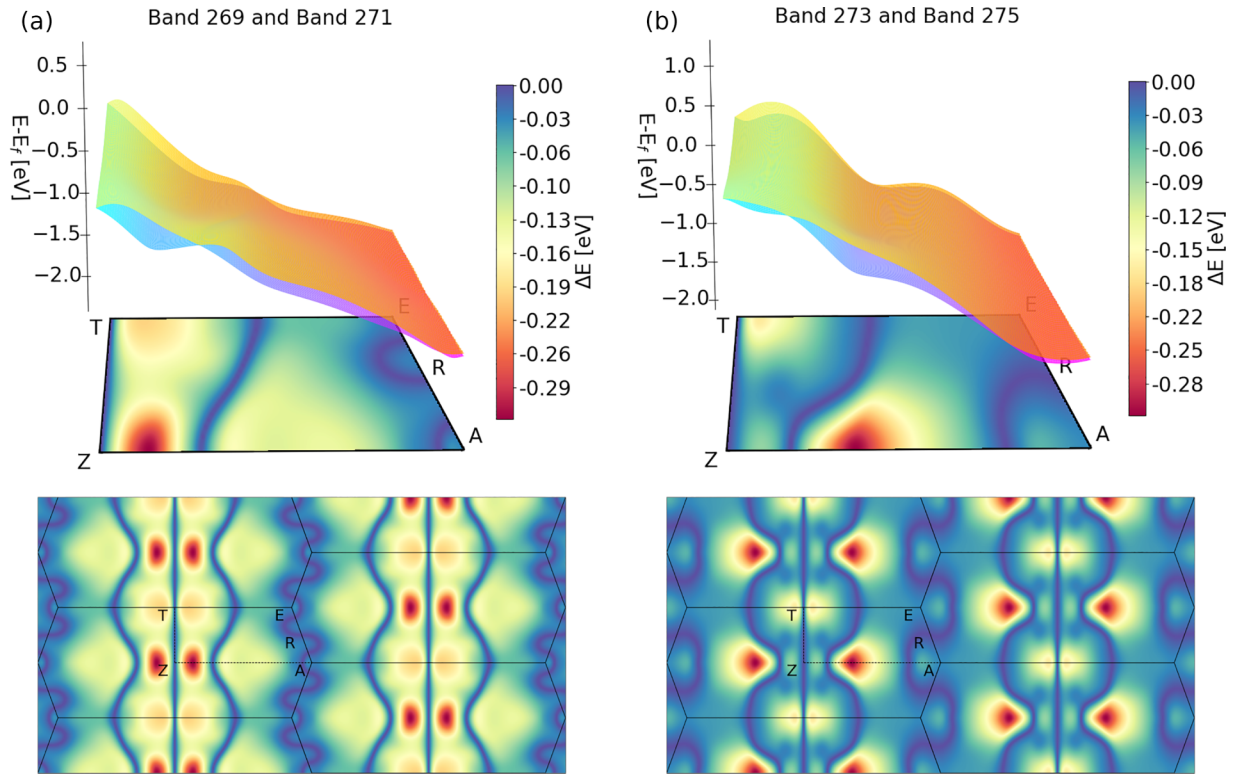


FIG. 6. Band structure in TaPtTe₅ in the $k_z = \pm\pi/c$ plane including SOC with (a) illustrating band 269 and band 271, and (b) illustrating band 273 and band 275. The energetic difference between two bands is shown in the contour plots below. For better visualization, the contour plot is extended to multiple Brillouin zones. One can clearly distinguish three nodal lines in both cases: one straight line in Z - T , one curve that does not intersect any high-symmetry points, and one curve along the Brillouin zone boundary connecting the high-symmetry points in R . Crystal symmetries protect the nodal line along Z - T and the nodal point in R . The numerical results shown here are consistent with those shown by Xiao *et al.* [38].

V. CONCLUSION

In this work we presented numerical results that show the existence of fourfold degenerate Dirac nodal lines in the $k_z = \pm\pi/c$ plane in the Brillouin zone of TaPtTe₅. After including spin-orbit coupling, this degeneracy is mostly lifted except at the high-symmetry line Z - T among others. The de Haas–van Alphen frequencies extracted from magnetic torque measurements allow to obtain a complete picture of the Fermi surface and hence indirectly confirm the band structure in this material. Particularly, the shape and size of the Fermi sheet arising from band 269 can be confirmed. Although the Berry phases cannot be reliably extracted from the data presented here or in the literature, high-field measurements should in principle be able to reach the quantum limit of the lowest-frequency branch arising from band 269, and confirm the presence of nontrivial Berry phases, and other signatures often found in Dirac semimetals.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: CHARACTERIZATION

Basic characterization of flux grown TaPtTe₅ samples are shown in Fig. 5. Needles with lengths of around 1 mm show good agreement with the stoichiometry of 1:1:5.

APPENDIX B: NODAL LINES IN THE $k_z = \pm\pi/c$ PLANE

Numerical illustration of band touching lines in the $k_z = \pm\pi/c$ plane shown in Fig. 6. These verify the existence of nodal lines in this material.

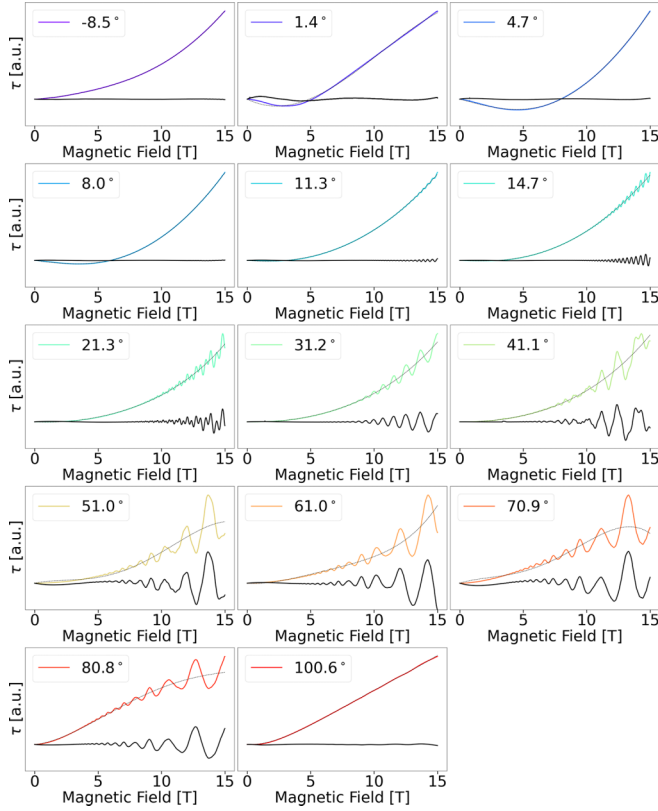


FIG. 7. Additional magnetic torque data for a TaPtTe₅ sample rotated in the b - c plane. The whole dataset was fitted with a fourth-degree polynomial (dashed black line), and the background-subtracted data are given as a solid black line. 0° corresponds to the magnetic field being aligned with the c axis. Although performed with the magnetic field in the same plane as given in Fig. 2, this dataset was acquired using a different piezoresistive cantilever which can explain the distinct background signal.

APPENDIX C: dHvA OSCILLATIONS IN THE MAGNETIC TORQUE

Together with Fig. 2, the data included in this Appendix form the basis for the frequency peaks shown in Fig. 4. Additional data in the b - c plane are given in Fig. 7, and fast Fourier transforms for both Figs. 2 and 7 are included in Fig. 8. Data for dHvA oscillations in the a - b plane are given in Fig. 9 with the respective FFT in Fig. 10.

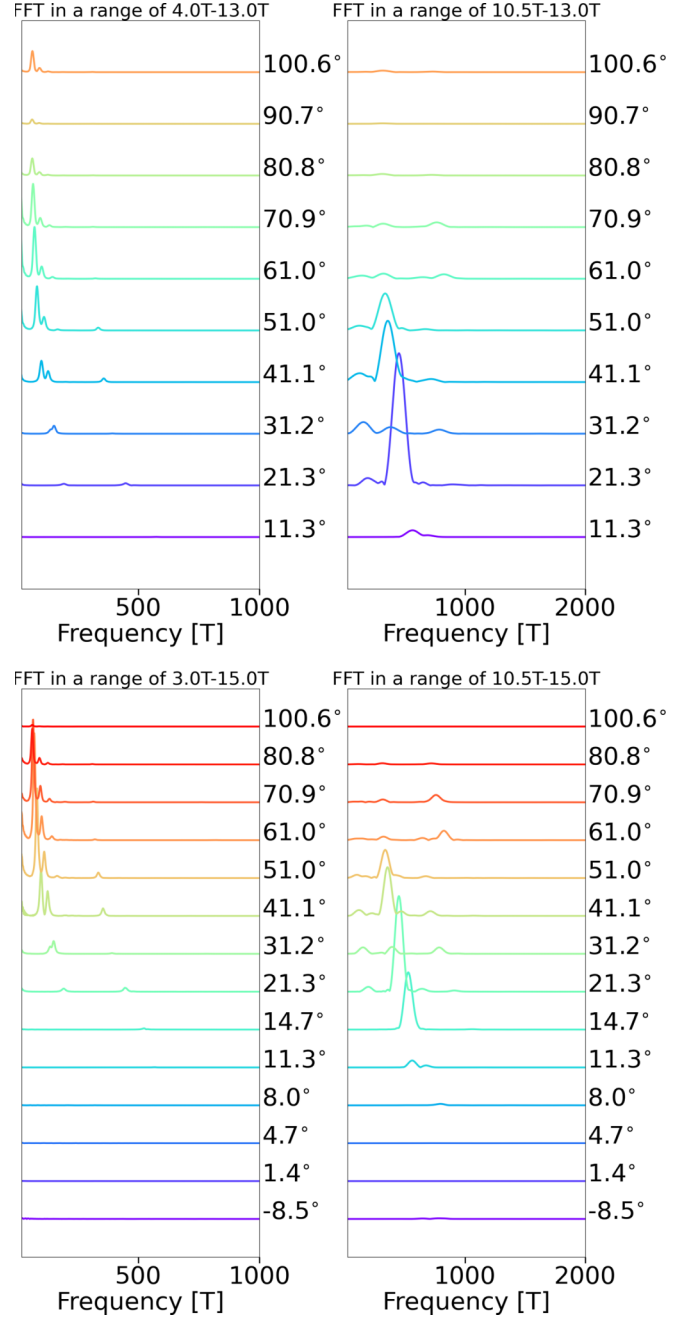


FIG. 8. Fast Fourier transform (FFT) for TaPtTe₅ in the b - c plane. 0° corresponds to the magnetic field being aligned with the c axis. The top row shows data from measurements up to 13 T (Fig. 2), while the bottom row shows data from measurements up to 15 T (Fig. 7).

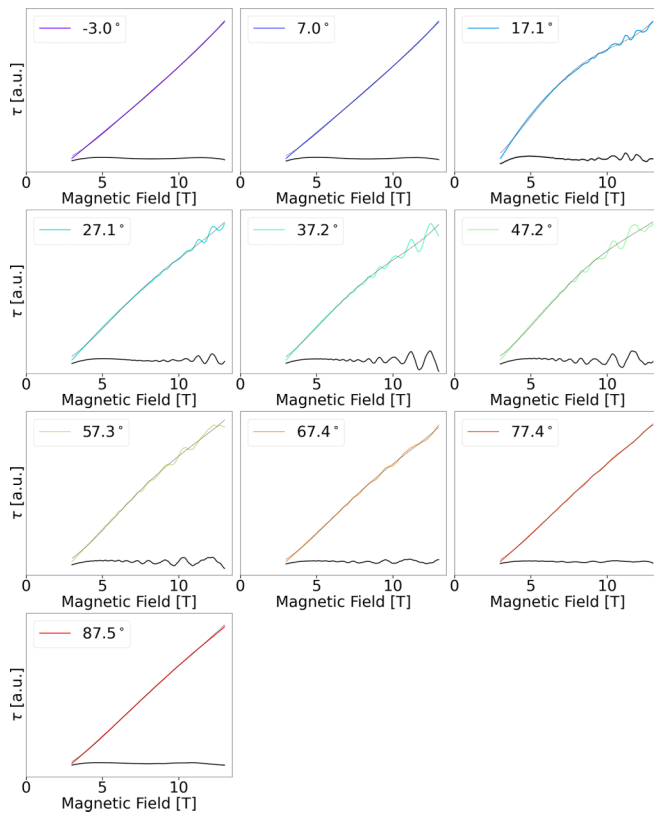


FIG. 9. Magnetic torque of a TaPtTe₅ sample rotated in the a - b plane. The whole dataset was fitted with a fourth-degree polynomial (dashed black line), and the background-subtracted data are given as a solid black line. 0° corresponds to the magnetic field being aligned with the a axis.

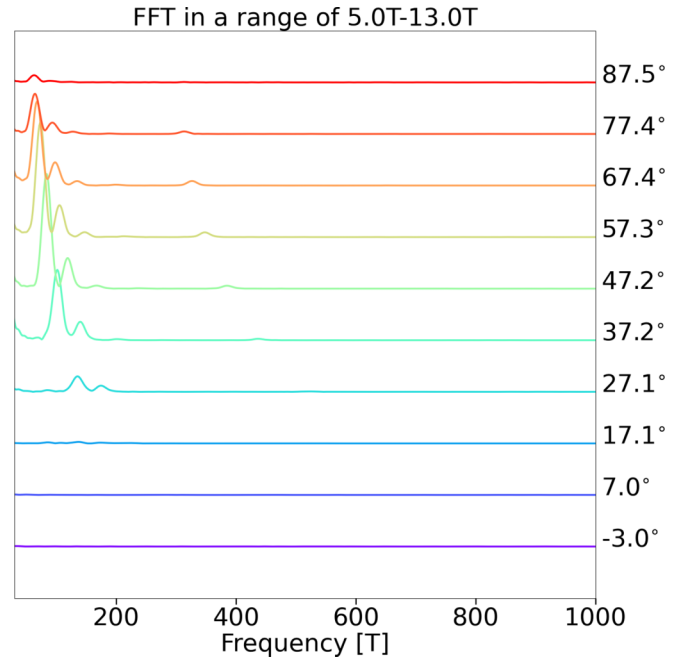


FIG. 10. Raw Fast Fourier Transform (FFT) for the data shown in Fig. 9 for TaPtTe₅ in the a - b plane. 0° corresponds to the magnetic field being aligned with the a axis.

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