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Evidence for Weyl fermions in a canonical heavy-fermion semimetal YbPtBi

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The manifestation of Weyl fermions in strongly correlated electron systems is of particular interest. We report evidence for Weyl fermions in the heavy fermion semimetal YbPtBi from electronic structure calculations, angle-resolved photoemission spectroscopy, magnetotransport and calorimetric measurements. At elevated temperatures where 4f-electrons are localized, there are triply degenerate points, yielding Weyl nodes in applied magnetic fields. These are revealed by a contribution from the chiral anomaly in the magnetotransport, which at low temperatures becomes negligible due to the influence of electronic correlations. Instead, Weyl fermions are inferred from the topological Hall effect, which provides evidence for a Berry curvature, and a cubic temperature dependence of the specific heat, as expected from the linear dispersion near the Weyl nodes. The results suggest that YbPtBi is a Weyl heavy fermion semimetal, where the Kondo interaction renormalizes the bands hosting Weyl points. These findings open up an opportunity to explore the interplay between topology and strong electronic correlations.
The presence of topologically non-trivial electronic band structures in condensed matter systems leads to a number of unusual consequences\(^1\). A rich variety of phenomena have been discovered in gapless topological materials, such as those exhibiting Dirac-fermion excitations near the points of linear crossings of bands close to the Fermi energy \(E_F\). The breaking of either spatial inversion symmetry or time reversal symmetry splits the degeneracy of the Dirac points, leading to a pair of topologically protected Weyl points\(^2,3\). Weyl fermions have been found to cause distinct experimental signatures, such as the chiral anomaly in transport measurements\(^4,5\), a topological Hall effect\(^6-11\), and Fermi arcs\(^12\).

Weyl fermions have mainly been studied in weakly correlated electron systems, while strong electronic correlations are frequently found to lead to novel electronic properties beyond those of simple metals or insulators, and heavy fermion systems are the prototype examples showing phenomena characteristic for strongly correlated electron systems. Here, due to strong Kondo coupling between the \(f\)-electron and conduction-band states, below the Kondo temperature \(T_K\), the electronic bands in the vicinity of \(E_F\) may become strongly renormalized, showing a strong \(f\)-character and a huge enhancement of the quasiparticle mass. When the chemical potential lies within the hybridization gap, insulating behavior is found at low temperatures in the topological Kondo insulators, such as has been proposed for SmB\(_6\), the resulting electronic structure is topologically non-trivial, again leading to conducting states on the surface\(^3,13-15\). It is therefore of particular interest to look for topological heavy fermion semimetals with gapless excitations, i.e. Weyl fermions in the presence of strongly renormalized bands. Such a Weyl–Kondo semimetal phase has been predicted from calculations based on the periodic Anderson model with broken inversion symmetry\(^16,17\). While it was proposed that Ce\(_3\)Bi\(_4\)Pd\(_3\) displays the low-temperature thermodynamic signatures of a Weyl–Kondo semimetal\(^11,16,18\), other signatures of Weyl fermions such as the chiral anomaly have not been reported. A Weyl heavy fermion state was also proposed for CeRu\(_3\)Sn\(_6\) from ab initio calculations\(^19\), but no experimental evidence for Weyl fermions has been demonstrated. Consequently, whether Weyl fermions exist in the presence of a strong Kondo effect needs to be determined experimentally. Furthermore, the influence of electronic correlations on Weyl fermions is to be explored, specifically how such a system evolves from high temperatures, where the \(f\)-electrons are well localized, to low temperatures where there is a strong Kondo interaction and a reconstruction of the electronic bands.

The cubic half-Heusler compounds (space group \(F43m\)) can be tuned by elemental substitution from trivial to topological insulators\(^20,21\). It was recently found that the half-Heusler GdPtBi, which has a strongly localized \(4f\)-electron shell, shows evidence for Weyl fermions in an applied magnetic field due to the presence of the chiral anomaly\(^22\) and topological Hall effect\(^9\). Here, we examine the isostructural compound YbPtBi. Although at high temperatures the Yb \(4f\)-electrons are localized similar to GdPtBi, upon cooling YbPtBi becomes a prototypical heavy-fermion semimetal\(^23-25\), where the enormous Sommerfeld coefficient of \(\gamma \approx 8 \text{ J mol}^{-1} \text{K}^{-2}\) demonstrates the enhanced effective mass of the charge carriers\(^23\). This compound is therefore highly suited to look for Weyl fermions, which are strongly affected by electronic correlations.

In this work, we report evidence for Weyl fermions in YbPtBi, where the bands hosting the Weyl points are strongly modified as the Kondo coupling strengthens at low temperatures. Electronic structure calculations and angle-resolved photoemission spectroscopy (ARPES) measurements indicate the presence of triply degenerate fermion points in the high-temperature regime, which will each split into a Weyl node and a trivial crossing in applied fields. At these temperatures, evidence for the chiral anomaly is revealed by field-angle-dependent magnetotransport measurements. As the temperature is lowered, the chiral anomaly is not detected in the magnetotransport, but experimental signatures of Weyl fermions are found in measurements of the specific heat. This is consistent with a greatly reduced Fermi velocity due to the influence of the Kondo effect on the electronic bands near the Weyl points. Furthermore, the observation of a topological Hall effect contribution, which can arise from the Berry curvature generated by the Weyl nodes, provides additional evidence for the existence of Weyl fermions at both low and elevated temperatures.

### Results

**ARPES and electronic structure calculations.** At higher temperatures, the band structure of YbPtBi can be calculated treating \(f\)-electrons as core states, as displayed in Fig. 1. The bulk Fermi surface consists of hole pockets centered at the \(\Gamma\)-point and electron pockets slightly away from \(\Gamma\). Along \(\Gamma-L\), the four-fold degenerate \(\Gamma_8\) state splits into two non-degenerate hole bands, and a pair of degenerate \(\Lambda_6\) electron bands, mainly consisting of Yb\(-t_{2g}\) and Bi-\(p\) orbitals. The \(\Lambda_6\) bands cross the two hole bands near \(E_F\), forming two triply degenerate fermion points\(^26\). Under a

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**Fig. 1** Existence of triply degenerate fermion points in the high-temperature phase of YbPtBi from DFT and ARPES. **a** Bulk band structure of YbPtBi from DFT calculations along the [111] direction. Blue curves are doubly degenerate \(\Lambda_6\) states, while the red and cyan curves represent the non-degenerate hole states. A comparison is shown between **b** ARPES measurements and **c** projected bulk band structure calculations, which are in good agreement. The comparison was made for the Yb-terminated (111) surface along the in-plane \(\Gamma - M\) direction (\([112]\)). The flat \(f\) bands at energies of \(-0.9\) and \(-2.1\) eV are the surface \(f\) bands from the topmost Yb layer (Supplementary Fig. 12), which are not taken into account by the bulk DFT calculations.
magnetic field, each triply degenerate point will further split into a Weyl point and a trivial crossing, with energies close to the bottom of the electron bands. The calculated bulk band structure with triply degenerate points is in good agreement with the ARPES results in Fig. 1b, which shows the energy–momentum dispersion relations along the surface ΓM direction. Note that the sample can only be cleaved well with the [111] orientation. Along this orientation, a symmetry-equivalent bulk TL direction projects on the surface ΓM direction at a slanted angle, allowing for the dispersion in the vicinity of the triply degenerate points to be revealed via a careful comparison with the projected bulk band structure calculations (Fig. 1c). Two hole bands crossing $E_F$ can be clearly identified in the ARPES experiments, as well as an additional electron band with a band bottom right below $E_F$. These experimentally observed bands are confirmed to be three-dimensional bulk bands based on their photon energy dependence, and they correspond well to the theoretical calculations. The direct observation of both electron and hole pockets and their close proximity with different group velocities confirms the existence of the triply degenerate fermion points near $E_F$, which is not affected by the slight discrepancy between the experimental results and calculations. This discrepancy is mainly related to the details of the separation and slope of the two hole bands, which could be caused by the limitations of frozen f-shell calculations and correlation effects not taken into account by the local density approximation. The good correspondence between ARPES measurements and density functional theory (DFT) calculations therefore provides evidence for Weyl fermions at elevated temperatures.

**Probing the chiral anomaly using magnetotransport.** Magnetotransport measurements were performed to look for the chiral anomaly associated with Weyl fermions (Fig. 2). Figure 2a–d show the field dependence of the resistivity of YbPtBi at selected temperatures with a current $I$ along [100] and a magnetic field $B$ applied parallel and perpendicular to $I$. For temperatures between 25 K and 170 K, the longitudinal magnetoresistance ($B \parallel I$) is positive at low fields but becomes negative in the higher field region, while the transverse magnetoresistance ($B \perp I$) is positive, which together are evidence for the chiral anomaly. The negative longitudinal magnetoresistance cannot be explained by either current jetting (Supplementary Fig. 2 and Supplementary Note 1), nor the sample anisotropy since similar behavior is found for other current directions (Supplementary Fig. 3). The negative longitudinal magnetoresistance above 20 K could be well fitted using a conductivity $\sigma(B) = (1 + c_\alpha B^2)\sigma_{WAL}$ (Fig. 2a–c, Supplementary Fig. 4 and Supplementary Note 2), where $c_\alpha$ is the chiral constant and $\sigma_{WAL} = a \Delta B$ is due to the weak antilocalization. As shown in Fig. 2e, the temperature dependence of $c_\alpha$ is well fitted with the expected behavior of $c_\alpha \propto \nu_F^2 \tau_c/(T^2 + \mu^2/\pi^2)$, where $\tau_c$ is the chirality-changing scattering time and $\mu$ is the chemical potential, yielding $\nu_F^2 \tau_c = 134 \text{ m}^2 \text{s}^{-1}$. The extracted $c_\alpha$ for various angles $\theta$ between $B$ and $I$ are displayed in Fig. 2i–h as a function of $B^2$, where the high field linear behavior indicates a $B^2$ contribution, while the very small $a$ values lead to a negligible component $\propto B^2$ (Fig. 2e). As displayed in Fig. 2i (and Supplementary Fig. 5), the extracted $c_\alpha(\theta)$ shows the expected angular dependence of $c_\alpha(\theta) \sim \cos^2 \theta$. Therefore, both the angle and temperature dependence of the magnetoresistance are highly consistent with the presence of a chiral anomaly in YbPtBi.

Meanwhile either by changing the Bi flux concentration or by Au doping, the carrier concentration can be tuned, as shown in Fig. 3. The Hall resistivity for various samples shows that more strongly hole-doped samples exhibit one band behavior with larger hole densities ($n_{h1}$), but upon electron doping, $E_F$ is shifted...
and eventually crosses the electron bands, leading to two band behavior (Fig. 3a, Supplementary Figs. 6, 7). As shown in Fig. 3b, c, in the vicinity of the crossover between one and two band behavior, the negative longitudinal magnetoresistance is most prominent. For more strongly electron-doped or hole-doped samples, no negative magnetoresistance is seen at elevated temperatures, indicating that this negative longitudinal magnetoresistance arises when $E_F$ is close to the Weyl points (Figs. 1a, 3d). Measurements of the transverse resistivity (with the voltage measured perpendicular to $I$) for fields rotated in the plane of the voltage drop and $I$ ($\rho_{\text{xy}}^{\text{PAMR}}$) provide an alternative method for probing the chiral anomaly, which is much less sensitive to spin scattering than the magnetoresistance (Fig. 3e–h). For two samples with evidence for the chiral anomaly in the magnetoresistance (S7 and S9), the oscillation amplitude of $\rho_{\text{xy}}^{\text{PAMR}}$ is greatly enhanced above 20 K, while this remains small for the more electron-doped sample, which is another signature of the chiral anomaly in samples where $E_F$ is near the band crossing. Interestingly, at 2 K the oscillations have very small amplitudes and are not sample dependent (Fig. 3f). This suggests that evidence for the chiral anomaly disappears from these measurements at low temperatures, leaving only a small contribution likely from the orbital magnetoresistance. Similar conclusions are drawn from the magnetoresistance in Fig. 2d, which at low temperatures is negative at all $\theta$, and the behavior is well accounted for by single impurity Kondo scaling (Supplementary Fig. 9 and Supplementary Note 5). This disappearance may be related to the drop of the effective Fermi velocity to $v' \ll v_F$ as the quasiparticles gain mass in the heavy fermion state, since $c_F \propto v_F^2$ and therefore decreasing $v_F$ will greatly reduce the chiral anomaly contribution. As a result, the disappearance of the chiral anomaly at low temperatures suggests a significant modification of the Weyl points by the electronic correlations.

**Topological Hall effect.** Even in the case when $v_F$ is small, the Berry curvature induced by the Weyl points can still contribute to the anomalous Hall effect (AHE). We analyzed the Hall resistivity between 0.3 and 30 K by considering the total Hall resistivity as the sum of three terms $\Theta_{xy}=\Theta_{xy}^A+\Theta_{xy}^N+\Theta_{xy}^T$ (1)

where $\rho_{xy}^N$, $\rho_{xy}^A$, and $\rho_{xy}^T$ are the normal Hall effect, anomalous term from the magnetization, and the topological Hall effect term arising from the Berry curvature, respectively. Figure 4a shows the anomalous contribution to the Hall resistivity ($\rho_{xy}^A$, $\rho_{xy}^T$) after subtracting the ordinary band part $\rho_{xy}^N$; the data are taken from measurements of sample S6 which exhibits single band behavior and evidence for the chiral anomaly. Here the $\rho_{xy}^T$ term shown by the dashed lines is proportional to the magnetization, which dominates at higher temperatures due to an increased resistivity (Supplementary Fig. 8), while the topological part $\rho_{xy}^T$ gives rise to the maxima as shown in Fig. 4a at low temperatures. After subtracting $\rho_{xy}^N$, the topological Hall angle $\Theta_{xy}^T=\Delta\sigma_{xy}/\sigma_{xx}$ is obtained and is displayed in Fig. 4b. Here a peak in $\Theta_{xy}^T$ can be resolved up to temperatures of at least 30 K, which is very similar to the behavior observed in the magnetic Weyl semimetals GdPtBi$^9$ and Mn$_3$Sn$^{11}$. The large maximum value in $\Theta_{xy}^T$ of 0.18 at 0.3 K in YbPtBi is comparable to the respective values of 0.17 and 0.4 for the two other compounds$^9,11$. We note that in the regions where the Hall resistivity is linear (below around 0.2 T
Evidence for Weyl nodes from the specific heat. Evidence for the presence of Weyl points in the heavy fermion state is also found in specific heat measurements. While in zero field there is an upturn of $C(T)/T$ prior to the onset of antiferromagnetic order in zero-field at 0.4 K (Supplementary Fig. 10), for larger applied fields $C(T)/T$ reaches a maximum before decreasing at lower temperatures. However, as also shown by the solid lines in Fig. 4c, the low temperature $C(T)/T$ at higher fields deviates from a spin-1/2 resonance-level model for Kondo impurity systems (Supplementary Note 6), where two levels of width $\Delta$ are split by a Zeeman field. This model can be widely applied in heavy fermion systems, both in the coherent heavy Fermi liquid state and the dilute limit. In higher fields, $C/T$ of the Kondo impurity model becomes nearly temperature independent at low temperatures, but the data are instead well described by a $T^3$ dependence of the specific heat, $C \sim (k_B T / h v_F^2)$ (Fig. 4d), which was proposed for a Weyl–Kondo semimetal, as a result of the linear dispersion $\epsilon_k = h v_F k$ in the vicinity of the Weyl nodes. We note that this term is too large to arise from acoustic phonons since it would correspond to an unreasonably small Debye temperature of $\Theta_D = 32$ K, compared to the much larger value of $\Theta_D = 190$ K for isostructural LuPtBi. With increasing field there is a decrease of the Sommerfeld coefficient $\gamma$ and an increase of $v_F$, consistent with the applied field reducing the effective mass of the quasiparticles (Supplementary Table 1). However, even at $B = 13$ T a value of $\gamma = 89 \text{ mJ mol}^{-1} \text{K}^{-2}$ is obtained, indicating that a significant mass enhancement persists in this field region, which is consistent with the single impurity Kondo scaling present up to the maximum measured field of 9 T (Supplementary Fig. 9). Correspondingly, fitting the data yields low effective Fermi velocities of $v_F = 213 \text{ m s}^{-1}$ at 7 T and $v_F = 394 \text{ m s}^{-1}$ at 13 T, which are significantly reduced compared to the Fermi velocity of $v_F = 2.3 \times 10^5 \text{ m s}^{-1}$ estimated from $v_F = (\hbar / m_e) (3\pi^2 n_i)$ at 50 K (Fig. 3c).

Discussion

Based on the above experimental findings, we propose the diagram shown in Fig. 5 to describe the Weyl fermions in YbPtBi. At high temperatures there are Weyl nodes formed from the conduction bands, while the $f$ electrons are well localized. This is consistently shown from electronic structure calculations, ARPES, and magnetotransport measurements. At lower temperatures, the strong band renormalization due to Kondo coupling enhances the effective quasiparticle mass, which modifies the dispersion of...
the bands in the vicinity of the topologically protected Weyl points, as shown schematically in the diagram. The renormalization also leads to a greatly reduced effective Fermi velocity $v_F$ compared to the bare band value, which eventually causes the disappearance of the chiral anomaly in transport measurements, but allows for the observation of a sizeable specific heat contribution $C \sim \left( k_B T / \hbar v_F \right)^3$. Importantly, there is evidence for the Berry curvature associated with the Weyl nodes from the anomalous Hall effect, which can be detected in both the intermediate and low-temperature regimes.

Our results highlight the existence of Weyl fermions in YbPtBi, where we find evidence for their modification as the Kondo coupling is strengthened upon lowering the temperature. How precisely the Weyl points are modified as the electronic correlations become stronger needs to be determined by future studies. While the topological Hall effect and specific heat provide evidence for the survival of Weyl fermions at low temperatures, looking for spectroscopic evidence from ARPES or scanning tunneling microscopy is very important. One possible approach to reveal Weyl fermions in the heavy fermion state from $f$-bands is resonant photoemission. However, our measurements across the Yb N edge do not show obvious resonance contrast (Supplementary Fig. 11). Although ARPES measurements with $\hbar \nu > 100$ eV (including with soft X-rays) indeed reveal the bulk $f$-bands near $E_F$ (Supplementary Fig. 12), resolving the (fine) hybridized bands deep inside the heavy fermion state is still challenging, and therefore further ARPES measurements with greater energy and momentum resolution are highly desirable.

The presence of Weyl fermions in YbPtBi is different from the cases of both CeSb38 and GdPtBi22, where the bands hosting Weyl fermions do not have a significant $f$-electron contribution. Meanwhile, evidence for Weyl fermions has also been found in some magnetic d-electron systems such as Mn$_3$Sn29 and YbMnBi$_2$40,41, where in the case of Mn$_3$Sn a significant topological Hall effect is also observed10,11. On the other hand, it is of great interest to look for the kind of dichotomy observed here for YbPtBi in other potential Weyl heavy-fermion semimetals, such as Ce$_2$Bi$_2$Pd$_3$, where a similarly small $v_F$ was inferred from the specific heat15, yet evidence for the chiral anomaly at elevated temperatures has not yet been reported. Furthermore, the strength of the Kondo interaction in heavy fermion systems can be readily tuned by non-thermal control parameters, such as pressure and magnetic field, and in particular, a quantum critical point can be reached in YbPtBi at a critical field of 0.4 T35. Therefore, our findings may open up the opportunity to explore the exciting relationship between Weyl fermions, electron–electron correlations and quantum criticality.

**Methods**

**Sample synthesis.** Single crystals of YbPtBi were prepared using a Bi self flux.42 Elemental Yb, Pt, and Bi were combined in a range of molar ratios from 1:17 to 1:20 and heated to 1150 °C, before being slowly cooled to 500 °C at a rate of 4 °C/h. For some samples, Au was also added up to a maximum ratio of Au:Pt = 1:19. The single crystal quality and orientation were checked using Laue diffraction, which was measured along the [100] direction (Supplementary Fig. 1).

**Physical properties characterization.** The magnetotransport was measured using the four-probe method in a Quantum Design Physical Property Measurement System (9T-PPMS) with the sample rotation option, where Pt wires were attached to the sample. Hall effect measurements for determining the AHE were performed in a $^3$He cryostat with a 15 T magnet. As shown in Supplementary Fig. 2, for some samples multiple voltage contacts were made, so as to rule out current inhomogeneities and the current jetting effect. The temperature dependence of the resistivity was checked for several samples (Supplementary Fig. 1), which are similar to previous reports35. The resistivities at 2 K range from 27 to 37 $\mu$Ω-cm with $\rho(300 K)/\rho(2 K) = 10$.

Specific heat measurements were performed using a 14T-PPMS using a $^3$He option, while magnetization measurements were carried out using the vibrating sample magnetometer (VSM) option. The magnetic susceptibility data are well fitted by the Curie–Weiss expression between 10 and 300 K (Supplementary Fig. 1), yielding a Curie–Weiss temperature of $\theta_{C/W} = -2.3 \pm 0.5$ K and an effective moment of $4.29 \mu_B$/Yb, again consistent with previous results35.

**ARPES measurements and electronic structure calculations.** ARPES measurements, including resonant photocurrent emission across the Yb N edge, were performed at the Advanced Light Source, BL7 micro-ARPES beamline. The (111)-oriented YbPtBi samples were cleaved in situ and measured at around 20 K with 75 eV photons, unless noted otherwise. A detailed photon energy dependence study was carried out to confirm the bulk nature of the bands reported here. The typical domain size after cleavage is only a few tens of $\mu$m. The surface termination (either Yb or Bi terminated) is determined by core level analysis as the Kondo interaction as the Kondo temperature is $T_K = 10$ K (Supplementary Fig. 1), which was measured along the [100] direction (Supplementary Fig. 1).

**Data availability**

All the data supporting the findings are available from the corresponding author upon reasonable request.

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**Fig. 5** Schematic phase diagram for Weyl fermions in heavy fermion systems. Illustration of the evolution of the contributions from different experimental probes of Weyl fermions in heavy fermion systems; the chiral anomaly $c_{ch}$, electronic specific heat $C_v$ and topological Hall effect $\rho_{xy}^T$. When the electronic bands in the vicinity of the Weyl points become heavy at low temperatures, the massive reduction of the effective Fermi velocity $v_F$ leads to the chiral anomaly contribution $c_{ch}$ becoming undetectable, yet gives a significant contribution from Weyl nodes to the electronic specific heat $C_v$, which is otherwise not detectable in weakly correlated materials. Meanwhile the topological Hall effect $\rho_{xy}^T$ which arises from the Berry curvature can be detected both when the $f$-electrons are well localized, as well as deep inside the heavy fermion state.
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