Extremely large magnetoresistance and compensated Fermi surfaces in the antiferromagnetic semimetal YbAs

W. Xie,1 Y. Wu,1 F. Du,1 A. Wang,1 H. Su,1 Y. Chen,1 Z. Y. Nie,1 S.-K. Mo,2 M. Smidman,1 C. Cao,1 Y. Liu,1,4,* T. Takabatake,1,5 and H. Q. Yuan1,4,†

1Department of Physics and Center for Correlated Matter, Zhejiang University, Hangzhou 310058, China
2Advanced Light Source, E. O. Lawrence Berkeley National Lab, Berkeley, California 94720, United States
3Department of Physics, Hangzhou Normal University, Hangzhou 310036, China
4Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China
5Department of Quantum Matter, AdSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

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We report the synthesis of single crystals of YbAs using a flux method, the properties of which were studied using magnetotransport and angle-resolved photoemission spectroscopy (ARPES) measurements, together with density functional theory (DFT) calculations. We observe an extremely large magnetoresistance (XMR) for both YbAs and the nonmagnetic counterpart LuAs, and construct a temperature-field phase diagram for YbAs. The Fermi surfaces of YbAs are probed via angle-dependent Shubnikov-de Haas oscillations, ARPES, and DFT calculations, which reveal that the Fermi surface consists of three symmetry-equivalent electron pockets and two hole pockets within the Brillouin zone. These can account for the presence of electron-hole compensation, which is also concluded from the analysis of the magnetoresistance and Hall resistivity. Our results indicate that electron-hole compensation is the primary mechanism giving rise to the XMR in both YbAs and LuAs. Furthermore, ARPES and DFT calculations find no evidence for band inversions in YbAs, indicating that the electronic structure is topologically trivial.

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1. I. INTRODUCTION

An extremely large magnetoresistance (XMR) reaching values up to $\sim 10^4$ to $10^6\%$ has been observed in some semimetals in moderately high magnetic fields [1–6]. This effect has mainly been attributed to electron-hole compensation [1, 7–9] or the presence of topologically non-trivial surface states [2–4]. In addition, other mechanisms have also been proposed, such as open Fermi surfaces [5], mobility imbalance with moderate compensation [6], and particular spin textures with free backscattering [10].

The $LnX$ series ($Ln =$ rare-earth and $X =$ As, Sb or Bi) is a large family of semimetals exhibiting XMR, crystallizing in the cubic NaCl-type structure [8, 11–23]. In LaSb, a field-induced upturn of the resistivity and a low temperature plateau were observed [11], which resembles that found in the proposed topological Kondo insulator SmB$_6$, where it was explained as arising due to the presence of topological surface states at low temperatures [24, 25]. Subsequently, XMR at low temperatures was also reported for isostuctural LaBi and LaAs [8, 17]. In LaBi, multiple Dirac cones were detected near the Fermi level [26], indicating a nontrivial band topology, whereas LaAs was reported to be topologically trivial with the XMR being accounted for by electron-hole compensation [17]. More recently, the LaX series were again measured using ARPES, which confirmed that LaBi has a nontrivial topology and LaAs is trivial, while LaSb was found to be on the verge of a band inversion [27]. This indicates the presence of a topological phase transition within the family of La-monopnictides. Furthermore, substituting nonmagnetic La with other lanthanides gives rise to additional interesting phenomena. For instance, evidence was found that CeSb hosts Weyl fermions in the field-induced ferromagnetic state [13], while PrSb also exhibits XMR but was found to be topologically trivial from an analysis of the Berry phase [18]. NdSb was reported to be a Dirac semimetal with antiferromagnetic (AFM) order, where a field-induced change of the Fermi surface is observed once the system reaches the spin-polarized state in high magnetic fields [14–16]. Meanwhile XMR was also found in SmSb, but here the analysis of the Shubnikov-de Haas (SdH) oscillations gives evidence for a topologically nontrivial band structure [20]. Topological electronic structures were detected using ARPES for several rare-earth mono-bismuthides (Ce, Pr, Sm, Gd)Bi, showing tunable bulk band inversions and corresponding surface states [28], while the bulk band inversion and surface states were found to be absent in the antimonides (Pr, Sm)Sb [29]. For the topological properties, the ARPES results agree well with density functional theory (DFT) calculations which assume that the $f$-electrons are localized [30]. Moreover, a combined ARPES and transport study of (Pr, Sm)Sb and (Pr, Sm)Bi suggested that electron-hole compensation is the origin of the observed XMR [29]. However, the XMR phenomenon in Yb monopnictides has not yet been reported. Since Yb$^{3+}$ has a $4f^{13}$ configuration, which corresponds to the hole counterpart of Ce$^{3+}$ (with $4f^1$), it is of particular interest to examine if these Yb-based compounds exhibit XMR and/or topological behaviors.
YbAs is a member of the $LnX$ series \cite{31}, which was initially reported to be a typical heavy fermion antiferromagnet with a Néel temperature $T_N = 0.5$ K. Heat capacity measurements revealed an entropy at $T_N$ of only 0.2Rln2 \cite{32} and an enhanced Sommerfeld coefficient of $\gamma = 270$ mJ/mol K$^2$ \cite{33}. The zero-field magnetic structure below $T_N$ was determined to be type-III AFM with a propagation vector of $k = [1, 0, 1/2]$ \cite{34}. Meanwhile both neutron scattering and Mössbauer spectroscopy show that there is a reduced ordered moment of around 0.85$\mu_B$/Yb \cite{34, 35}, likely due to the Kondo effect. Furthermore, an inelastic neutron scattering (INS) study revealed the development of short-range spin correlations below around 20 K, which is far above $T_N$ \cite{36, 37}. The splitting of the first excited crystalline-electric field (CEF) $\Gamma_8$ quartet upon cooling below about 80 K was explained by a giant quadrupolar interaction \cite{38}.

The heavy fermion nature of this compound was also indicated by the huge value of the nuclear spin relaxation rate in nuclear magnetic resonance (NMR) measurements and DFT calculations revealed an entropy at $T_N$ of $\gamma \sim 10^{20}$ cm$^{-3}$, only about 1% of that of the magnetic Yb-ions, which is far less than that required for full Kondo screening \cite{40}. A de Haas-van Alphen (dHvA) effect study revealed the presence of three ellipsoidal electron pockets and one spherical hole pocket within the Brillouin zone \cite{41}. In order to account for the large Sommerfeld coefficient, it was proposed based on $p$-$f$ mixing theory that there are additional hole pockets with large effective masses \cite{41}. To explain the experimental results, various theoretical scenarios have been proposed, such as the interplay of the Kondo effect and magnetic exchange interaction \cite{35, 42, 43}, a $p$-$f$ mixing model \cite{40, 44}, magnetic polaron formation \cite{45}, spin density wave formation \cite{45, 46}, pair Jahn-Teller distortion and charge dipolar ordering \cite{47}, indicating intricate physics in this compound.

Here we have grown high-quality single crystals of YbAs and LuAs using a flux method. XMR and SdH oscillations were observed at low temperatures for both YbAs and LuAs. The XMR of YbAs was compared with that of LuAs, revealing additional low-temperature features, while its scaling behavior shows that Kohler’s rule is valid in YbAs. Fitting the magnetoresistance (MR) and Hall resistivity with a two-band model indicates the presence of electron-hole compensation, as well as a large enhancement of mobilities of both electrons and holes upon cooling below around 70 K. The analysis of the angle-dependent SdH oscillations in the MR reveals similar Fermi surfaces for both YbAs and LuAs. ARPES measurements and DFT calculations confirm these findings, and find no evidence for the band inversions necessary for topological surface states. Our study indicates that the XMR, originating from electron-hole compensation and high carrier mobilities, is affected by the presence of 4$f$-electrons, most likely due to the presence of short-range magnetic correlations.

II. EXPERIMENTAL DETAILS

Single crystals of YbAs and LuAs were prepared using eutectic Pd-As binary phases as a flux, in contrast to previous studies where samples were grown using the Bridgman method \cite{48}. Yb (or Lu) powder, Pd powder and prereacted PdAs$_2$ were placed in an alumina crucible in the molar ratio 1:2:2. The crucible was sealed in an evacuated quartz tube. The mixture was slowly heated to 1000°C in a muffle furnace and held there for one day. The furnace was then slowly cooled to 800°C at a rate of about 1.8°C/h, before the quartz tube was centrifuged to separate the crystals from the flux. Shiny single crystals with a typical size of about $1 \times 1 \times 1$ mm$^3$ were obtained, as shown in the inset of Fig. 1(a).

The crystal structure and orientation were confirmed using x-ray diffraction (XRD) on a cleaved crystal using a PANalytical X’Pert MRD powder diffractometer with Cu $K_{\alpha1}$ radiation monochromated by graphite. The chemical composition was determined by energy-dispersive x-ray spectroscopy (EDS) using a Hitachi SU-8010 Field Emission scanning electron microscope. The resistivity and angle-dependent magnetotransport were measured using a Quantum Design Physical Property Measurement System (PPMS) with a sample rotation option. Four Pt wires were attached to the sample using silver paste. The specific heat was also measured using a PPMS. The low-temperature MR between 0.275 K and 10 K was measured using a $^3$He system in fields up to 15 T. The Hall measurements were performed using a PPMS, utilizing a four-wire-method on a piece of single crystal with the applied field perpendicular to the (111) plane and the current in this plane, where the transverse resistivity contribution was subtracted.

High-resolution ARPES measurements were carried out on the beamline 10.0.1 at the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory (USA). The typical energy and angular resolution were about 15 meV and 0.2°, respectively. A photon energy range from 30 eV to 200 eV was used during the measurements. Single crystals of YbAs were cleaved in situ at around 20 K and measured at the same temperature. Temperature-dependent scans were performed from 13 K up to 80 K, but no obvious temperature dependence was found in the ARPES spectra. All measurements were performed in an ultrahigh vacuum with a base pressure lower than $1 \times 10^{-10}$ torr.

Density functional theory (DFT) calculations were performed using the Vienna Abinitio Simulation Package (VASP). A plane-wave basis up to 380 eV and $12 \times 12 \times 12$ $\Gamma$-centered K-mesh were used to make sure the total en-
energy converges to 1 meV per unit cell. The modified Becke-Johnson (mBJ) potentials were used with the effect of spin-orbit coupling (SOC) considered. The $f$-electrons are treated as core states in all the calculations, which gives good agreements with experimental results.

III. RESULTS AND DISCUSSION

A. Sample characterization

Figure 1(a) shows an XRD pattern of a newly-cleaved single crystal, in which the diffraction peak positions correspond to the (001) plane of YbAs, indicating the correct phase of our crystals with the [001] direction perpendicular to the cleaved face. Figure 1(b) shows the normalized temperature dependence of the resistivity $\rho_{xx}(T)/\rho_{xx}(300 \text{ K})$ from 300 K to 1.9 K for YbAs and LuAs. The absolute resistivity of YbAs is shown in the inset, where the residual resistivity at 1.9 K is about 0.4 $\mu\Omega$ cm. The metallic behavior for YbAs is consistent with previous reports [41]. However, the residual resistivity ratio RRR ($= \rho_{xx}(300 \text{ K})/\rho_{xx}(1.9 \text{ K})$) of 260 is more than one order of magnitude higher than previous studies [48], while the RRR of LuAs is about 180, which is also higher than that reported for polycrystalline samples [49]. The magnetic contribution to the heat capacity $C_{\text{mag}}/T$ (Fig. 1(c)), obtained by subtracting the $C/T$ of LuAs from that of YbAs, begins to increase below 20 K with a more rapid increase below about 8 K.

![FIG. 1. (Color online) (a) XRD pattern of an YbAs single crystal with a surface perpendicular to the $c$ direction. The inset shows a piece of single crystal with typical dimensions. (b) Normalized temperature dependent resistivity $\rho_{xx}(T)$ for YbAs and LuAs in zero applied field. The inset of (b) displays the absolute value of $\rho_{xx}(T)$ of YbAs, where there is a small residual resistivity of 0.4 $\mu\Omega$ cm at 1.9 K. (c) Low temperature heat capacity as $C/T$ of YbAs and LuAs. The blue solid line displays the magnetic contribution to the heat capacity of YbAs.](image1)

![FIG. 2. (Color online) Temperature dependence of the resistivity $\rho_{xx}$ under various applied magnetic fields down to 1.9 K for (a) YbAs and (b) LuAs, with $B \perp I \parallel [100]$. Several characteristic temperatures are marked. The insets of (a) and (b) show the low temperature part of the zero field resistivity of YbAs and LuAs down to 0.3 K, respectively.](image2)
B. XMR and $B$–$T$ phase diagram

In the main panel of Fig. 2, $\rho_{xx}(T)$ under different applied magnetic fields is displayed for YbAs and LuAs down to 1.9 K. The field direction is perpendicular to the crystallographic plane and current direction, with $I \parallel [100]$ and $B \perp [100]$. As shown in the insets of Fig. 2, the zero field resistivity $\rho_{xx}(T,0)$ flattens below around 15 K for LuAs, while $\rho_{xx}(T,0)$ of YbAs has a gradual change of slope at about 20 K, and decrease at a greater rate below 8 K, close to the temperature below which $C_{\text{mag}}/T$ (Fig. 1(c)) also begins to increase more rapidly. The temperature dependent resistivity $\rho_{xx}(T, B)$ of both YbAs and LuAs starts to upturn below a temperature denoted as $T_{\text{min}}$ once a field is applied, which increases with applied field. For LuAs, a resistivity plateau develops below about 15 K, which is similar to other non-magnetic XMR materials such as LaX [8, 11, 17]. However, the in-field resistivity of YbAs continues to increase with decreasing temperature, and there is a more rapid increase below around 8 K, which is not present in the data of LuAs. Since $\rho_{xx}(T,0)$ decreases more rapidly below this temperature, this suggests that the low-temperature anomalous XMR of YbAs shares the same origin as the zero field resistivity behavior. We note that INS measurements indicate that anomalous short-range antiferromagnetic spin correlations onset below 20 K, and the INS peak intensity increases more strongly with decreasing temperature below about 8 K [36, 37]. Therefore, we attribute the unsaturated in-field resistivity of YbAs at low temperatures to the short-range spin correlations developing in the same temperature range. These correlations were suggested to lead to part of the magnetic entropy being released above $T_N$, and the small ordered moment could therefore be due to the coexistence of the short-range correlations with long-range order [36, 37]. Our results also suggest that the short-range correlations are not sensitive to field, as also evidenced by the weak field dependence of the broad peak in $C(T)$ in fields up to 10 T [50].

From low-temperature resistivity measurements in applied transverse fields, we determined the field dependence of $T_N$. Although $\rho_{xx}(T,0)$ shows no detectable anomaly at $T_N = 0.5$ K (inset of Fig. 2(a)), clear jumps can be resolved in the in-field data. As shown in Fig. 3(a), $T_N$ decreases with applied field up to 9 T, while above 11 T, a different anomaly appears in $\rho_{xx}$ (denoted as $T_M$), which moves to higher temperature with increasing field. The solid black arrows in Fig. 3(a) denote the cooling and warming process of the resistivity measurements. While a negligible thermal loop is found at $T_N$, above 11 T a loop occurs at $T_M$, which becomes larger with increasing field. Note that the magnitude of the anomaly at the transition increases with field for both $T_N$ and $T_M$. Based on $\rho_{xx}(T)$ and $\rho_{xx}(B)$, the $B$–$T$ phase diagram of YbAs was constructed, as shown in Fig. 3(b). The first order transition at $T_M$, as well as a drastically different field-dependence, indicates a different nature from that at $T_N$. Considering the strong quadrupolar interaction reported previously in YbAs [38, 51], it may be that $T_M$ corresponds to quadrupolar ordering. The quadrupolar moments could originate from the mixture of the CEF ground state $\Gamma_0$ and the first excited CEF state $\Gamma_8$ under applied magnetic fields [51]. Other examples of field-induced quadrupolar ordering in rare earth compounds include Dy$_3$Ru$_4$Al$_{12}$ [52] and HoFe$_2$Al$_{16}$ [53]. However, this proposal is to be confirmed by further studies, such as ultrasound measurements.

C. Kohler’s rule scaling and Hall resistivity

The MR ($= (\rho_{xx}(T, B) - \rho_{xx}(T, 0))/\rho_{xx}(T, 0) \times 100\%$) of YbAs was analyzed to look for the presence of Kohler’s rule scaling, as performed for other XMR materials [8, 9, 17]. Figure 4(a) displays the isothermal MR measured at various temperatures between 300 K and 1.9 K, which is plotted as a function of $B/\rho(T, 0)$ in Fig. 4(b). It is apparent that the data at different temperatures fall onto a single line, showing that Kohler’s rule is valid in YbAs [54]. Similar to WTe$_2$, this excludes the scenario of a metal-insulator transition being the origin of the field-induced resistivity upturn [9]. For WTe$_2$, the overall resistivity upturn behavior can be explained by Kohler’s
rule scaling,

\[ MR = \alpha (B/\rho (T, 0))^m, \tag{1} \]

with \( m \approx 2 \), which can be derived from a two-band model with electron-hole compensation [9]. For YbAs as shown in Fig. 4(b), when the data are plotted on a double logarithmic scale, there is an apparent change of slope around 50–70 K, while below 50 K the data scale well linearly, with a fitted value of \( m = 1.75 \). Changes of the carrier concentration and/or mobility in the temperature range of 50–70 K may account for this change of slope \([8, 9]\). Since the presence of Kohler’s scaling shows that \( \rho(T, B) \) is solely determined by \( \rho(T, 0) \), this suggests that in YbAs the unsaturated temperature dependence of the in-field resistivity is a reflection of the continuous decrease of \( \rho(T, 0) \) shown in Fig. 2(a).

The Hall resistivity \( \rho_{xy}(T, B) \) was also measured, so as to probe whether there is change of carrier concentration or mobility with temperature. As displayed in Fig. 5(a), \( \rho_{xy}(B) \) for \( T > 50 \) K exhibits a near linear field dependence, while it is non-linear below 50 K.

For a two-band model \([8, 54]\), \( \rho_{xy}(B) \) and the MR can be expressed as

\[ \rho_{xy} = \frac{B}{e} \frac{(n_h \mu_h^2 - n_e \mu_e^2) + (n_h - n_e)(\mu_e \mu_h)^2 B^2}{(n_h \mu_h + n_e \mu_e)^2 + (n_h - n_e)^2 (\mu_e \mu_h)^2 B^2}, \tag{2} \]

\[ MR = \frac{n_e \mu_e n_h \mu_h (\mu_e + \mu_h)^2 B^2}{(n_h \mu_h + n_e \mu_e)^2 + (n_h - n_e)^2 (\mu_e \mu_h)^2 B^2}. \tag{3} \]

where \( n_e \) and \( n_h \) are the carrier concentrations of electrons and holes, respectively, while \( \mu_e \) and \( \mu_h \) are the respective mobilities. Both \( \rho_{xy}(B) \) and the MR were simultaneously fitted using Eqs. (2) and (3), and the fitted curves at several temperatures are displayed in Fig. 5(a). Due to the large number of parameters, \( n_e \) was fixed to the value of 4.74×10^{20} \text{ cm}^{-3} \) from the analysis of the SdH oscillations (see below). In Fig. 5(b), the temperature dependence of the fitted values of \( n_e/n_h, \mu_e, \) and \( \mu_h \) are displayed. It can be seen that both \( \mu_e \) and \( \mu_h \) show a significant increase upon cooling below about 70 K, which may explain the change of exponent in the Kohler’s rule.
to resistance at low temperatures. Note that these mobiles can be fitted with the L-K formula. Of the SdH oscillation amplitudes of the two hole bands (\(B \geq 9\) T. SdH oscillations can be resolved for \(T > T_\alpha\) the thick lines for the FFT analysis of the angle dependent MR in the field range of 6–9 T. The fitted curves described in the main text are shown by 6–15 T) and \(\theta = 0^\circ\) in fields up to 15 T. SdH oscillations can be resolved for \(B \geq 6\) T. (d) The SdH oscillation frequencies as a function of \(\theta\), obtained via an FFT analysis of the angle dependent MR in the field range of 6–9 T. The fitted curves described in the main text are shown by the thick lines for the \(\alpha\) and \(\alpha'\) bands, while the other thin lines are guides to the eye. (e) FFT analysis at three temperatures, both above and below \(T_N\) or \(T_M\), which show negligible differences in the oscillation frequencies. (f) Temperature dependence of the SdH oscillation amplitudes of the two hole bands (\(\beta\) band and \(\gamma\) band) down to 0.275 K. The solid lines show the results of fitting with the L-K formula.

The large values of the mobilities, reaching 4–6 m²/(V·s) at 1.9 K, can also account for the large magnetoresistance at low temperatures. Note that these mobilities are quite different from previous results [35], where only the electron mobility displays a weak increase below about 80 K, and the values are an order of magnitude lower. We ascribe this difference to the higher quality of our single crystals, manifested in the RRR value of 260. The fitted electron- and hole-carrier densities are nearly compensated across the whole temperature range (\(n_e/n_h \approx 1\)), in agreement with previous reports [35].

D. SdH oscillations and Fermi surfaces

Clear SdH oscillations are observed in the MR at temperatures up to \(\sim 10\) K in fields above 6 T. To further study these oscillations, we performed MR measurements in fields up to 15 T, at temperatures down to 0.275 K, and the results are displayed in Fig. 6(a). After subtracting the background, we performed a fast-Fourier-transform (FFT) analysis on the data in the field range of 6–15 T. As shown in Fig. 6(b), we find the presence of five principal frequencies (\(\alpha, \alpha', \alpha'', \beta, \) and \(\gamma\)) and some harmonic frequencies, indicating multiple Fermi surface pockets in YbAs. Note that when the field is applied along [001] (\(\theta = 0^\circ\)), \(\alpha''\) coincides with \(\alpha'\).

Angle dependent MR measurements were also performed down to 1.9 K, by rotating the sample, which are displayed for several field directions in Fig. 6(c). The directions of the applied current and fields are illustrated in the inset of Fig. 6(a), where \(I \parallel [100]\) and \(\theta\) is the angle between the applied field and the [001] direction. The corresponding angle dependence of the SdH frequen-
cies is displayed in Fig. 6(d), obtained from performing an FFT analysis on the data in the field range of 6–9 T. There are five fundamental frequencies, corresponding to the different Fermi pockets, where the cross-sectional areas of the extremal orbits \( A_{\text{ext}} \) change upon rotating the field direction according to the Onsager relation \( F \equiv (\Phi_0/2\pi^2) A_{\text{ext}} \), where \( \Phi_0 \) is the magnetic flux quantum. The dispersions shown here are consistent with the dHvA results reported for YbAs in Ref. [41] as well as those of LaAs [17]. In Ref. [41], four angle-dependent dispersion lines are observed, corresponding to three ellipsoidal electron pockets and only one spherical hole pocket, which correspond to the \( \alpha \), \( \alpha' \), \( \alpha'' \) pockets and the \( \beta \) pocket in our results, respectively. They also proposed that at least one more hole pocket with a large effective mass must exist based on the \( p-f \) mixing model [41]. Here we find that an extra hole pocket is indeed present (labelled as \( \gamma \)), which likely corresponds to a jack shape, as observed in LaAs [17, 41].

Based on the above, we calculated the carrier concentrations \( n \) of both electrons and holes, which are proportional to the volume \( V_F \) of the Fermi pockets via \( n = V_F/4\pi^3 \). Here the angular dependence of \( A_{\text{ext}} \) was used to extract the lengths of the semi-major and semi-minor axes of the ellipsoidal pockets, as well as the radius of the spherical pocket. For the irregularly shaped \( \gamma \)-pocket, \( V_F \) was estimated following the method used for LaAs in Ref. [17]. The calculated carrier densities are \( n_e = 4.74 \times 10^{20} \text{ cm}^{-3} \) and \( n_e/n_h = 1.082 \) for YbAs, which also gives support for the presence of electron-hole compensation.

For three-dimensional ellipsoidal pockets, the angular dependent quantum oscillation frequency \( F(\varphi) \) can be described by [56]

\[
F(\theta) = A\pi ab/\sqrt{\sin^2(\theta + \varphi) + (a^2/b^2) \cos^2(\theta + \varphi)},
\]

where \( a \) and \( b \) are the lengths of the semi-major axis and semi-minor axis of the ellipsoidal \( \alpha \) pockets, respectively, \( A \) is a constant, and \( \varphi \) is an angular shift [56]. By using the above derived parameters \( a \) and \( b \), it is shown in Fig. 6(d) that the angular dependence of the \( \alpha \) and \( \alpha' \) band frequencies can be well accounted for by Eq. (4), with fitted values of \( A = 3.35 \times 10^4 \text{Å}^2 \) and \( \varphi = -1.26^\circ \).

To examine the influence of the transitions at \( T_N \) and \( T_M \) on the Fermi surface, we analyzed the FFT in several temperature and field ranges, corresponding to different phases in the \( B-T \) phase diagram shown in Fig. 3(b). The results displayed in Fig. 6(c) indicate that the SdH frequencies are nearly unchanged, suggesting that the Fermi surface volume is not modified upon crossing \( T_N \) or \( T_M \). The temperature dependence of the amplitudes for the two hole bands were extracted from the FFT analysis in the range 6–11 T, which were fitted using the Lifshitz-Kosevich (L-K) formula [57], as shown in Fig. 6(f). For the \( \gamma \) band, the L-K fit yields an effective mass of \( 0.541 m_0 \) (\( m_0 \) is the free electron mass) and no anomaly is observed upon crossing \( T_N \). However, for the \( \beta \) band which has a lighter effective mass of \( 0.256 m_0 \), an abrupt increase of the amplitude is observed upon decreasing the temperature below \( T_N \). The origin of this increase currently remains to be determined. An anomalous temperature dependence of SdH amplitudes is also found in SmSb upon crossing \( T_N \), which is not found in dHvA measurements [20]. In SmSb, evidence for a \( \pi \) Berry phase is found, and hence a topologically nontrivial band structure was suggested [20]. However, as described below, ARPES measurements and band structure calculations indicate that YbAs is topologically trivial.

We also performed similar measurements and analysis for LuAs, as a comparison. In Figs. 7(a)-(c), we show \( \rho_{xx}(B) \) at \( \theta = 0^\circ \) and \( 45^\circ \), the corresponding FFT results, and the angle dependent dispersions of the FFT frequencies, respectively. The angular dependence and absolute values of the FFT frequencies of LuAs are very similar to those of YbAs. This indicates that YbAs has a similar Fermi surface to LuAs and therefore the 4\textit{f}-electrons are well localized in the studied temperature range down to 0.275 K. The similar Fermi surfaces between magnetic YbAs and non-magnetic LuAs also suggests that the additional features observed in \( \rho_{xx}(T,B) \) for YbAs at low temperatures are not related to differences in the Fermi surface.

### E. DFT calculations and ARPES measurements

To further study the Fermi surfaces of YbAs, we performed DFT calculations and ARPES measurements. In Figs. 8(a) and (c), we show the calculated band structure and Fermi surface of YbAs. Figure 8(b) displays the ARPES energy vs momentum cut along the \( k_z \) direction at \( k_y = 0 \) and \( k_z \approx 0 \), while Fig. 8(d) shows the Fermi surface map in the \( k_z-k_y \) plane at \( k_z \approx 0 \). The ARPES spectra were taken at 60 eV, which corresponds to the \( k_z = 0 \) condition. From comparing the calculated results with the measured data, it is clear that the Fermi surfaces consist of two concentric hole pockets at the \( \Gamma \) point and three symmetry-equivalently electron pockets at the \( X \) points, which are consistent with the results of our FFT analysis. In general, the ARPES spectra are in good agreement with the DFT calculations, indicating that the \( \textit{f} \) electrons are mostly localized. In Figs. 8(a) and (b), no band inversion along the \( \Gamma-X \) direction can be observed, unlike the rare-earth monobismuthides [28], indicating the topologically trivial nature of YbAs, similar to LaAs [17].

To highlight the different parts of the Fermi surface, we show the separated pockets in Fig. 9 together with the calculated angle-dependent dispersions of the FFT frequencies. These dispersions agree well with our FFT
FIG. 7. (Color online) (a) $\rho_{xx}(B)$ of LuAs in fields up to 9 T measured at several temperatures with $\theta = 0^\circ$ and 45$^\circ$. $\theta$ is the angle between the field direction and [001], as illustrated in the inset of Fig. 4(a). (b) FFT results of the observed oscillations in panel (a) for $\theta = 0^\circ$ and 45$^\circ$. (c) Variation of the oscillation frequency of LuAs with $\theta$ obtained from the FFT analysis of the angle dependent MR. The thin solid lines are guides to the eyes. The frequencies for $\theta > 90^\circ$ are mirrored from the 0–90$^\circ$ data, in order to compare with those of YbAs in Fig. 6(d).

FIG. 8. (Color online) (a) The calculated band structure of YbAs along high-symmetry lines. (b) ARPES energy-momentum cut along the $k_x$ direction (Γ-X) at $k_y = 0$ and $k_z \approx 0$, to be compared with the Γ-X direction in (a). (c) The calculated 3D Fermi surfaces at $k_z = 0$ viewed from the $z$-direction. (d) Experimental Fermi surface in the $k_x$–$k_y$ plane near $k_z = 0$. The photon energy used for (b) and (d) is 60 eV, which corresponds to the $k_z = 0$ cut. The broken red line sketches the Brillouin Zone (BZ).

FIG. 9. (Color online) (a) The calculated Fermi surfaces of YbAs, including electron pockets (dark yellow) at the X points and hole pockets (dark red and dark green) around the Γ point in the Brillouin zone. (b) The calculated angle dependent dispersions of the FFT frequencies based on the Fermi pockets shown in (a).

analysis displayed in Fig. 6(d), while the systematic differences in the values of the frequencies may arise from the presence of correlations in YbAs.

Furthermore, Fig. 8(b) shows that no coherent bulk 4f band, i.e., the Kondo resonance peak, can be observed near the Fermi level, which indicates that the heavy fermion state has not developed. To confirm that the absence of a Kondo resonance peak is not due to a diminishing photoexcitation cross section, we employed a large range of photon energies (from 30 eV up to 200 eV)
to search for any weak signature of a Kondo resonance peak near the Fermi level. Nevertheless, all our ARPES spectra show similar flat $f$ bands at -1 and -2.1 eV (as shown in Fig. 8(b)), which are far away from the Fermi level and therefore are different from the bulk Kondo resonance that always resides near the Fermi level. A large-energy-range spectrum with its angle-integrated energy distribution curve is shown in Fig. 10, which reveals multiple intense Yb$^{3+}$ peaks ranging from -12 eV to -6 eV, and weak Yb$^{2+}$ peaks at -1 and -2.1 eV, respectively. The sharp Yb$^{3+}$ peaks confirm that the valence of Yb is mainly trivalent in YbAs, while the weak peaks at -1 and -2.1 eV are most likely due to surface Yb$^{2+}$ contributions, as seen in many other Yb-based heavy fermion compounds [58]. Temperature dependent scans were also performed from 13 K up to 80 K, but no signature of a Kondo resonance peak near the Fermi level can be observed and the band structure shows essentially no temperature dependence. This indicates that the many-body Kondo screening is rather weak at temperatures of 10 K and above.

IV. CONCLUSION

In summary, we have found XMR in high-quality single crystals of YbAs and studied the electronic structure. XMR was also observed for the nonmagnetic counterpart LuAs. By comparing with LuAs, however, distinct behaviors in the temperature dependence of $\rho_{xx}(T, B)$ are discerned for YbAs at low temperatures, likely related to the presence of short-range magnetic correlations from the Yb$^{3+}$ 4f moments, as revealed from INS measurements [36, 37]. From analyzing the MR and Hall resistivity, we find that the electron- and hole-carrier densities are nearly compensated, and that there is a significant enhancement of mobility for both electron and hole carriers below about 70 K, reaching 4–6 m$^2$/V·s at 1.9 K, which may give rise to the XMR at low temperatures. Analysis of SdH oscillations shows that the Fermi surface of YbAs consists of three symmetry equivalent electron pockets and two hole pockets within the Brillouin zone, which is also confirmed by ARPES measurements and DFT calculations. These findings can account for the electron-hole compensation of the Fermi surfaces. We further constructed a temperature–field phase diagram of YbAs for $B \perp [100]$. We find the presence of a different field-induced phase at high fields ($\geq 11$ T), the temperature of which increases with field. Importantly, both ARPES and DFT calculations did not find the presence of band inversions in YbAs and evidence for a Kondo-resonant flat band near the Fermi level is not found in our ARPES measurements down to 10 K.

Our results therefore indicate that the XMR phenomenon in YbAs originates from electron-hole compensation and high carrier mobilities, which is affected by the localized Yb 4f states, likely due to the influence of short-range spin correlations.

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* yangliuphys@zju.edu.cn
† hqyuan@zju.edu.cn
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