Quantum phase transition in the heavy-fermion compound YbIr$_2$Si$_2$

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(Dated: September 7, 2018)

We investigate the pressure-temperature phase diagram of YbIr$_2$Si$_2$ by measuring the electrical resistivity $\rho(T)$. In contrast to the widely investigated YbRh$_2$Si$_2$, YbIr$_2$Si$_2$ is a paramagnetic metal below $p_c \approx 8$ GPa. Interestingly, a first-order, presumably ferromagnetic, transition develops at $p_c$. Similar magnetic properties were also observed in YbRh$_2$Si$_2$ and YbCu$_2$Si$_2$ at sufficiently high pressures, suggesting a uniform picture for the former pressure can be described by Landau Fermi-liquid (NFFL) model. Moreover, evidence of a pressure-induced valence transition likely exists in the pressurized Yb-compounds. Furthermore, in YbRh$_2$Si$_2$ (see the inset, the dot marks its location at $p = 0$) AFM phase with weak magnetic moments exists below $p_c$ and vanishes at a QCP ($p_c$) where the LFL theory is violated.

The study of quantum critical phenomena has attracted considerable attention because of the fascinating physical properties caused by quantum fluctuations. In the Ce-based heavy fermion (HF) systems, unconventional superconductivity, most likely paired via antiferro magnetic (AFM) spin fluctuations, has been widely observed around a spin-density-wave (SDW) type quantum critical point (QCP) $^1$. On the other hand, YbRh$_2$Si$_2$ has been established as a model system to study quantum physics at a “local” QCP $^2$, around which no superconductivity has yet been observed at $T > 10$ mK. Recent efforts have been largely concentrated on weakly first-order quantum phase transitions (QPT), e.g., the ferromagnetic (FM) transition in MnSi $^3$-$^4$, the metamagnetic transition in Sr$_2$Ru$_2$O$_{2.9}$ $^5$, and the valence transition in CeCu$_2$(Si$_{1-x}$Ge$_x$)$_2$ $^6$.

The HF compound YbRh$_2$Si$_2$ undergoes an AFM transition at $T_N = 70$ mK $^7$. A small magnetic field or a slight expansion of the unit cell by substituting Si with Ge can eventually suppress the AFM order at a QCP $^2$-$^8$, at which the conventional LFL theory breaks down (see the inset of Fig. 1). As tuning away from the QCF LFL behavior immediately recovers at the lowest temperature. On the other hand, the weak AFM transition in YbRh$_2$Si$_2$ is stabilized by applying pressure $^7$-$^9$, $^{10}$. In particular, the magnetic phase undergoes a first-order transition from a small-moment state (FM-type) to a large-moment state around 10 GPa $^9$. Furthermore, it was argued that in YbRh$_2$Si$_2$ FM quantum critical fluctuations dominate over a wide range in the phase diagram except for the close vicinity of the AFM QCP $^{11}$-$^{12}$. In order to better understand the nature of the “local” QCP, YbIr$_2$Si$_2$, a sister compound of YbRh$_2$Si$_2$, was recently synthesized by Hossain et al. $^{13}$. YbIr$_2$Si$_2$ (I-type) is a moderate HF compound with a paramagnetic ground state at zero pressure and, therefore, was expected to cross a magnetic QCP by applying a small pressure of the order 2–3 GPa to compress the unit cell volume of YbIr$_2$Si$_2$ to that of YbRh$_2$Si$_2$ at $p = 0$ $^{13}$.

In this letter, we present the first high-pressure study for YbIr$_2$Si$_2$. Surprisingly, YbIr$_2$Si$_2$ exhibits properties distinct from YbRh$_2$Si$_2$ and shows no evidence for the existence of an AFM QCP at low pressures (see Fig. 1). However, a similar (likely ferro-) magnetic transition is found at high pressures ($p > p_c \approx 8$ GPa). LFL behavior, characterized by $\Delta \rho \sim T^2$, survives in the lowest temperature region. These findings are consistent with the NFFL model $^4$ and suggest that a first-order FM QPT likely exists in the pressurized Yb-compounds. Furthermore, evidence of a pressure-induced valence transition

FIG. 1: (Color online) Schematic phase diagram for the Yb compounds other than YbRh$_2$Si$_2$. A large-moment order, presumably FM-type, develops at a critical pressure $p_c$.

The ground-state properties in both the high-$p$ phase and the paramagnetic state can be described by LFL theory. Uniquely, in YbRh$_2$Si$_2$ (see the inset, the dot marks its location at $p = 0$) AFM phase with weak magnetic moments exists below $p_c$ and vanishes at a QCP ($p_c$) where the LFL theory is violated.
The electrical resistivity \( \rho(T) \) (I \( \parallel \) ab) for YbIr\(_2\)Si\(_2\) at various pressures. The downward curvature in \( \rho(T) \) as marked by the arrows at \( T_m \) indicates the occurrence of a magnetic transition above 8.3 GPa. Inset: The resistivity \( \rho(T) \) plotted as a function of \( T^2 \) at \( p = 6.4 \) GPa.

is revealed in YbIr\(_2\)Si\(_2\).

High quality single crystals of YbIr\(_2\)Si\(_2\) have been grown from In flux in closed Ta crucibles [13]. Depending on the synthesis conditions, YbIr\(_2\)Si\(_2\) can crystallize either in the I-type ThCr\(_2\)Si\(_2\) (I4/mmm) as in YbRh\(_2\)Si\(_2\) or in the P-type CaBe\(_2\)Ge\(_2\) (P4/nmm) structure. The P-type YbIr\(_2\)Si\(_2\) is magnetically ordered below 0.7 K, whereas the I-type is a paramagnet [13]. Here we investigate the properties of the I-type YbIr\(_2\)Si\(_2\). High sensitivity, AC four-point measurements of the electrical resistivity under high pressure were carried out in a miniature Bridgman cell (\( p \leq 10 \) GPa) and a piston-cylinder cell (\( p < 3 \) GPa), filled with either steatite (the former) or fluorinert (the latter) as pressure medium [14]. The pressure is determined from the superconducting transition temperature of Pb (or Sn) mounted inside the cell together with the samples. The experiments were carried out in a PPMS (down to 1.8 K), a home-made adiabatic demagnetization cooler (\( \sim 250 \) mK) and a commercial dilution refrigerator (\( \sim 50 \) mK).

Fig. 2 shows \( \rho(T) \) (I \( \parallel \) ab) of YbIr\(_2\)Si\(_2\) at various pressures. At \( p = 0 \), the residual resistivity \( \rho_0 \) of this sample is about 5\( \mu \Omega \text{cm} \) (RRR \( \simeq 35 \)). At \( p < 8 \) GPa, YbIr\(_2\)Si\(_2\) is a paramagnet showing a LFL ground state with \( \Delta \rho(T) = \rho(T) - \rho_0 = AT^2 \) at \( T \leq T_{FL} \) \( (T_{FL} = 150 \sim 200 \) mK) (see inset). With increasing temperature, the resistivity deviates from LFL behavior, following \( \Delta \rho(T) \sim T^\alpha \) with \( \alpha \sim 1 \). It is noted that no evidence of magnetism and superconductivity has been detected down to 50 mK even in highly pure samples (\( \rho_0 \sim 0.3 \mu \Omega \text{cm}, \ \text{RRR} \simeq 350 \)) measured in a hydrostatic piston-cylinder cell. For \( p > 8 \) GPa, a weak kink at \( T_m \) as marked by the arrows in Fig. 2 is observed in the resistivity \( \rho(T) \), which becomes more pronounced with increasing pressure. This transition closely resembles the magnetic transitions as found in other Yb-compounds [7, 9, 10, 15], suggesting a magnetic nature of the transition at \( T_m \). In this context, \( T_m \) is determined as the temperature below which \( \rho(T) \) shows a downward deviation from the \( T \)-linear resistivity as indicated by the dashed lines in Fig. 2.

In Fig. 3a, the derived values for \( T_m \) and \( T_{FL} \) are plotted as a function of pressure for YbIr\(_2\)Si\(_2\). Also included in the figure is the value of \( T_{max} \) at which \( \rho(T) \) reaches a maximum attributed to the onset of coherent Kondo scattering. The value of \( T_{max} \) usually scales with the Kondo temperature \( T_K \). In contrast to the Ce-based HF systems, \( T_{max} \) of YbIr\(_2\)Si\(_2\) monotonically decreases with increasing pressure \( (dT_{max}/dp = -11.3 \) K/GPa), becoming saturated at \( p_c \simeq 8 \) GPa above which a magnetic transition appears. Similar features of \( T_{max}(p) \) were observed also in YbCu\(_2\)Si\(_2\) [15], but not in YbRh\(_2\)Si\(_2\) [7, 8] and YbNi\(_2\)Ge\(_2\) [16]. In the latter two compounds, the
resistivity maximum at $T_{\text{max}}$ is split into two maxima under pressure, corresponding to the contributions from the Kondo effect and the crystalline-electric-field (CEF) as frequently observed in the Ce-based HF compounds.

For comparison, the magnetic transitions $T_m(p)$ of YbRh$_2$Si$_2$ (the high-pressure phase only) and YbCu$_2$Si$_2$ are included in Fig. 3(a). In all these compounds, a magnetic transition appears to abruptly develop above a certain critical pressure ($p_c \sim 8$ GPa), showing a uniform magnetic phase diagram and suggesting a first-order QPT at $p_c$. Note that one can not completely exclude the possibility that the weak magnetic transition is smeared out by the enhanced residual scattering while approaching $p_c$. The magnetic properties of these different Yb compounds appear to be rather similar at sufficiently high pressures, and one may speculate about the nature of the magnetic transition at $T_m$ from the following experimental facts: (i) In both YbIr$_2$Si$_2$ and YbRh$_2$Si$_2$, the Sommerfeld-Wilson ratio is strongly enhanced compared to other HF systems, indicating that these Yb compounds are close to a FM instability. (ii) The NMR results demonstrated that AFM fluctuations compete with FM fluctuations in YbRh$_2$Si$_2$. Upon applying pressure, FM fluctuations may dominate and, therefore, favor a FM-type magnetic structure. (iii) In YbRh$_2$Si$_2$, the $^{170}$Yb Mössbauer effect measurement suggests that the large magnetic moments in the high-pressure phase are aligned along the $c$-axis. All these features indicate that the pressure-induced transition at $T_m$ is likely of FM nature even though other possibilities can not be totally excluded at this moment. Further experiments, e.g., neutron scattering, are required to confirm its true nature.

In the NFFL model, it is predicted that the conventional LFL behavior survives well below a crossover temperature $T^*$ in both the paramagnetic state and the FM state. Above $T^*$, the NFFL model reduces to a marginal Fermi-liquid model which allows one to explain the non-Fermi-liquid (NFL) behavior observed at $T > T_{FL}$. $T^*$ usually vanishes as a magnetic QCP is approached: $T^*$ is inversely proportional to the magnetic correlation length $\xi$ which becomes divergent at a QCP. However, in the case of a first-order magnetic transition near $p_c$, $T^*$ will be finite. The experimentally observed FL behavior in the pressurized YbIr$_2$Si$_2$ is in fact consistent with the NFFL model, further supporting a FM-type transition at $T_m$.

Fig. 3b shows, for YbIr$_2$Si$_2$, the pressure dependence of $\rho_0$ and the resistivity coefficient $A$. One notes that the base temperature for data collected in the Bridgman cell is down to 250 mK for $p \leq 6$ GPa and 50 mK for $p > 6$ GPa. The fit of $A\rho = AT^2$ over 0.25K $T \leq 0.5$K can give a reasonable estimation to the coefficient $A$ for $p \leq 6$ GPa, as evidenced by the good agreement with data at lower temperatures measured either in the piston-cylinder cell ($p < 2$ GPa) or in the Bridgman cell at higher pressures ($p > 6$ GPa). An important feature here is the steep increase of both $\rho_0$ and $A$ setting in, upon increasing pressure, around 6 GPa. Similar phenomena were also observed in YbCu$_2$Si$_2$ and MnSi, the latter of which was regarded as a typical example to study the FM QPT. Since the characters of the quasiparticles, e.g., the FL ground state with a nearly pressure-independent $T_{FL}$, appears to be hardly affected while crossing $p_c$, it is unlikely that here the enhancement of both $\rho_0$ and $A$ is mainly due to spin fluctuations as usually discussed for systems at a magnetic QCP. Note that $T_{FL}$ dramatically increases as tuning away from the QCP in MnSi. Alternatively, the occurrence of these unique features in YbIr$_2$Si$_2$ might be related to a valence change as discussed below.

In most cases, intermediate-valence compounds have a much lower KW ratio $A/\gamma^2$ ($\sim 0.4 \mu\Omega cm$ mol$^2$ K$^2$ J$^{-2}$) than the HF compounds (10 $\mu\Omega cm$ mol$^2$ K$^2$ J$^{-2}$) due to the full degeneracy of the ground state. In YbIr$_2$Si$_2$ and YbCu$_2$Si$_2$, the CEF splitting $\Delta_{CEF}$ is comparable to the Kondo temperature, leading to a moderate value of the KW ratio: $A/\gamma^2 = 2 - 5 \mu\Omega cm$ mol$^2$ K$^2$ J$^{-2}$. Upon applying pressure, $T_K$ is reduced and the ground state could be strongly affected by the CEF effect. As a result, the KW ratio can be enhanced due to the reduction of the $f$-orbital degeneracy. Since $T_{\text{max}} \sim T_K \sim \gamma^{-1}$, the value of $A/\gamma^2$ can be measured by $AT_{\text{max}}^2$. In Fig.4, we plot $A$ vs. $T_{\text{max}}$ in a log-log plot, in which the dashed lines follow $A \sim T_{\text{max}}^2$. One can see that a transition takes place around $p = 6$ GPa, on either side of which $A \sim T_{\text{max}}^2$. The decrease of $A/\gamma^2$ around 6 GPa indicates a weak valence transition attributed to the change of $f$-orbital degeneracy. This assertion is further supported by the the resistivity isotherms $\Delta\rho(T,p) =$
\( \rho(T, p) - \rho_0(p) \) as shown in Fig. 5. The large decrease of \( \Delta \rho(T, p) \) (at low-\( T \)) and \( A \) below \( p \leq 6.4 \) GPa implies a weakening of electronic correlations as a result of the delocalization of \( f \)-electrons at lower pressures.

Similar features of \( \Delta \rho(T, p) \), \( \rho_0 \) and the coefficient \( A \) as demonstrated in \( \text{YbIr}_2\text{Si}_2 \) were previously found in \( \text{CeCu}_2(\text{Si}_1-x\text{Ge}_x)_2 \) at a weak first-order volume-collapse transition \( \rho_0 \). Indeed, a theoretical model based on valence fluctuations predicts a pronounced enhancement of \( \rho_0 \) and \( A \) as well as the \( T \)-linear resistivity above a crossover temperature \( T_v \) at a valence transition \( \rho_0 \), consistent with our findings here. How these two (magnetic and valence) transitions are interacting with each other remains an interesting question which can not, however, be answered based on the available results. For example, in \( \text{YbCu}_2\text{Si}_2 \) the magnetic transition appears around 8 GPa, but \( \rho_0 \) and \( A \) peak at 10 GPa, where the KW relation starts to deviate \( \rho_0 \). On the other hand, in \( \text{YbIr}_2\text{Si}_2 \) the valence transition appears prior to the magnetic transition. Interestingly, the valence transition seems to be accompanied by a strong enhancement of \( \rho_0 \) and \( A \).

The cause for the unique appearance of the low-pressure AFM phase in \( \text{YbRh}_2\text{Si}_2 \) \( \rho_0 \) and \( \rho_0 \) (and possibly also in \( \text{YbNi}_2\text{Ge}_2 \) \( \rho_0 \)) remains unclear. One possibility might be related to the band structure, e.g., the distinct values of the density of state (DOS) at the Fermi energy \( N(E_F) \), originating from the different electronic configurations of \( \text{Rh} \) and \( \text{Ir} \). While the intrasite coupling constant \( J \) between \( f \)- and conduction- electrons may experience similar modulation under pressure, the value of \( N(E_F)J \) may vary from compound to compound because of the different values of \( N(E_F) \). In \( \text{YbRh}_2\text{Si}_2 \), \( N(E_F) \) can be small because the DOS peaks just below \( E_F \). The resulting small value of \( N(E_F)J \) may favor magnetic ordering even at low pressures, while in \( \text{YbIr}_2\text{Si}_2 \) and \( \text{YbCu}_2\text{Si}_2 \) the Kondo effect may dominate in the same pressure region, leading to a nonmagnetic ground state \( \text{YbCu}_2\text{Ge}_2 \) \( \rho_0 \). These arguments are compatible with the pressure dependence of \( \rho_{max} \). \( \rho_{max} \) reaches a few kelvins in \( \text{YbRh}_2\text{Si}_2 \) \( \rho_0 \) and \( \rho_{max} \) in \( \text{YbIr}_2\text{Si}_2 \) and \( \text{YbCu}_2\text{Si}_2 \) \( \rho_0 \) at \( p_c \), indicating a predominant RKKY interaction in \( \text{YbRh}_2\text{Si}_2 \). The intersite RKKY coupling can change sign and, therefore, give rise to different type of magnetic ordering under pressure.

In summary, we have shown that a FM-type quantum phase transition is likely to exist in the \( \text{Yb} \)-compounds under sufficiently high pressure and that the related properties may be well described within the NFFL model. These findings will be essentially important for understanding the unusual properties of \( \text{YbRh}_2\text{Si}_2 \), especially its complex \( p - T \) phase diagram, and will stimulate further exploration of FM quantum criticality in the HF systems. Moreover, a weak valence transition accompanied by a huge enhancement of \( \rho_0 \) and the resistivity coefficient \( A \) appears to exist in these pressurized \( \text{Yb} \)-systems. To elucidate these remarkable properties, further experimental and theoretical efforts are highly desired.

We thank Q. Si and M. B. Salamon for stimulating discussions. HQY acknowledges the ICAM fellowship.

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