Fermi Surface Instability and Symmetry Breaking in Heavy-Fermion Compound YbBiPt

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We report resistivity measurements on the cubic heavy-fermion compound YbBiPt at ambient and hydrostatic pressures to ≈ 6 kbar and in magnetic fields to 1 T. Resistivity anisotropy sets in below the phase-transition temperature $T_c = 0.4$ K. We interpret a rise of resistivity below 0.4 K as due to partial gapping of the Fermi surface with the weak coupling energy gap of $\Delta_0/k_B T_c = 1.65 \pm 0.15$. Effects of hydrostatic pressure and magnetic field on the phase transition and heat capacity data are consistent with a spin density wave formation in a very heavy electron band at $T = 0.4$ K.

Interest in the compound YbBiPt has been sparked by the very large coefficient of the linear-in-temperature contribution to the heat capacity, $\gamma = 8$ J/mole K^2, that develops at low temperatures [1]. Inelastic neutron scattering [2] suggests that some fraction of this large γ may be due to the existence of low-lying crystal-field excitations. However, separation of these and intrinsic heavy-fermion contributions has not been possible. An intriguing aspect of this material is the existence of a magnetic phase transition at 0.4 K that manifests itself as a small but rather sharp peak in specific heat. Unlike Ce− or U− based heavy-fermion antiferromagnets, in which magnetic order creates an internal magnetic field that reduces γ below the Néel temperature, the large γ in YbBiPt persists below 0.4 K. Muon spin resonance experiments [3] have placed an upper limit on the ordered moment of $0.1\mu_B$ which is consistent with the absence of a nuclear Schottky anomaly in the very low temperature specific heat and with the absence of a strong suppression of γ below 0.4 K [1]. Although small-moment magnetism is found in heavy-fermion materials, it appears in many cases to coexist with superconductivity, e.g., in UPt$_3$, U$_{1-x}$Th$_x$Be$_{13}$, and CeCu$_2$Si$_2$ [4]. This is not the case in YbBiPt, which makes it particularly interesting. To address questions of the nature of the magnetic transition in YbBiPt and its ground state, we have studied the electrical resistivity as a function of pressure and applied magnetic fields and we argue that these results, combined with specific heat measurements, are consistent with the development of a spin density wave (SDW) below 0.4 K in a heavy-mass band of conduction electrons.

Single-crystal samples of YbBiPt were grown from an excess Bi flux [5]. X-ray diffraction confirms the samples to be face-centered cubic with the half-Heusler structure at room temperature. Neutron diffraction shows no evidence for a structural transition to 27 K [2]. Resistance measurements were made in standard 4-probe and Montgomery [6] configurations. Pressure was generated in a self-clamping Be-Cu cell [7] with Flourinet FC-75 as the hydrostatic pressure medium. The pressure at low temperatures was established from the shift in the superconducting transition of a piece of high purity lead mounted

near the sample. Specific heat was determined on ≈ 16 mg of YbBiPt using a semiadiabatic technique.

Results of 4-probe ac resistivity measurements are displayed in Fig. 1(a) for several rod-shaped samples in which the current flow was close to being parallel to the (100) crystallographic direction. Below the phase transition temperature T_c of 0.4 K, the resistivity curves no longer fall on top of one another; either an increase or a decrease in resistivity is observed for different samples. The rise in resistivity below T_c, found in most samples, suggests a decrease in the number of conduction electrons that could arise from partial gapping of the Fermi surface. To ascertain whether the different behavior among samples shown in Fig. 1(a) is a sample-to-sample variation or an inherent property of YbBiPt, we performed resistivity measurements on a single-crystal square platelet in Montgomery arrangement [6]. The two pairs of the long edges of the platelet were found to be closely parallel to crystallographically equivalent (100) and (010) directions. We pass excitation current along
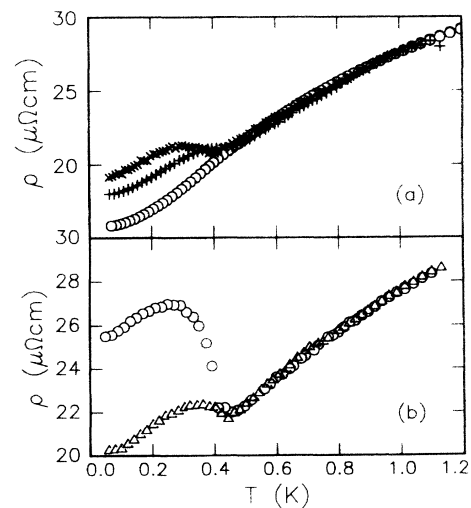

FIG. 1. Resistivity of the YbBiPt: (a) three different rod-shaped samples, (b) Montgomery type thin platelet sample, with excitation current applied along (100) and (010) directions.

one of the edges of the sample and detect the voltage drop along the opposite edge for both pairs of edges. We can then extract resistivities in the directions along the two edges [6]. The result of such a measurement and analysis on one sample is shown in Fig. 1(b). We see that the resistivity becomes markedly anisotropic, and the cubic symmetry, apparent above T_c by the coincidence of the two resistivity curves, is broken below $T_c = 0.4$ K. Behavior similar to that shown in Fig. 1(b) has been observed [8] in face-centered cubic Cr, which exhibits an SDW transition at 311 K. This SDW gaps part of the Fermi surface along the direction of the SDW ordering vector $\vec{Q}$, with a corresponding increase in resistivity along the same direction. However, in the case of Cr the anisotropy must be brought out by applying magnetic field or uniaxial stress to the sample to align randomly oriented [with $\vec{Q}$ along three equivalent (100) directions] domains. In YbBiPt, however, we see anisotropy without changing external parameters (magnetic field or stress), which is a highly unusual situation. It implies that there are very few large domains in the sample or that the domains are oriented to a high degree, perhaps by internal stress developed during material growth.

Hydrostatic pressure has been an important tool for investigating the SDW transition in Cr. The transition temperature is suppressed rapidly by pressure, at the rate of $(dT_N/dP)_{P\to 0} = -5.1$ K/kbar [9]. Such a strong dependence on pressure is seen as a consequence of the delicate Fermi-surface nesting that results in an SDW transition. Figure 2 shows the effect of hydrostatic pressure on the resistivity of YbBiPt. Application of a rather small pressure, between 0.78 and 1.20 kbar, suppresses any resistive signature for the low-temperature phase transition. Such high sensitivity to relatively small pressure again is consistent with the 0.4 K transition in YbBiPt being due to a Fermi-surface instability.

Extending the analogy with Cr, we have analyzed the resistivity curve shown by open circles in Fig. 1(b) following McWhan and Rice's [10] approach to Cr. If the total conductivity is $\sigma = \sigma_1 + \sigma_2$, where indices 1 and 2 refer to the ungapped and gapped regions of the Fermi surface at zero pressure and magnetic field, then the change in conductivity produced by the SDW is given by

$$\frac{\sigma_p - \sigma_g}{\sigma_p} = \frac{R_g - R_p}{R_g} = \frac{\sigma_{2p}}{\sigma_p}\left(1 - \frac{\sigma_{2g}}{\sigma_{2p}}\right). \quad (1)$$

Here the subscripts g and p refer to the case when the region 2 of the Fermi surface is gapped or made paramagnetic, respectively, by application of pressure. In using Eq. (1), we assume that neither relaxation times nor σ_1 are affected by the ordering [10], and that R_p, the paramagnetic background that has to be subtracted, is given by the $p = 1.2$ kbar curve of Fig. 2. The ratio σ_{2g}/σ_{2p} is given by [11]
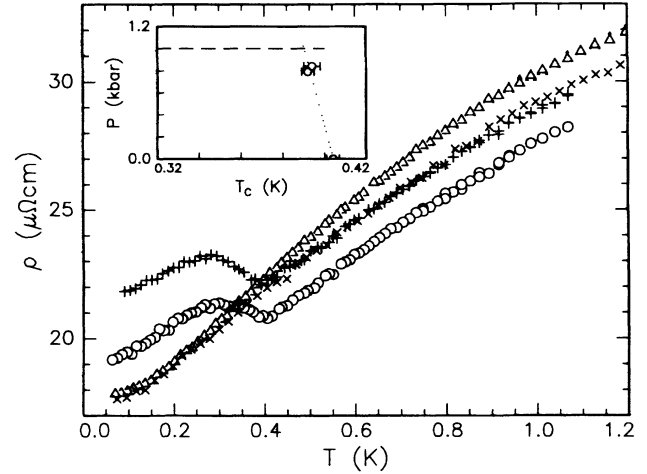

FIG. 2. Resistivity of a single-crystal rod-shaped sample of YbBiPt under hydrostatic pressure: ○, 0 kbar; +, 0.78 kbar; ×, 1.20 kbar; △, 4.20 kbar. Inset: transition temperature T_c versus applied hydrostatic pressure, obtained from the kinks in the curves of the main body of figure. Dashed line: approximate pressure that suppresses the low temperature phase. Dotted line passes through the data points, with a slope $(dT_c/dP)_{P\to 0} = -14$ mK/kbar. The low temperature phase is suppressed by pressure between 0.84 and 1.20 kbar.

$$\frac{\sigma_{2g}}{\sigma_{2p}} = \int_{-\infty}^{+\infty} d\xi \frac{\Delta^2}{E^3}\frac{1}{e^{\beta E} + 1}, \quad (2)$$

where $E^2 = \xi^2 + \Delta^2$, $\beta = 1/k_B T_c$, and $\Delta(T)$ is the temperature-dependent gap opened on the Fermi surface by the SDW. In the model [12] used to derive Eq. (2), the gap equation is identical to a Bardeen-Cooper-Schrieffer (BCS) equation and, therefore, $\Delta(T)/\Delta(T = 0) = f_{BCS}(T/T_c)$, where $f_{BCS}(T/T_c)$ is the BCS function for the temperature dependence of the gap with $f_{BCS}(0) = 1$. Analyzing the data in this way, we find (Fig. 3) that the ratio $\sigma_{2p}/\sigma_p = 0.33$. Best fits to the data in Fig. 3 are obtained with $\Delta_0/k_B T_c = 1.65 \pm 0.15$. This is close to the minimum value of 1.764 for the two-band model of itinerant antiferromagnetism [12] used by McWhan and Rice. However, Δ_0 can appear to be suppressed if the magnitude of the gap varies substantially over the Fermi surface area that takes part in ordering. For comparison, in Cr it was found [10] that $\Delta_0/k_B T_N = 2.3$ and $\sigma_{2p}/\sigma_p = 0.3$.

To further investigate this transition we performed a series of resistance measurements in a magnetic field. The two samples used were of a "Montgomery type" thin square platelets, each oriented to have one pair of long edges along the magnetic field. Figure 4 displays the resulting magnetic-field–temperature phase diagram for the low-temperature phase of YbBiPt. For both the temperature and magnetic field sweeps the phase transition was marked by a kink in the V/I traces [13]. The solid curve is a BCS energy gap scaled to pass through the points $(T_c = 0.4 \text{ K}, H = 0)$ on the x axis and
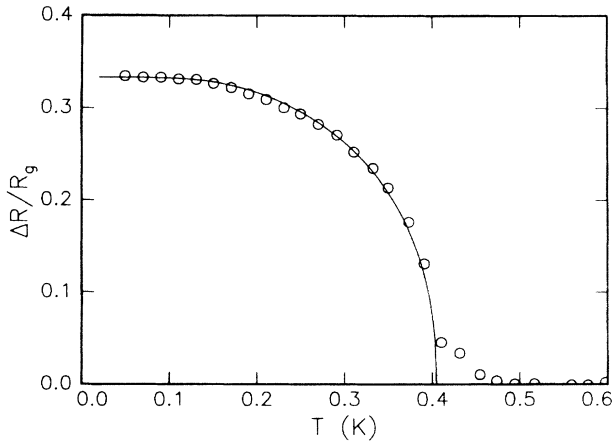
FIG. 3. Relative resistivity increase for the sample of Fig. 1(b), for the direction of the larger increase. The solid line is the result of Eqs. (1) and (2) with $\sigma_{2p}/\sigma_p = 0.333$ and $\Delta_0/k_B T_c = 1.6$.
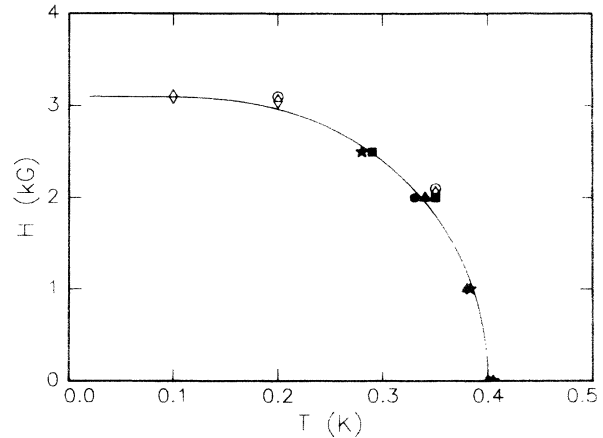

FIG. 4. Magnetic-field–temperature phase diagram for low-temperature phase of YbBiPt. The solid and open symbols are results of the temperature and magnetic field sweeps, respectively. Different symbols correspond to several different samples studied. The solid line is a BCS curve fixed by the points $(H, T = 0)$ and $(H = 0, T_c)$.

$(T = 0, H = 3.1$ kG) on the y axis. The curve fits the data very well, indicating the weak-coupling nature of the transition in the whole temperature range studied. In contrast to Cr, in which T_N is independent of magnetic fields up to $H = 16$ T [14], YbBiPt follows mean-field prediction expected of an itinerant antiferromagnetism.

Within an SDW picture of the 0.4 K phase transition in YbBiPt, it is now possible to make a rough estimate of the heavy-fermion contribution to the low-temperature specific heat, which as mentioned is one of the central issues raised by YbBiPt. Figure 5 shows C_p vs T near T_c, which is similar to the data reported previously [1]. An equal-area construction, shown by the dashed line, gives the ideal change in heat capacity at T_c of $\Delta C = 0.47 \pm 0.1$ J/mole K. The resistivity analyses above indicate that YbBiPt follows weak-coupling BCS theory, and consequently $\Delta C/\gamma T_c$ should be equal to 1.43. To proceed further we need an estimate of the percentage of the Fermi surface that is gapped. This estimation is complicated by the formation of large domains that are responsible for anisotropic resistance below T_c. In polydomain samples (like Cr) the resistivity is averaged with respect to the direction of the SDW wave vector, and it can serve as a good estimate of the gapped fraction of the Fermi surface. We obtain an "effective polydomain" estimate by averaging relative resistivity changes at $T = 0$, similar to that shown in Fig. 3, for all available data on different samples. The relative resistivity change so obtained is $(\Delta R/R_g)_{\text{ave}} = (\sigma_{2p}/\sigma_p)_{\text{ave}} \approx 0.16$. Taking this number as an approximate percentage of the Fermi surface that is gapped, i.e., contributing to ΔC, the weak-coupling relation gives a Sommerfeld coefficient $\gamma \approx 5$ J/mole K^2. This rough estimate indicates that the heavy fermion contribution can account for most (if not all, within uncertainties coming principally from the estimated

fraction of the Fermi surface that is gapped) of the low-temperature Sommerfeld coefficient γ in YbBiPt.

YbBiPt is not the first heavy-fermion system where the existence of an SDW phase has been suggested. The first and only other candidate so far has been the $T_0 = 17.5$ K phase transition in URu_2Si_2 [15], where a rise in resistivity at the transition temperature and an exponentially decreasing heat capacity below T_0 have been interpreted within SDW hypothesis. Analysis of the heat capacity data gave a value of the energy gap as $\Delta_0 = 7.2 k_B T_0$, with about 40% of the Fermi surface removed by the formation of the SDW state [15]. In spite of extensive experimental and theoretical work on the nature of the 17.5 K phase transition in URu_2Si_2 since original investigation, the pre-
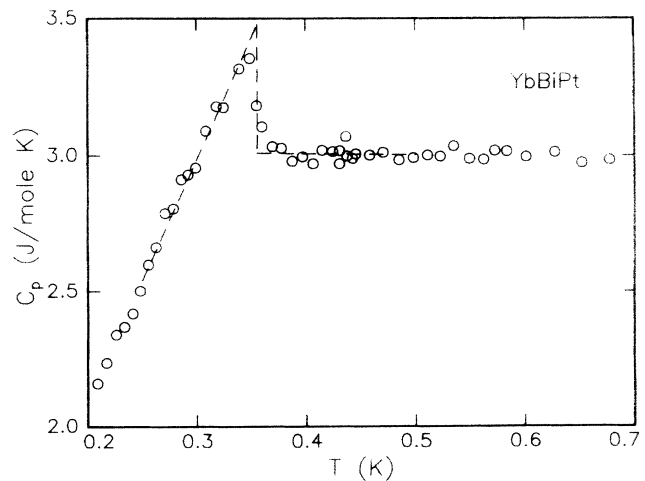

FIG. 5. Heat capacitance of YbBiPt, with equal area construction for estimating the jump in C_p at T_c.

cise picture of the magnetic order below $T_0 = 17.5$ K "remains an enigma" [16]. Consensus, however, is shifting towards a complicated ordering of local moments. Given that YbBiPt may be the first clear case of a heavy-fermion system where antiferromagnetism is of itinerant character, with Fermi surface nesting occurring in the very heavily renormalized bands.

In summary, below $T_c = 0.4$ K the resistivity of YbBiPt becomes highly anisotropic, indicating that the cubic symmetry is broken below T_c. The rise in resistivity along some directions of the lattice is consistent with partial gapping of the Fermi surface. From an analysis of the temperature dependence of the resistivity increase below T_c, we conclude that the gap is described by a weak-coupling energy gap $\Delta(T) = \Delta_0 f_{BCS}(T/T_c)$ with $\Delta_0/k_B T_c = 1.65 \pm 0.15$. The H-T phase diagram is that of a classic weak-coupling transition, with the phase boundary closely following BCS theory. We suggest that these observations are consistent with a spin-density wave transition in YbBiPt at 0.4 K that gaps a part of the Fermi surface. This identification is supported further by the extreme pressure dependence of the transition temperature. Analysis of the specific heat near T_c in view of this interpretation indicates that the SDW occurs within a strongly renormalized band of heavy fermions that accounts for much of the low temperature Sommerfeld coefficient $\gamma \approx 8$ J/mole K^2.

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