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Quantum criticality in $YbRh_2Si_2$

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Abstract

We discuss recent low-temperature measurements on single-crystalline samples of the heavy fermion compounds $YbRh_2(Si_{1-x}Ge_x)_2$ ($T_K = 30$ K) with $x = 0$ and 0.05 (nominal). Both show weak antiferromagnetic (AF) order at $T_N = 70$ and 20 mK respectively. At the field-induced quantum critical point (QCP) that occurs at $B = B_c \approx 0.06$ T ($B \perp c$) for the pure compound, non-Fermi-liquid properties are observed down to the lowest accessible temperatures (≈10 mK). These are caused by quantum critical AF fluctuations predominating over the competing ferromagnetic ones. At $B = 0$ and for $T_N < T < 0.3$ K, both compounds show a magnetic susceptibility which follows a Curie–Weiss law with a surprisingly large effective moment of 1.4 μ_B, and a Sommerfeld coefficient of the electronic specific heat which deviates towards large values from the theoretically expected $(-\log T)$ dependence observed above $T = 0.3$ K. This observation is in striking contrast to the linear T dependence of the electrical resistivity found down to $T \approx 10$ mK. It suggests a break up of the heavy fermion in the approach to the $B = 0$ QCP that occurs at a slightly larger Ge concentration.

1. Introduction

Heavy fermion (HF) metals are ideally suited to studies of quantum criticality which has become of increasing interest, especially after the discovery of high-temperature superconductivity in the cuprates. HF metals contain a dense lattice of certain lanthanide (4f) or actinide (5f) ions which are, at sufficiently low temperatures ($T \ll T_K$, the Kondo temperature), strongly coupled to the surrounding Fermi sea of delocalized (s, p, d) conduction electrons.

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In this way the local magnetic 4f(5f) moments that exist well above T_K are eventually screened by the conduction electrons, yielding the formation of unusual electronic quasiparticles, the 'heavy electrons' or 'heavy fermions'. These are 'composite fermions' consisting of a dominating local f ('spin') part which is complemented by an itinerant conduction electron ('charge') component.

HF metals sometimes lie so close to an antiferromagnetic (AF) instability that a modest pressure or chemical doping is sufficient to bring the metal to its quantum critical point (QCP), at which $T_N \to 0$ in a continuous way. In the vicinity of the QCP, pronounced deviations from the behaviour of a heavy Landau Fermi liquid (LFL) with regard to physical properties are observed. These so-called non-Fermi-liquid (NFL) phenomena are related to the action of strong low-lying AF spin fluctuations (associated with the QCP) that mediate the coupling between the quasiparticles. Two different theoretical scenarios have been proposed to describe this AF QCP: a spin density wave (SDW) and a localized moment (LM) scenario. In the former scenario [1–7], magnetic properties are associated with the spin polarization of the Fermi surface, and NFL behaviour results from the scattering of quasiparticles off the quantum critical spin fluctuations in the magnetization. Three-dimensional (3D) spin fluctuations only couple strongly to quasiparticles along *hot lines* around the Fermi surface separated by the wavevector $\boldsymbol{Q}$ of the AF order. The remaining part of the Fermi surface is largely unaffected by the quantum critical fluctuations. Only in the case of strong magnetic frustration may the 3D system of AF spin fluctuations ('spin fluid') be decoupled into 2D spin fluids. In this case only, all quasiparticles on the Fermi surface may be scattered by the quantum critical fluctuations (2D SDW scenario). Very recent inelastic neutron scattering (INS) experiments on $CeCu_{6-x}Au_x$ ($x = 0.1$) have revealed an anomalous energy over temperature, E/T, scaling in the critical component of the AF spin fluctuations, found to be virtually independent of wavevector, i.e. local in nature [8, 9]. This has led to the proposal [9–11] that the LM scenario, in which the internal structure of the composite fermions is seriously taken into account, is more adequate for HF metals than the (itinerant) SDW scenario.

2. Field-induced quantum critical point: $YbRh_2Si_2$

The compound $YbRh_2Si_2$ (tetragonal $ThCr_2Si_2$ structure) appears to be another exemplary system to demonstrate the applicability of the LM scenario. This material lies remarkably close to a QCP [12]. It exhibits a tiny AF ordering temperature $T_N = 70$ mK that can be suppressed by a small magnetic field $B_c \approx 0.06$ T (applied perpendicular to the c-axis, figure 1(a)). For this configuration, i.e. for the field applied in the easy magnetic plane, the low-T isothermal magnetization $M(B)$ shows a strongly nonlinear response (figure 2). For $T < T_N$ a pronounced reduction in the slope of $M(B)$ occurs above B_c, which indicates the suppression of AF order and the transition into a field-aligned state. A smooth extrapolation of $M(B)$ from $B \gtrsim 0.06$ T towards $B = 0$ reveals a tiny value of the ordered moment, $\mu_s \lesssim 10^{-2}\,\mu_B$, in agreement with results of recent μSR experiments [13]. It is this same small moment which becomes polarized by a field $B \gtrsim B_c$, while the major fraction of the magnetic Yb^{3+} moments are undergoing quantum fluctuations constituting a heavy LFL state on either side of the critical field [14]. For fields applied along the magnetic hard direction, $B \parallel c$, the magnetization shows an almost linear behaviour (figure 2) which was found to extend to fields as high as about 56 T [15]. For $T < T_N$, a miniscule decrease in the $M(B)$ slope is observed at ≈ 0.7 T, which determines the critical field for this configuration according to $\rho(T)$ measurements [14, 15].

The two variants of an LFL state, the weakly AF ordered one for $B < B_c$ (figure 2) and the weakly polarized one for $B > B_c$, are almost degenerate as shown by the low value

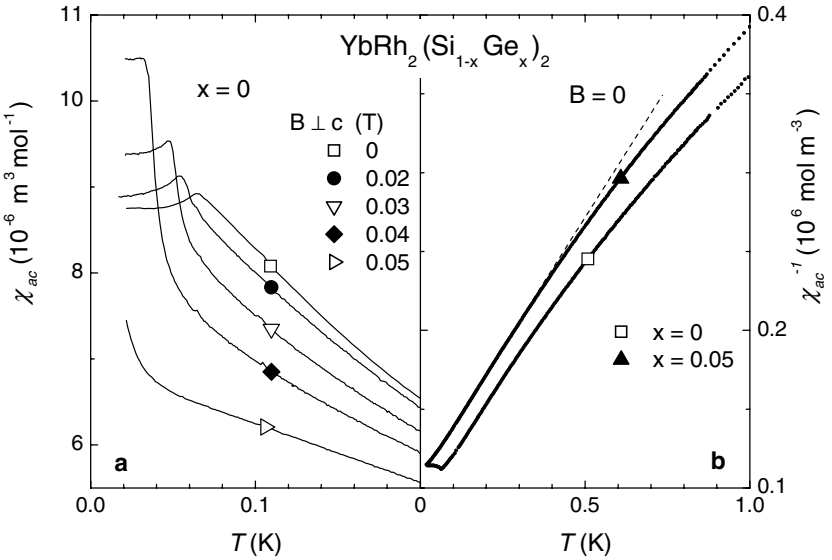

Figure 1. AC susceptibility of $YbRh_2(Si_{1-x}Ge_x)_2$ measured along the basal plane. (a) χ_{ac} versus temperature T at various superimposed dc fields for $x = 0$. (b) Inverse of the ac susceptibility χ_{ac}^{-1} versus T for $x = 0$ and 0.05. The dashed curve indicates Curie–Weiss behaviour.

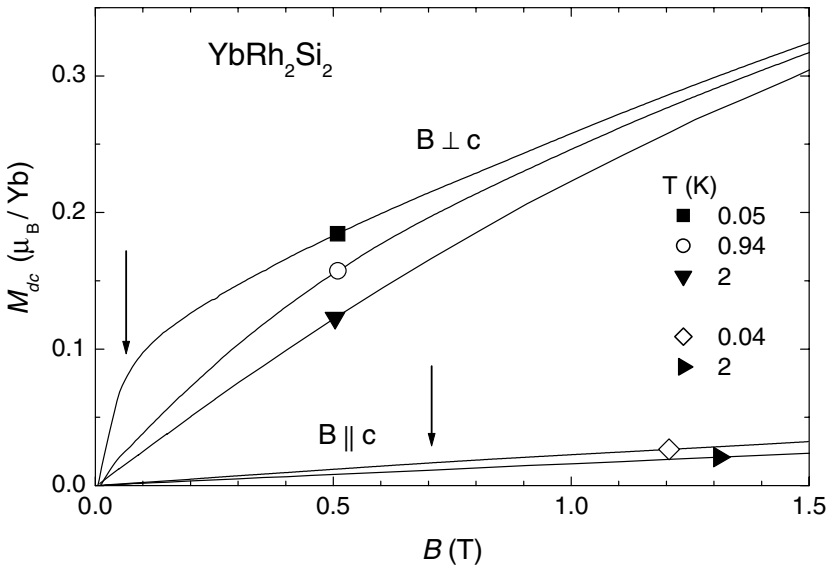

Figure 2. Isothermal dc magnetization M_{dc} of $YbRh_2Si_2$ measured at varying temperatures for fields applied along and perpendicular to the c-axis. The arrows mark the critical fields $B_c = 0.06$ and 0.7 T for $B \perp c$ and $B \parallel c$ respectively.

of the critical field. Both the pronounced increase in $\chi(T)$ which is observed in a finite field $B < B_c$ at the AF ordering temperature (figure 1(a)) and the large slope of the low-T magnetization curve at $B < B_c$ hint at the presence of *ferromagnetic* ($\boldsymbol{q} = 0$) fluctuations that are competing with the AF ones already in the magnetically ordered state ($B < B_c$). Both

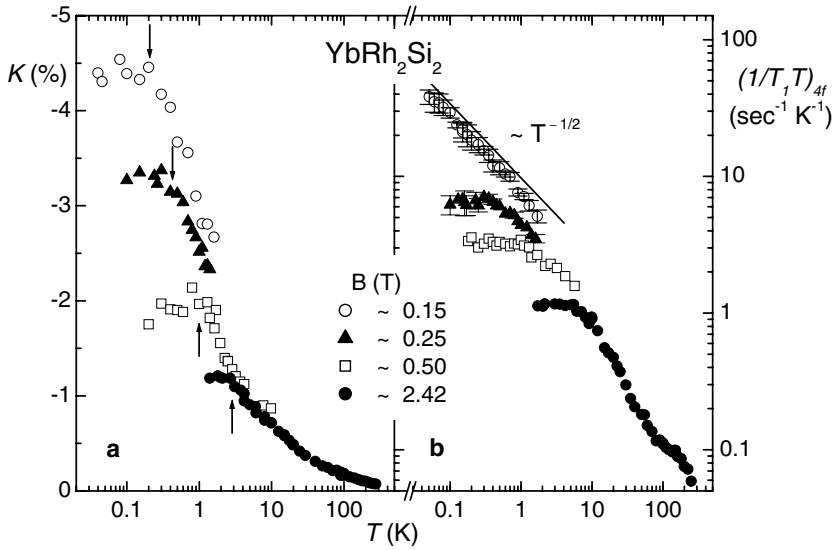

Figure 3. Results of a ^{29}Si NMR study on $YbRh_2Si_2$ at various B-fields applied perpendicular to the c-axis. (a) T dependence of the Knight shift K in a semi-log plot. Arrows indicate the temperatures below which $K(T)$ saturates. (b) T dependence of the 4f contribution of $1/T_1T$ at various fields in a double-log plot.

kinds of fluctuations have been carefully probed for $B > B_c$ by ^{29}Si NMR measurements [16]. The latter have been used to determine the Knight shift, K, which is probing the uniform static spin susceptibility $\chi'(\boldsymbol{q} = 0, \omega = 0)$ as well as the nuclear spin–lattice relaxation rate $(1/T_1)$ of ^{29}Si, which yields a $\boldsymbol{q}$ average of the dynamical spin susceptibility $\chi''(\boldsymbol{q}, \omega)$. As displayed in figures 3(a) and (b), at $B \geqslant 0.25$ T ($B \perp c$) both K versus T and $(1/T_1T)_{4f}$ versus T saturate below certain cross-over temperatures that increase with the field in either case; $(1/T_1T)_{4f}$ originating from the Yb^{3+} fluctuations only [16]. The T-independent values of K and $(1/T_1T)_{4f}$ display the field-induced LFL state. However, when approaching $B_c \approx 0.06$ T, i.e. for $B = 0.15$ T, disparate behaviour of K and $(1/T_1T)_{4f}$ is observed: while $K(T)$ flattens below $T \approx 0.2$ K, $(1/T_1T)_{4f}$ continues to increase, roughly $\propto T^{-1/2}$, upon cooling to $T \approx 40$ mK. This proves the presence of critical spin fluctuations with finite $\boldsymbol{q}$ vector near the field-induced QCP at $B = B_c$. In fact, pronounced NFL behaviour is observed [14, 17] right at the critical field for $T > 20$ mK in $\Delta\rho(T) = \rho(T) - \rho_o$ (ρ_o being the residual resistivity) as well as for $T > 40$ mK in $\gamma(T) = C_{el}(T)/T$, where the electronic specific heat has been obtained by subtracting from the raw data both the phonon contribution (determined from measurements on $LuRh_2Si_2$) and the nuclear (quadrupolar and Zeeman) contributions [18].

3. Exploring the vicinity of the B = 0 quantum critical point: $YbRh_2(Si_{1-x}Ge_x)_2$

By a small expansion of the unit-cell volume realized through low doping of the larger Ge atoms on Si sites one can, in principle, fine-tune the Néel temperature T_N and the critical field B_c to zero without significantly changing either the electronic structure or the disorder in the material. A nominal Ge concentration $x = 0.05$ (corresponding to an effective one of $\leqslant 0.02$) was recently shown to push T_N down to 20 mK and B_c to ≈ 0.027 T ($B \perp c$) [18]. Both $YbRh_2Si_2$ and $YbRh_2(Si_{1-x}Ge_x)_2$, $x = 0.05$ (nominal), show very similar behaviour at $B = 0$ in their corresponding paramagnetic states. For $T > 0.3$ K, the magnetic susceptibility

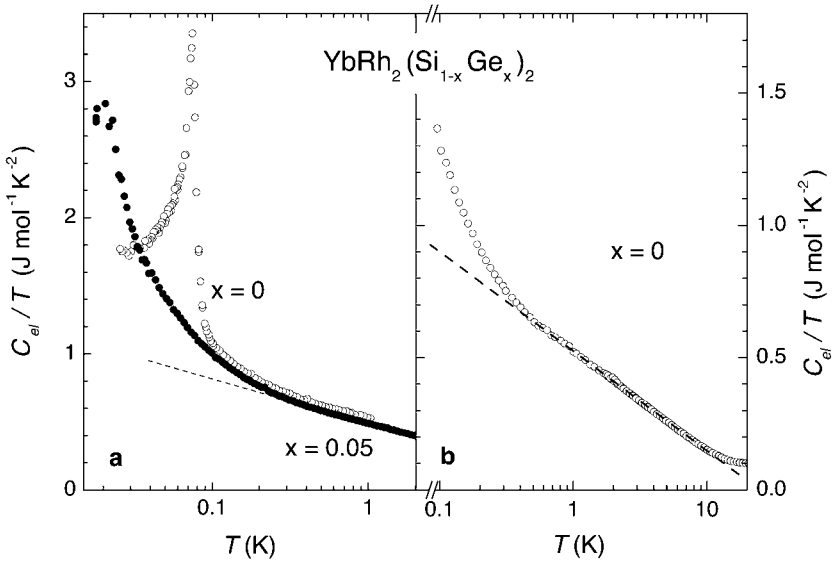

Figure 4. Zero-field electronic specific heat divided by temperature for $YbRh_2(Si_{1-x}Ge_x)_2$ as a function of temperature (on a logarithmic scale): (a) $x = 0$ and 0.05 (0.01 K $\leqslant T \leqslant$ 2 K); (b) $x = 0$ (0.1 K $\leqslant T \leqslant$ 20 K).

follows $\chi^{-1} \propto T^{\alpha}, \alpha \approx 0.75$, up to $T \approx 1.5$ K, while $\gamma(T) \propto -\log T$ up to $T \approx 10$ K (figure 4(b)). These results support the conclusions drawn from earlier measurements on the quantum critical material $CeCu_{6-x}Au_x$ ($x = 0.1$) [9] and the underlying recently proposed LM scenario [10, 11].

However, at lower temperatures $T_N < T < 0.3$ K, both $\chi(T)$ and $\gamma(T)$ deviate from the behaviour described above: the uniform magnetic susceptibility is well described by a Curie–Weiss law implying a surprisingly large effective moment $\mu_{\rm eff} \approx 1.4\ \mu_B$ and a Weiss temperature $\Theta \approx -0.3$ K for both compounds (figure 1(b)). This paramagnetic moment exceeds the small ordered moment by more than two orders of magnitude. It appears hardly affected by the Kondo interaction which is most surprising in view of the fact that our experiments are carried out at temperatures two orders of magnitude lower than the Kondo temperature $T_K \approx 30$ K [18]. Whether or not this unique feature is yet another consequence of the ferromagnetic component in the magnetic fluctuation spectrum discussed above has to be explored by future INS experiments. Below $T = 0.3$ K, where $\chi(T)$ follows a Curie–Weiss law, the Sommerfeld coefficient of the electronic specific heat starts to deviate towards larger values departing from the $-\log T$ dependence (figure 4(a)). This 'upturn' continues in $YbRh_2(Si_{0.95}Ge_{0.05})_2$ to $T \approx 20$ mK if a small critical field $B_c = 0.027$ T ($B \perp c$) is applied. Related volume thermal expansion $\beta(T)$ measurements revealed a similar observation. The low temperature ratio $\beta(T)/T$ deviates stronger than logarithmically to absolute larger values. Since thermal expansion is insensitive to both impurity and hyperfine contributions, the low-T upturn in $\beta(T)/T$ supports the intrinsically electronic, rather than extrinsic or nuclear, origin of the upturn in $\gamma(T)$. We therefore ascribe this unique feature to the critical fluctuations associated with the zero-field quantum phase transition that exists at a slightly larger Ge concentration.

In contrast to $\gamma(T)$, which deviates from the canonical $-\log T$ dependence below $T \approx 0.3$ K, the electrical resistivity follows a strictly linear T dependence from $T \leqslant 10$ K down to $T = 10$ mK, the lowest temperature accessible in the experiment (figure 5). This striking

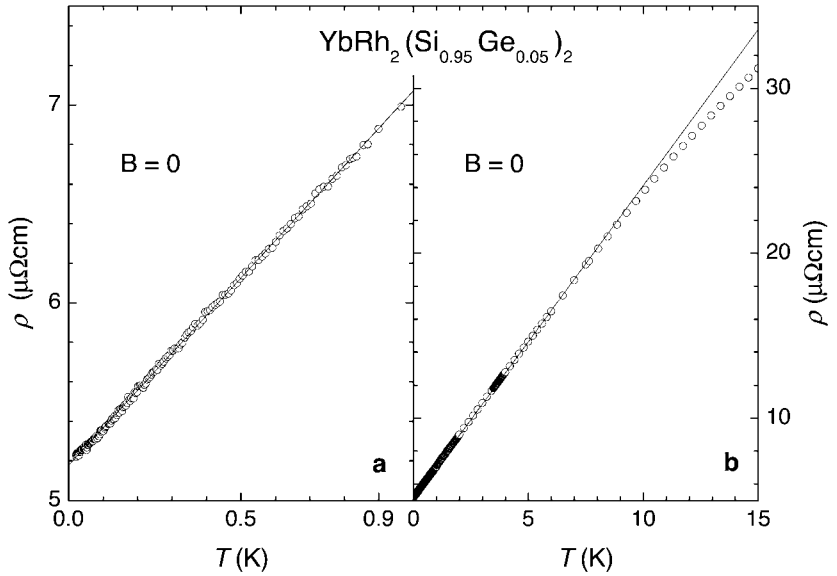

Figure 5. Zero-field electrical resistivity ρ of $YbRh_2(Si_{0.95}Ge_{0.05})_2$ versus temperature T for $T < 1$ K (a) and up to 15 K (b). The solid line represents $\Delta\rho = (\rho - \rho_o) \propto T$. The onset of AF ordering at $T_N \approx 20$ mK is masked by the alloying-induced disorder which causes a residual resistivity $\rho_o \approx 5.2\ \mu\Omega$ cm (cf also [12]).

disparity at low T between the thermodynamic quantity $\gamma(T)$ and the transport property $\Delta\rho(T)$ suggests that the dominating local f component of the composite fermions, probed by $\gamma(T)$, is more sensitive to the nearby AF order than is their itinerant counterpart, probed by $\Delta\rho(T)$. The observed disparity may thus be viewed as a direct manifestation of a real break-up of the composite fermion in the approach to the QCP.

4. Conclusion

We have discussed a number of challenging observations on samples of undoped and slightly Ge-doped $YbRh_2Si_2$:

(1) A very low critical field separates, for $T \ll T_N \approx 70$ mK in the pure compound, two almost degenerate heavy LFL states from each other. Both the weakly AF ordered one ($B < B_c$) and the weakly polarized one ($B \gtrsim B_c$) show competing ferromagnetic and AF fluctuations, the latter becoming critical and dominating the NFL behaviour observed at the field-induced QCP ($B = B_c$).

(2) For both $x = 0$ and 0.05 (nominal), the zero-field uniform susceptibility follows, in the range $T_N < T < 0.3$ K, a Curie–Weiss law with an almost unquenched paramagnetic moment of $\mu_{eff} \approx 1.4\ \mu_B$, in spite of the high Kondo temperature $T_K = 30$ K.

(3) Disparate temperature dependences in the Sommerfeld coefficient of the electronic specific heat and the electrical resistivity in the same temperature range where $\chi(T)$ obeys the Curie–Weiss law, suggest a disintegration of the HF into its local f-spin part and its itinerant conduction electron component.

Acknowledgments

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