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Field and pressure response of Yb compounds close to a quantum critical point

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Abstract. $YbCu_{5-x}Al_x$ provides the possibility to tune ground state properties by a change of the valence due to the Cu/Al substitution, by pressure as well as by the application of a magnetic field. Near to the critical concentration $x_{cr} \approx 1.5$ non-Fermi-liquid properties (NFL) are obvious, obeying hyperscaling. If magnetic order sets in for $x > 1.5$, the application of moderate magnetic fields quenches order and again NFL features become evident. Hyperscaling in this case indicates strongly interacting spin fluctuations.

Keywords. $YbCu_{5-x}Al_x$; non-Fermi-liquid; scaling analysis.

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1. Introduction

Phase transitions which occur at zero temperature are presently the subject of thorough theoretical and experimental studies. For recent reviews see e.g., refs [1,2]. By applying some non-thermal parameters like pressure, chemical composition, or magnetic field to appropriate systems, a phase transition like that from the magnetically ordered to the paramagnetic state may be driven continuously towards $T \to 0$. Such transitions are called quantum phase transitions (QPT) and are controlled by quantum fluctuations as a consequence of Heisenberg's uncertainty principle.

The majority of real objects used to study the various extraordinary features associated with a QPT is actually selected from the group of heavy fermion compounds. Such systems are thought to be defined from a subtle interplay of the Kondo coupling strength ($T_K \propto \exp[-1/JN(E_F)]$) and the RKKY interaction ($T_{RKKY} \propto [JN(E_F)]^2$), where $N(E_F)$ is the density of states of the conduction band at the Fermi energy E_F and J the s–f coupling constant. For a certain intermediate value of $JN(E_F)$, both mutual processes may bring about magnetic ordering at $T = 0$, providing a model class of compounds for the study of QPT. The pronounced spin fluctuations associated with the QPT eventually cause a breakdown of the Fermi liquid (FL) scenario and non-Fermi-liquid (NFL) behavior possibly becomes observable. NFL is generally believed to represent a new type of a ground state in metals and is usually characterized by a number of specific low temperature features such as $C/T \propto -\ln T$ (C heat capacity) or $\rho(T) = \rho_0 + AT^n$ (ρ, electrical resistivity, ρ_0, residual resistivity); A and n are constants with $n < 2$. These particular dependencies and appropriate critical parameters associated with the phase transition have been corroborated in various theoretical studies [3–6].

In the case that heavy fermion systems are driven by substitution, pressure or magnetic fields across the quantum critical point (QCP), two different scenarios are conceivable [2]: (i) The QCP is a spin-density wave instability of the Fermi surface and NFL behavior results from Bragg scattering of electrons off a critical spin density wave. In this weak coupling approach, the electrons which form the Fermi surface on the paramagnetic and the antiferromagnetic side of the QCP are closely related to one another. (ii) In the strong coupling model, the heavy fermions of a Kondo lattice are considered to be bound states between local moments and high energy conduction electrons, which disintegrate at the QCP. Thus, the Fermi surface in the antiferromagnetic and the paramagnetic state involve different quasiparticles.

Here we aim to evaluate physical properties around the quantum critical point of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$ which are derived by substitution, magnetic fields or hydrostatic pressure. Synthesis of the samples and experimental details are described elsewhere [7,8].

2. Results and discussion

In a number of recent investigations, we have shown that owing to the Cu/Al substitution in $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$, a significant change of the electronic configuration (EC) of the Yb ion, in this series of hexagonal compounds, takes place [7,8]. While YbCu_5 behaves almost divalent ($\nu \approx 2.2$), hence the Yb ion takes up the non-magnetic $4f^{14}$ EC, an increasing Al content drives the system towards the 3+ state of Yb, which can be associated with the magnetic $4f^{13}$ EC. A particular variation of $\nu(x)$ can be read off from figure 1a, where the valence ν of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$, as derived from L_{III} measurements, is plotted at $T = 300$ and 10 K, respectively. The large change of the EC throughout the series is accompanied by a corresponding change of the various physical properties. Most impressive, long range magnetic order sets in above a critical concentration $x_{\mathrm{cr}} \approx 1.5$, with both an increase of the ordered moment and an increase of the antiferromagnetic transition temperature on further increasing the Al content [7].

The evolution of physical quantities upon the change of the Yb valence, as the temperature dependent electrical resistivity ρ, is illustrated in figure 1b. Overall shape of the $\rho(T)$ measurements demonstrates intermediate valence behavior for small values of x. For increased Al content typical features of a Kondo lattice are obvious, with a maximum in $\rho(T)$ at $T_\rho^{\max}$. Since, according to Cox and Grewe [9], $T_{\mathrm{K}} \sim T_\rho^{\max}$, a significant decrease of T_{K} on increasing values of x becomes evident. Thus, the reduction of T_{K} makes it likely that long range magnetic order is possible beyond $x_{\mathrm{cr}} \approx 1.5$.

The Al related decrease of T_{K} cannot be attributed to chemical pressure, since the Cu/Al substitution enlarges the unit cell volume [8]. Hence, changes of the electronic structure, associated with the Cu/Al substitution, may influence details of $JN(E_{\mathrm{F}})$. Optical reflectivity measurements [10] evidence that the increase of Al in $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$, depletes n/m^* continuously where n is the carrier density and m^* the carrier effective mass. In conjunction with a reduction of the plasma frequency, a decrease of $|JN(E_{\mathrm{F}})|$ *via* the decrease of $N(E_{\mathrm{F}})$ can be concluded.

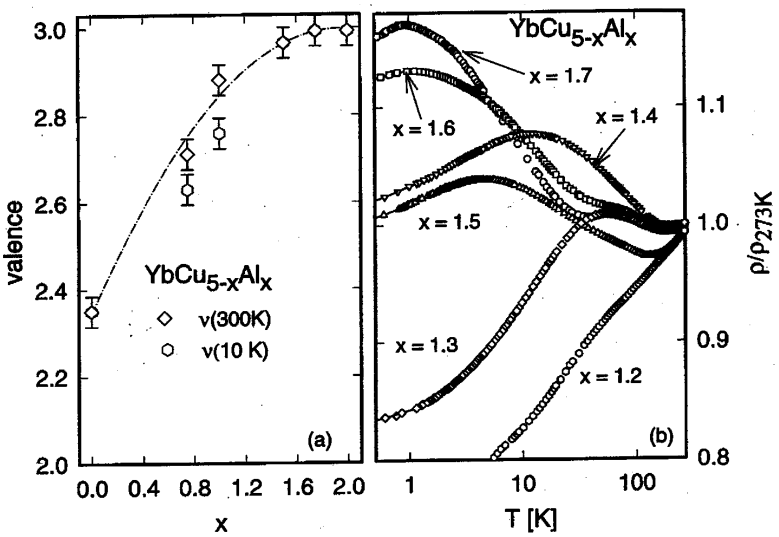

Figure 1. (**a**) Concentration and temperature dependence of valency ν of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$. (**b**) Temperature dependence of electrical resistivity ρ of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$.

2.1 *Concentration induced NFL in* $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$

Previous studies of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$ substantiated that the critical concentration for the appearance of magnetic order is $x_{\mathrm{cr}} \approx 1.5$ [8]. Outlined in figures 2a–c is the temperature dependent specific heat $C(T)$ of $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$ for different magnetic fields. Figure 2a shows $\Delta C/T$ vs. log T, where ΔC is observed from the raw data after subtracting a core contribution. At zero external fields $\Delta C/T$ behaves logarithmically down to about 300 mK; below this temperature, however, $\Delta C/T$ tends to flatten out. As the external magnetic field rises, the logarithmic behavior vanishes and an almost temperature independent behavior becomes evident, signalling a FL scenario.

In order to test whether or not $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$ is at the quantum critical point, the self-consistent renormalization (SCR) model of Moriya and Takimoto [5] can be taken to describe $C(T)$. A least squares fit to the experimental data is displayed in figure 2a, revealing $T_0 = 3.5$ K, $y_0 = 0.05$ and $y_1 = 11$, where y_0 measures the distance to the QCP. The finite – although small – value of y_0 indicates that $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$ is not directly at the QCP; nevertheless it proves that this sample is next to a phase transition at $T = 0$.

To additionally survey the proximity to a phase transition at $T = 0$, a Grüneisen analysis is applied to the pressure dependent resistivity measurements performed on various concentrations of $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$, where $T_\rho^{\max}(x, p)$ serves as the characteristic temperature. The electronic Grüneisen parameter Γ_e follows from $\Gamma_e = -\partial \ln T_{\mathrm{K}}/\partial \ln V = B\partial \ln T_{\mathrm{K}}/\partial p$ [11] where B is the bulk modulus of the system, and becomes unusually large for systems at the QCP. Previously we have shown that Γ_e exhibits a maximum for $\mathrm{YbCu}_{3.6}\mathrm{Al}_{1.6}$ ($\Gamma_e \approx -150$) [8], while $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$ shows $\Gamma_e \approx -80$. Comparing both values proves the SCR analysis that $\mathrm{YbCu}_{3.5}\mathrm{Al}_{1.5}$ is slightly away from the QCP of this series.

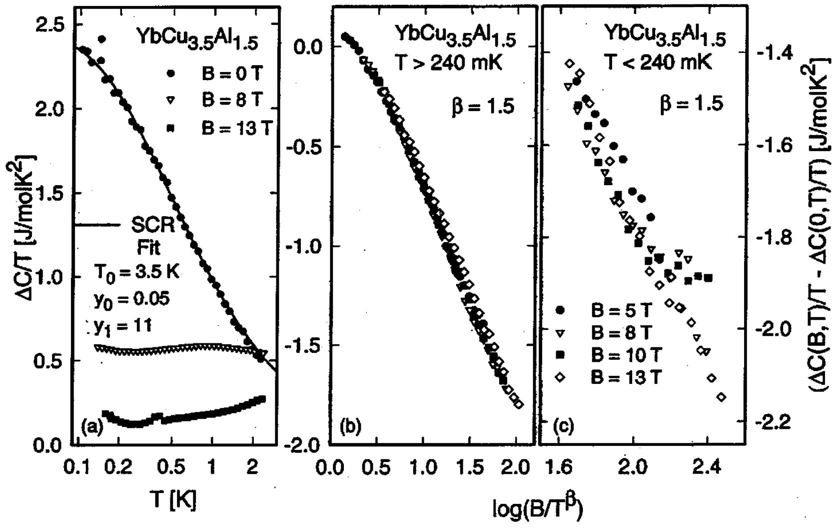

Figure 2. (**a**) Temperature dependent specific heat of $YbCu_{3.5}Al_{1.5}$ plotted as $\Delta C/T$ vs. log T for various values of applied magnetic fields. The solid line is a least squares fit of the SCR model. (**b**), (**c**) Scaling plots of the specific heat of $YbCu_{3.5}Al_{1.5}$.

According to Tsevlik and Reizer [3], scaling is possible for the specific heat with a critical exponent β. Plotted in figure 2b is $\Delta C(B,T)/T - \Delta C(0,T)/T$ vs. $\log(B/T^{\beta})$. By choosing $\beta = 1.5$, data for the various magnetic fields collapse onto a single graph above temperatures of about 240 mK. Below this temperature, scaling is not possible with any choice of β (figure 2c). A comparison shows that scaling breaks down at that temperature where $\Delta C(B,T)/T$ can no longer be described by a $-\log(T)$ behavior. In the scope of the SCR theory, weakly interacting spin fluctuations dominate, which, however do not result in hyperscaling. On the contrary, only systems with strongly interacting spin fluctuations, characterized by $\Delta C(B,T)/T \propto -\log(T)$, provide scaling behavior. One, therefore, may conclude that $YbCu_{3.5}Al_{1.5}$ is characterized by a crossover from strong to weak interactions when the temperature is lowered below 240 mK.

2.2 *Field driven NFL in* $YbCu_{3.25}Al_{1.75}$

According to earlier investigations [7], $YbCu_{3.25}Al_{1.75}$ orders magnetically at $T_N = 1$ K, where the Yb moments are locked in a simple antiferromagnetic structure with $\vec{k} = (1/2, 1/2, 0)$ and $\mu \approx 1\ \mu_B$.

Shown in figure 3a is the low temperature specific heat plotted as $\Delta C/T$ vs. $\log T$ for various external magnetic fields. ΔC was obtained by subtracting the nuclear contribution. Results obtained in this specific manner evidences that the phase transition at $T = 1$ K becomes suppressed and at a critical field value $B_{cr} \approx 1.4$ T, the specific heat behaves proportional to $-\log(T)$ which indicates a NFL ground state. A further increase of the field strength, however, recovers a FL.

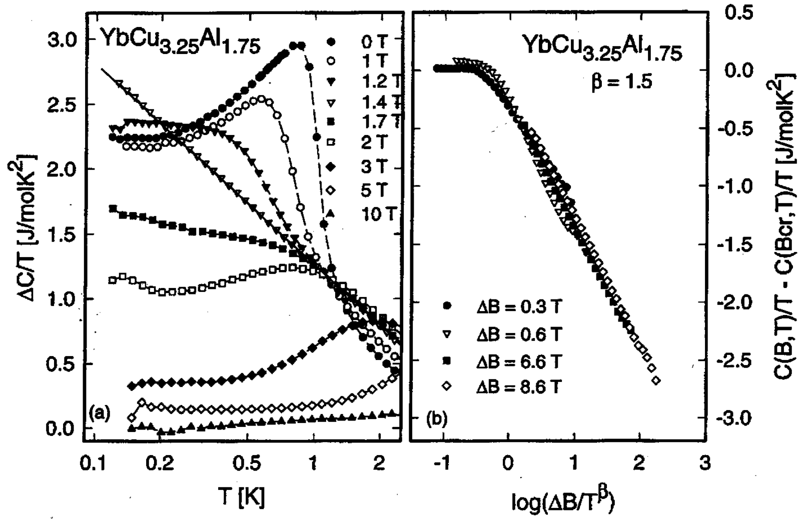

Figure 3. (**a**) Temperature dependent specific heat of $YbCu_{3.25}Al_{1.75}$ plotted as $\Delta C/T$ vs. $\log T$ for various values of applied magnetic fields. (**b**) Scaling plot of the specific heat of $YbCu_{3.25}Al_{1.75}$. The reference data are taken at $B = B_{cr} = 1.4$ T.

To decide whether field induced NFL behavior results from single ion effects or collective spin fluctuations, the specific heat data for upper critical fields ($B > B_{cr}$) are shown in figure 3b in a plot similar to figure 2, except that the zero field data are exchanged with those at the critical field. Again, the data match a single unique curve if the exponent is chosen as $\beta = 1.5$. Since $\beta > 1$, single ion effects can be ruled out as origin of the observed NFL behavior. It should be noted that scaling with the same exponent β holds also for the cases $x = 1.6$ and 1.7 [10,12].

2.3 *Concentration vs. field induced non-Fermi liquid*

The above presented data for hexagonal $YbCu_{5-x}Al_x$ reveal, unambiguously, a dramatic breakdown of the usual low temperature FL picture. This is obtained on a sample where due to substitution of Cu/Al long range magnetic order sets in at $T = 0$ ($x_{cr} = 1.5$), as well as on samples ($x > x_{cr}$) where long range magnetic order is suppressed by moderate magnetic fields. For each of the already studied members of both groups, hyperscaling of the specific heat and magnetization is observed and the relevant exponent $\beta = 1.5$ references, in both cases, to collective spin fluctuations as the origin of the observed NFL. A drastic difference between concentration and field induced NFL scenarios, however, occurs when comparing the scaling behavior in the whole temperature range: while for the field induced case hyperscaling is observed over the entire low temperature region, hyperscaling breaks down for the concentration induced example $x = 1.5$ at temperatures below about 240 mK. This observation may be associated with the fact that roughly around this temperature, $C(T)$ crosses over from the $-\log(T)$ dependence to a $\sqrt{T}$ behavior, while in the former case $-\log(T)$ is observed for the specific heat down to 100 mK. Distinct differences are also resolved for the exponent η of the low temperature susceptibility. While for the concentration induced case $\eta = 0.74$, this exponent is about $\eta \approx 0.9$ if NFL is derived via the suppression of magnetic order due to magnetic fields. A similar enhancement of η in the case of field induced NFL was also found for single crystalline Ce(Cu, Ag)$_6$ [13].

3. Summary

A number of studies on $\mathrm{YbCu}_{5-x}\mathrm{Al}_x$ evidence a valence-driven change from a nonmagnetic to a magnetically ordered ground state when the Al content increases from $x = 0$ to $x = 2$. Near to the critical concentration where magnetic order sets in ($x_{\mathrm{cr}} \approx 1.5$), significant deviations of physical properties from the FL behavior are observed and attributed to a QCP with $T_{\mathrm{N}} = 0$. Optical conductivity data [10] seem to exclude substitution related disorder as a relevant mechanism to originate NFL. While the concentration driven NFL state can be accounted for in terms of the SCR model, incorporating weakly interacting spin fluctuations, the case where long range magnetic order at finite temperatures is suppressed by externally applied magnetic fields calls for a proper description of collective and strongly interacting fluctuations. The scenario invoking the spin density wave model would therefore be in line with the former case and the composite fermion picture possibly accounts for the latter, where e.g., diverging effective masses at the QCP may be found. A signature could be the logarithmic dependence of the heat capacity.

Acknowledgements

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