Two energy scales and slow crossover in $YbAl_3$

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Abstract

We present results for $YbAl_3$ which show that the susceptibility $\chi(T)$, 4f occupation number $n_f(T)$ and the entropy $S(T)$ exhibit a slow crossover between the Fermi liquid and local moment regimes. In addition both $\chi(T)$ and the linear specific heat coefficient $\gamma = C/T$ exhibit low temperature peaks that imply that in addition to the Kondo scale ($T_K \approx 500$K) there is a second low temperature scale ($T_{coh} \approx 50$K) for the onset of coherence. We discuss these results in the context of Nozieres' exhaustion in the Anderson lattice.

Key words:
Intermediate valence, Anderson lattice, exhaustion

Recent theoretical studies of the Anderson lattice (AL) suggest that as the background conduction electron density n_c decreases a new low temperature scale T_{coh} for the onset of Fermi liquid coherence emerges where T_{coh} is significantly smaller than the high temperature Kondo scale T_K[1]. On this low temperature scale new peaks (in addition to those expected on the high temperature scale T_K) are predicted for the susceptibility and specific heat. Second[2], as n_c decreases, the crossover from low temperature Fermi liquid behavior to high temperature local moment behavior becomes slower than predicted for the Anderson Impurity Model (AIM). This theoretical work was motivated by the desire to understand "Nozieres exhaustion"[3], i.e. how the conduction

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electrons can screen the $4f$ spins when the number of conduction electrons n_c is smaller than the number n_f of $4f$'s in the lattice. A number of years ago, we gave evidence[4] based on the susceptibility and transport behavior, for the existence of two energy scales in the IV compound $CePd_3$. More recently we have given evidence[5] for a slow crossover of the susceptibility and 4f occupation number in the IV compounds YbXCu$_4$ (X= Ag, Cd, Mg, Tl, Zn). In this paper we give evidence *both* for two energy scales *and* for a slow crossover in the IV compound $YbAl_3$.

In Fig. 1 we plot the susceptibility and the linear coefficient of the 4f specific heat, where $\gamma_m = C_m/T$ and $C_m = C(YbAl_3)$ - $C(LuAl_3)$. The broad peaks near 100K are typical of Yb IV compounds with $T_K \sim 500$K. In addition, there is a peak at 15K in the susceptibility (first reported by Heiss *et al.*[6]) and a peak in the specific heat coefficient at $T = 0$. These additional peaks are the basic evidence for the existence of a low temperature scale, $T_{coh} \lesssim 50$K below which there is a significant change in the behavior of the compound. Evidence for this change of character can also be seen in the Hall effect, whose derivative dR$_H$/dT changes sign at 50K[7].

To demonstrate that the crossover from Fermi liquid behavior to local moment behavior is slower than predicted by the AIM (calculated in the non-crossing approximation or NCA) we proceed as in Ref. 5. We compare the data to the AIM result that holds for the measured ground state values of the susceptibility and $4f$ occupation number (which was measured using Yb L_3 x-ray absorption (XRA)). We fixed the spin-orbit splitting ($\Delta_{so} = 1.3$eV) and we fixed the width W of the conduction band, assumed Gaussian $N(E) = e^{-E^2/W^2}/\sqrt{\pi}W$, to give the same specific heat coefficient that we observed in $LuAl_3$ ($\gamma =$ 4mJ/mol-K^2). The values of the f-level energy E_f and the 4f/conduction hybridization V that yield the measured $n_f(0)$ and $\chi(0)$ then can be determined uniquely. The values of the parameters are given in Fig.2; T_K is determined from the formula

$$T_K = (\frac{V^2}{\sqrt{\pi}W \mid E_f \mid})^{1/8}(\frac{W}{\Delta_{so}})^{6/8} W e^{\sqrt{\pi}W E_f/8V^2}$$

which includes the effect of spin orbit splitting but ignores crystal field splitting since $T_K \ll T_{cf}$.

Fig. 2 clearly demonstrates that the crossover to local moment behavior is slower than expected based on the Anderson Impurity Model and Fig. 1 demonstrates the existence of a new low temperature scale for $YbAl_3$. In the theory of the Anderson lattice, such results are expected[1,2] as the conduction electron density decreases from the value $n_c = 1$ appropriate to a half-filled band when $n_f = 1$. In our recent work[5] on YbXCu$_4$ we assumed a one-band model and deduced n_c from the value for the corresponding Lu compound us-

ing the formula $n_c = 1/eR_H(\mathrm{Lu}X\mathrm{Cu}_4)$. We then found that the slow crossover emerged when the number of electrons per atom (the number per formula unit divided by the number of atoms in the formula unit) decreased below the value unity. The strongest deviations occurred for $YbMgCu_4$ where $n_c \sim 0.5$/atom. Using the same approximations for $YbAl_3$ we deduce from the Hall coefficient of $LuAl_3$[7] that $n_c \sim 0.5$/atom. Hence, while the conduction electron density is not low for $YbAl_3$, it is (in this approximation) as low as other compounds where strong deviations from the AIM are observed. (We note in passing that the conduction electron density of $CePd_3$, the other IV compound where two energy scales are clearly observed, is less than 0.1 carrier/atom[4].)

Measurement of the spin dynamics through inelastic neutron scattering is crucial for understanding the microscopic differences that occur on the low temperature scale. Results[8] in polycrystals indicate that in addition to the usual Lorentzian excitation centered at $E_0 = 40$meV, which energy corresponds to the high temperature Kondo scale (for the parameters of Fig. 2 the AIM predicts $E_0 = 39.6$meV), a new excitation centered at 30meV arises below 50K. Further work on single crystals is needed to address this issue.

Work at UC Irvine was supported by UCDRD funds and by the UC/LANL Personnel Assignment Program. Work at Polytechnic was supported by DOE FG02ER84-45127. Work at Lawrence Berkeley National Laboratory was supported by DOE DE-AC03-76SF00098. Work at Los Alamos, as well as the XRA experiments which were performed at SSRL, was performed under the auspices of the DOE.

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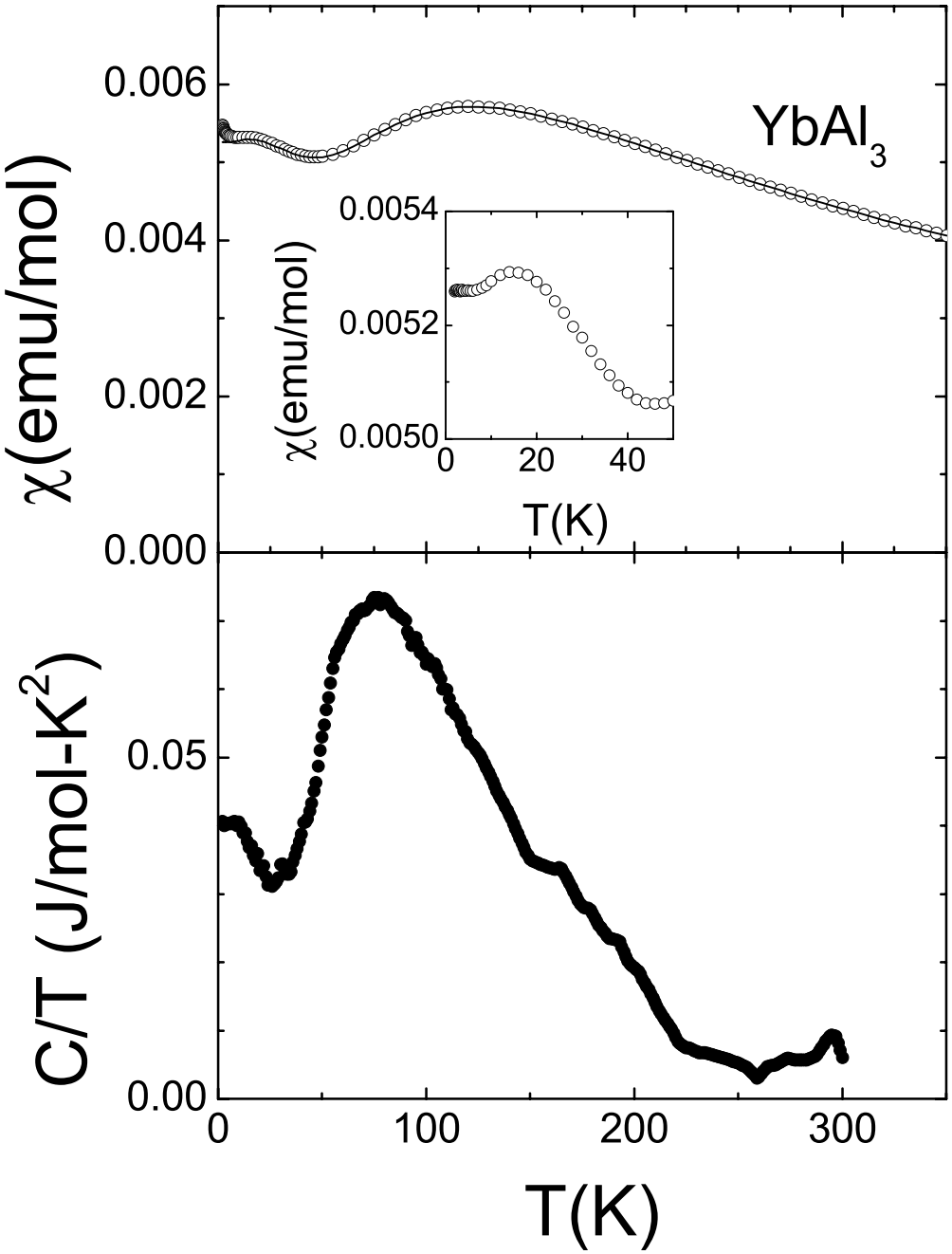
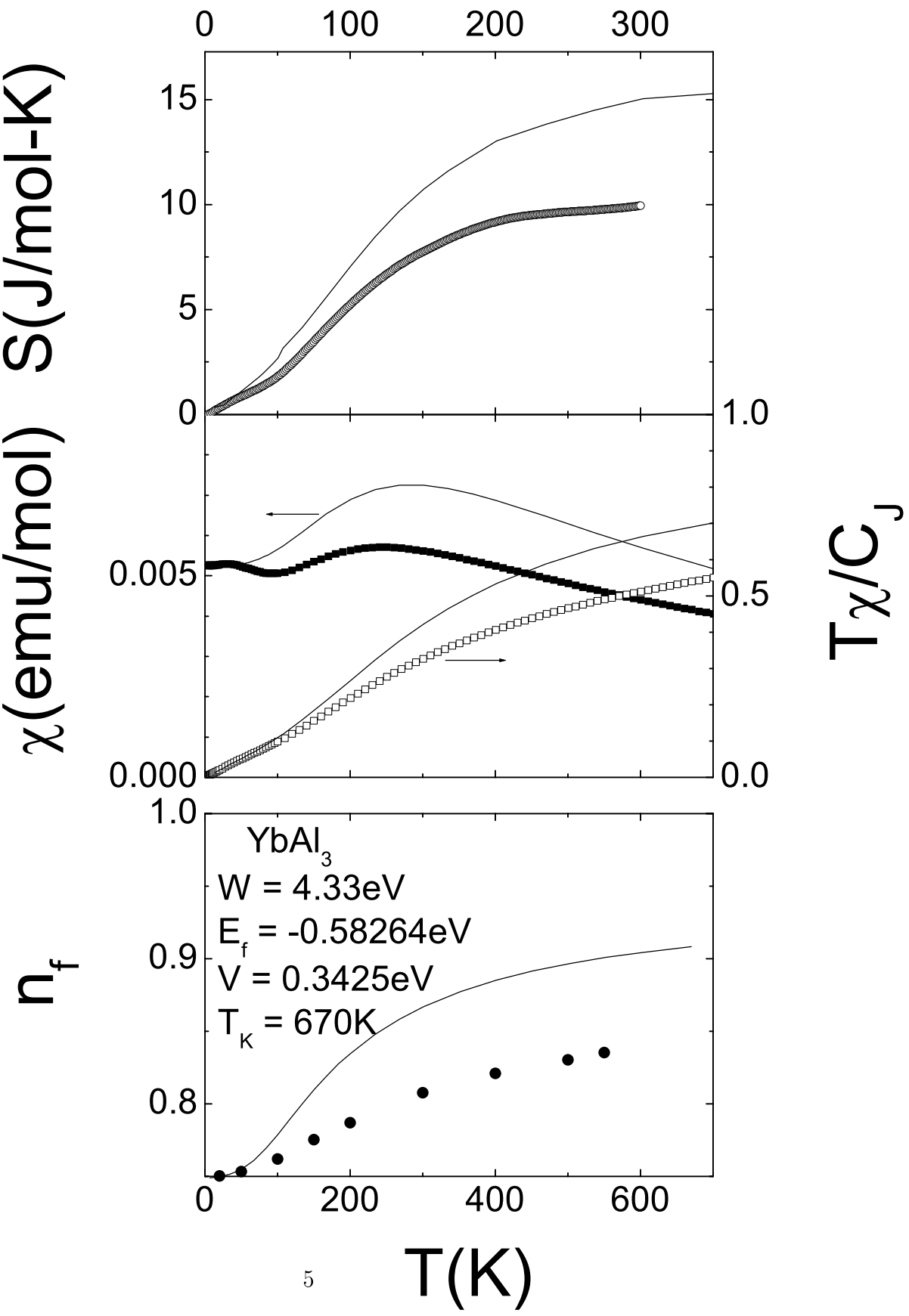

YbAl3
χ(emu/mol)
0.006
0.004
0.002
0.000
0.0054
0.0052
0.0050
0
20
40
T(K)
C/T (J/mol-K2)
0.05
0.00
0
100
200
300
T(K)


0
100
200
300
15
10
5
0
1.0
0.5
0.0
0.005
0.000
S(J/mol-K)
χ(emu/mol)
Tχ/C_J
1.0
0.9
0.8
n_f
YbAl3
W = 4.33eV
E_f = -0.58264eV
V = 0.3425eV
T_K = 670K
0
200
400
600
T(K)