# PHOTOEMISSION IN $YbCu_2Si_2$: PROBLEMS WITH THE KONDO IMPURITY MODEL

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$YbCu_2Si_2$ is a heavy fermion compound with a Kondo temperature $T_K$ of order 50K. It provides a very important test case for the Kondo impurity model of photoemission. A key prediction of this model is that there should be a "Kondo Resonance" (KR) in the valence band spectrum, located a distance $_kT_K$ below the Fermi level $\epsilon_F$ and with spectral weight proportional to $T_K$ at T = 0; furthermore the KR should renormalize to zero for $T > T_K$. We have measured the photoemission spectrum at $YbCu_2Si_2$ at 10, 77 and 300K, using the Los Alamos U3C Beam Line at NSLS. We find no temperature dependence over this interval even though a strong reduction in the $4f^{13}(J = 7/2)$ final state peak identified as the KR is predicted by the model. Furthermore, the width of the $4f^{13}(J = 7/2)$ peak is much larger than predicted for the KR. Taken together with recent photoemission results for cerium compounds these results raise serious doubts about the Kondo impurity explanation of heavy fermion photoemission.

# Photoemission in $YbCu_2Si_2$: Problems with the Kondo Impurity Model

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## Abstract

We report valence band photoemission results for $YbCu_2Si_2$. The $4f^{13}(J=7/2)$ final state peak, centered 60meV below the Fermi level $\epsilon_F$, lacks the temperature dependence and is broader than predicted for a Kondo resonance. Together with recent photoemission results for cerium compounds, these results raise serious doubts about the Kondo impurity explanation of heavy fermion photoemission.

The prevailing theory[1,2] of photoemission in heavy fermion compounds is the Kondo impurity theory in the 1/N approximation. This approach predicts that a resonance should appear in the spectrum, located (for cerium) a distance $T_K$ above the Fermi level $\epsilon_F$ (where $T_K$ is the Kondo temperature) with a spectral weight proportional $T_K$; the resonance should vanish as the temperature increases above $T_K$. We have recently shown[3] for a series of cerium compounds that there is no correlation between the spectral weights observed in the 4f peaks near $\epsilon_F$ and the known Kondo temperatures; furthermore the temperature dependence is negligible. This suggests that the spectra are not related to a Kondo resonance.

A problem for cerium compounds is that the resonance is expected to lie <u>above</u> $\epsilon_F$; hence, only the tail below $\epsilon_F$ can be observed in photoemission. For ytterbium compounds the resonance should be <u>below</u> $\epsilon_F$, and hence is directly observable[2]. In this paper we report results for $YbCu_2Si_2$, which has a Kondo temperature of order 50K as deduced from specific heat[4] or quasielastic neutron linewidth[5]. While a peak which might be identified as a Kondo resonance is observed, our main result is that we find <u>no</u> temperature dependence over a temperature interval [10,300K], and that the peak is substantially broader than predicted by Kondo theory.

Experiments were carried out at the Los Alamos U3C beamline at NSLS with supporting work at U. Wisconsin's SRC using an HA-50 hemispherical analyzer anu ERG monochromators. The total resolution varied from 60 to 180 meV depending on photon energy. Flux grown single crystals were cleaved in UHV ($7x10^{-11}$ torr). Further details are described elsewhere[3].

The spectrum at hν=182eV is shown in Fig. 1. The large peak near 4.5eV is due to Cu emission. The peaks in the interval 5-12eV arise from bulk $4f^{13}{\rightarrow}4f^{12}$ transitions while the two peaks within 3eV of the Fermi energy arise from $4f^{14}{\rightarrow}4f^{13}$ transitions, with the $4f_{7/2}$ final state closest to $\epsilon_F$ and the $4f_{5/2}$ transition at approximately 1.5eV binding energy[6]. Also included in Fig. 1 is a high resolution spectrum taken at hν=50eV. This shows that the $4f^{14}$ spectrum consisits of bulk and surface doublets, with the latter at higher binding energy. From the ratio of the $4f^{14}$ and $4f^{13}$ bulk transitions we estimate[6] that the Yb valence is 2.8-2.9 (the estimate varies somewhat with photon energy).

In the language of Kondo theory[2] the bulk $4f^{14}{\rightarrow}4f^{13}$ transitions are the Kondo resonance ($4f_{7/2}$, nearest $\epsilon_F$) and a spin -orbit sideband ($4f_{5/2}$, at 1.4eV). These should be highly temperature dependent on the scale of the Kondo temperature, 50K. To test for this we show in Fig. 2 high resolution spectra taken at hν=60eV for T=10K and 300K. (The spectra were normalized to the Cu emission peak, which should be temperature independent; the surface doublet was fitted to a pair of Gaussians and subtracted off.) It is clear that the temperature dependence is negligible.

A complication[2] arises from the known existence[7] of crystal fields in $YbCu_2Si_2$. The level scheme as deduced from neutron scattering[7] is shown in Fig. 3. The ground state doublet has a width 4meV. Excited state doublets at 12, 30 and 80meV have neutron linewidths of order 8meV; this width is believed to arise from Kondo scattering, and it gives the scale on which the crystal field Kondo sidebands should renormalize to zero[2]. The observed $4f_{7/2}$ peak near $\epsilon_F$ should be the sum of these sidebands, convoluted with instrumental resolution, as shown in Fig. 3. Direct comparison to our data for Figs. 2 and 3 demonstrates that there is no temperature dependence, neither on the scale of the ground state Kondo temperature, nor on the scale of the sideband Kondo temperature (100K); secondly the observed emission peak is substantially broader than the peak predicted by convoluting the sideband peaks with instrumental resolution.

The prediction of Kondo impurity theory that the Kondo resonance should renormalize to zero implies that the valence should approach the value 3 at high temperature[2]. Our results seem to imply that the valence remains constant. Perhaps in the Kondo <u>lattice</u> the valence is stabilized. Alternatively, photoemission may be incorrectly measuring valence, perhaps due to final state screening effects. In either case it is clear that Kondo impurity theory alone cannot explain the valence band photoemission results. Together with our results[3] for cerium compounds, this suggests serious problems for the Kondo impurity theory of heavy fermion photoemission.

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## Figure Captions

Fig. 1 Photoemission spectra of $YbCu_2Si_2$ taken at $h\nu$=182eV with 180meV resolution for T=10K. The inset, taken at $h\nu$=50eV with 60meV resolution, resolves the $4f^{13}$ final state into surface and bulk spin-orbit doublets. The peaks from 5 to 12eV represent the $4f^{12}$ final state. The valence estimated from this plot is 2.9.

Fig. 2 The $4f^{13}$ final state doublet at T=10K (closed circles) and T=300K (open circles). The photon energy is 60eV; the resolution is 90meV. The surface doublet has been fit to two Gaussians and subtracted out. No temperature dependence is observed.

Fig. 3 The $4f^{13}(J=7/2)$ final state peak, measured at $h\nu$=60eV with 60meV resolution and at T=20K. The dashed curve in both the bottom and top plots is a convolution of the reported crystal field sidebands with instrumental resolution. The data are substantially broader than this fit.

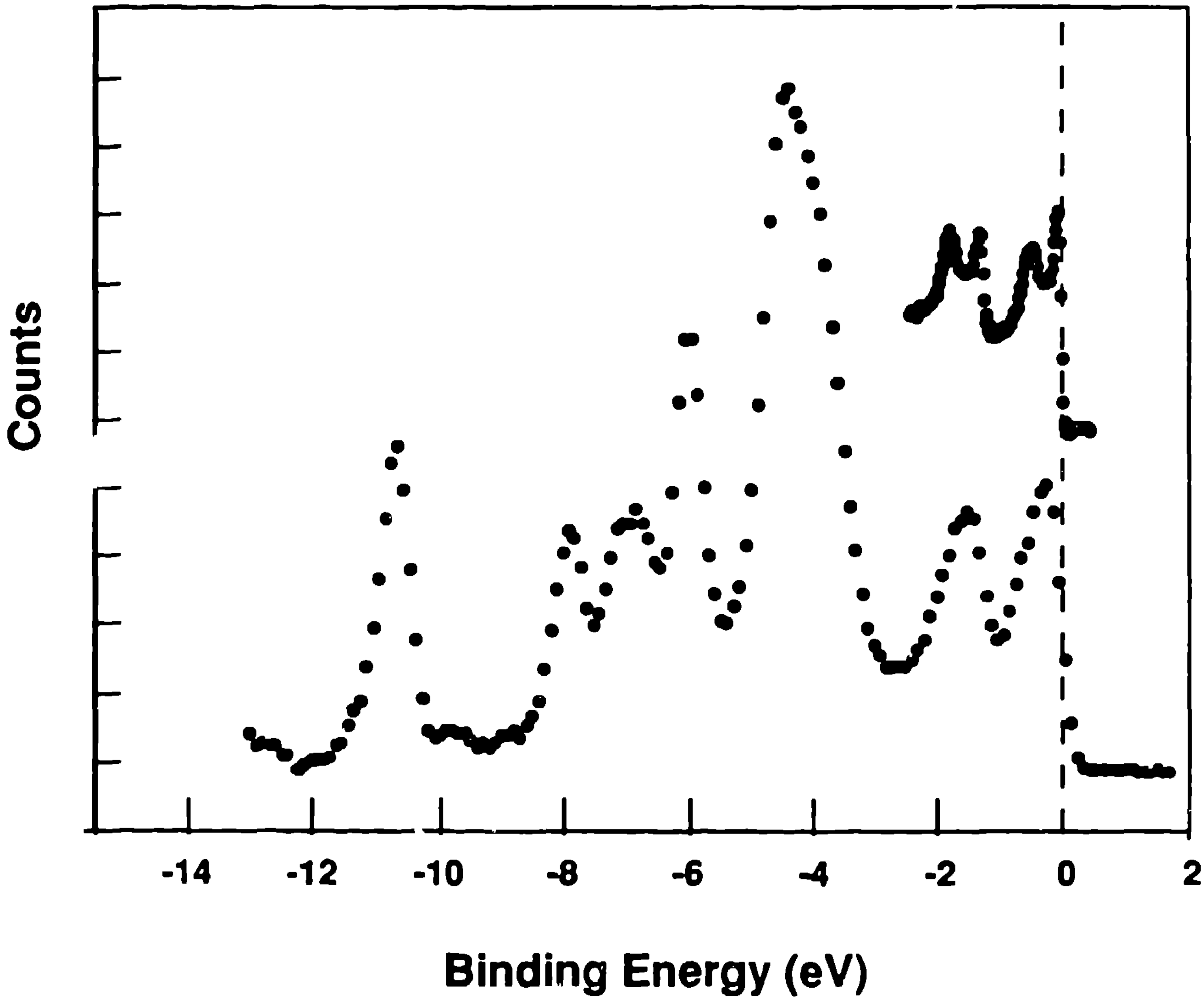


Fig 1

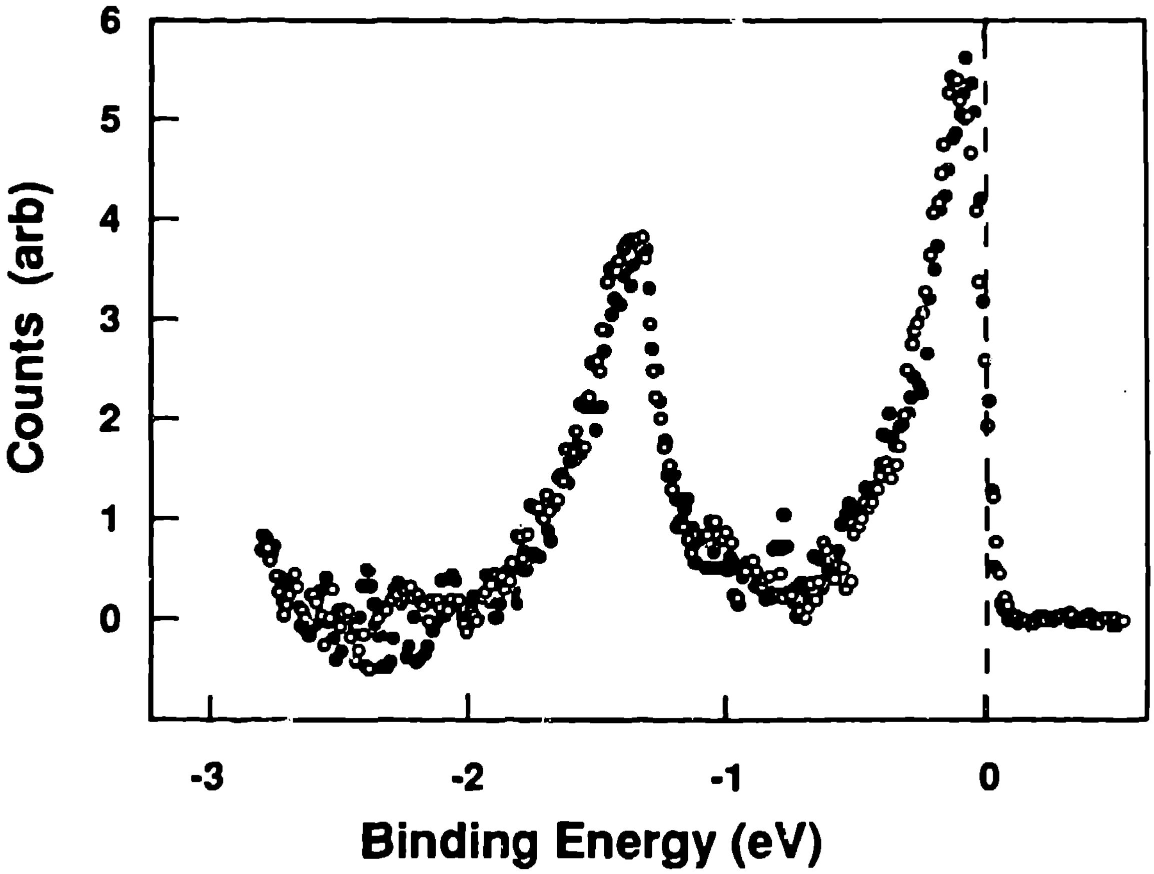


Fig. 2

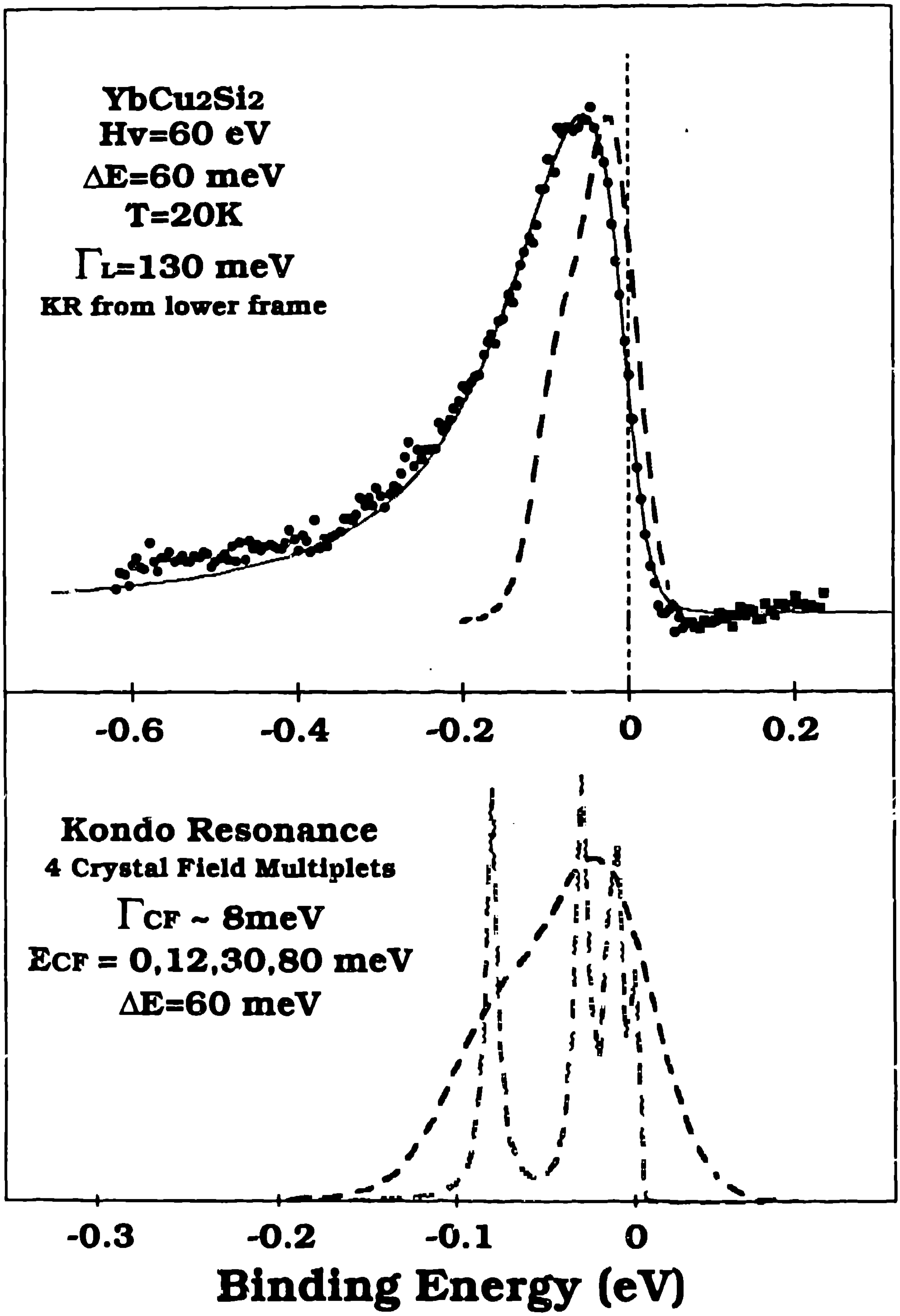
YbCu2Si2
Hv=60 eV
ΔE=60 meV
T=20K
ΓL=130 meV
KR from lower frame
-0.6
-0.4
-0.2
0
0.2
Kondo Resonance
4 Crystal Field Multiplets
ΓCF ~ 8meV
ECF = 0,12,30,80 meV
ΔE=60 meV
-0.3
-0.2
-0.1
0
Binding Energy (eV)

Fig 3