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IS YbAs A HEAVY FERMION SYSTEM?*

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Abstract

Using parameters extracted from a tight binding fit to an ab initio band structure, the specific heat anomaly observed in YbAs around 5 K is computed within the infinite U limit of the degenerate Anderson *impurity* model. Applying the renormalization procedure derived in variational treatments of the *periodic* Anderson model, a quasiparticle Fermi surface with strong nesting features and small mass enhancements is obtained. The results suggest that YbAs is not a "classical" heavy Fermion system.

Introduction

The occurence of a broad hump in the specific heat $c_p(T)$ of all Ytterbium pnictides around 5K [1,2], with no apparent relation to the Schottky anomaly expected from the crystal field splitting of the $4f^{13}\ ^2F_{7/2}$ ground state of the Yb ion measured by inelastic neutron scattering [3-5], together with the calorimetric observation of a phase transition below 1K, have lead to the conjecture that these compounds belong to the class of heavy fermion materials with a magnetically ordered ground state [6]. The magnetic origin of the phase transition was subsequently confirmed for YbP and YbAs by Mössbauer spectroscopy [7,8] and very recently a neutron diffraction experiment showed the ordering to be antiferromagnetic of type III in YbAs [9]. The existence of heavy quasiparticles in coherent Bloch states, on the other hand, has yet to be established, e.g. through a measurement of the de Haas von Alphen (dHvA) effect.

In the following we first show that the specific heat anomaly around 5K can be understood as resulting from the interplay between the crystal field and the Kondo effect on a single site. We limit our discussion to the case of YbAs, for which the growth of high quality single crystals seems to be the least problematic among all pnictides [10]. A detailed account of the method, with applications to YbN and YbP will appear elsewhere [11]. In a second step we consider the quasiparticle spectrum and in particular the effect the strong local Coulomb correlations on the area and cyclotron mass of a number of extremal orbits on the Fermi surface (FS).

The specific heat anomaly

Bethe Ansatz solutions for the Coqblin-Schrieffer (impurity) model in the presence of crystal fields [12-14] strongly suggest that the specific heat anomaly observed in the Yb pnictides around 5K is due to the Kondo effect for the ground state (Γ_6) doublet. To assess that picture we draw on our experience with the high energy spectroscopies for these compounds [15,16]

and consider the infinite U limit of the degenerate Anderson *impurity* model in the presence of CF:

$$H = H_{Band} + H_f + H_{Mix} \qquad (1)$$

where the parameters in H_{Band} and H_{Mix} are obtained from a tight binding fit to an ab initio band structure calculation. To compute the impurity partition function Z_f we introduce the empty- and occupied-site propagators $G_o(z)$ and $G_{\Gamma_i}(z)$ where Γ_i labels the CF-levels. In the non-crossing approximation (NCA) to the selfconsistent large-N (≡ degeneracy) expansion [17-20], these satisfy the following set of coupled integral equations:

$$G_o(z) = \{ z - \sum_i N_{\Gamma_i} \int |V_{\Gamma_i}(\varepsilon)|^2 G_{\Gamma_i}(z+\varepsilon) f(\varepsilon) d\varepsilon \}^{-1} \qquad (2a)$$

$$G_{\Gamma_i}(z) = \{ z - \varepsilon_{\Gamma_i} - \int | V_{\Gamma_i}(\varepsilon) |^2 G_o(z-\varepsilon) (1- f(\varepsilon)) d\varepsilon \}^{-1} \qquad (2b)$$

where ε_{Γ_i} denotes the position of the corresponding CF level (of degeneracy N_{Γ_i}) with respect to the Fermi energy and $f(\varepsilon)$ is the Fermi function. The important quantity here is $|V_{\Gamma_i}(\varepsilon)|^2$, which describes the hopping of a hole from the level Γ_i to any of the conduction bands and back. Its explicit form is given in ref. [11], and it is displayed in Fig. 1 for three CF levels of YbAs. From the relative amplitude of the coupling functions near the Fermi energy and eq. (2b) one expects the hybridisation with the conduction bands to induce a substantial shift in the position of the Γ_6 level, less so for the first excited (Γ_8) level, and almost none for Γ_7, which is consistent with the splittings $\Delta\varepsilon_{68}$ = 18 meV, $\Delta\varepsilon_{67}$ = 40 meV) observed by inelastic neutron scattering [4].

In terms of the spectral functions $\rho_o(\varepsilon)$ and $\rho_{\Gamma_i}(\varepsilon)$ associated with the propagators in eqs. (2a,b), the impurity partition function takes the form [17]:

$$Z_f = \int d\varepsilon\, e^{\beta\varepsilon} \left[\rho_0(\varepsilon) + \Sigma_i N_{\Gamma_i} \rho_{\Gamma_i}(\varepsilon) \right] \qquad (3)$$

c_p (T) is now obtained as the usual thermodynamic derivative [11,17] and as seen in Fig. 2, a peak is indeed found in the right temperature range.

The quasiparticle spectrum

Realistic quasiparticle spectra have been obtained for a number of Ce- and U-based heavy fermion systems, using the concept of renormalized bands [21-24]. The starting point in these treatments is a selfconsistent calculation in the local density approximation (LDA), with the Bloch states expanded in partial waves within atomic spheres. In its most sophisticated version [24] the renormalization consists in replacing the potential parameters for the l = 3 channel by a resonance of width T* (≡ condensation energy) for each CF level of the spin orbit ground multiplet and using the observed CF excitation energies to fix the band centers.

The simple (NaCl) crystal structure of the Yb-pnictides suggests an alternate approach, based on a tight binding fit to a fully relativistic selfconsistent LDA calculation. The resulting Slater Koster (SK) parameters can then be renormalized according to the rules derived from variational treatments of the *periodic* Anderson model [25-28]. These show that in the infinite U limit the latter is equivalent a lattice of virtual bound states, with the f-band mixing matrix elements reduced by a factor $q^{1/2}$ with respect to the original ones. For the present case of a doublet (Γ_6) localized level:

$$q = (1-n_f) / (1-n_f/2) \qquad (4)$$

where n_f is the average f (hole) occupation. From a careful analysis of the 3d core-level spectrum of YbAs [16], we find $n_f = 0.91 \pm 0.02$ and $q \approx 0.17$ (the tight binding value n_f^{TB} is 0.54, due to the contribution from the tails of neighbouring atoms to the $l = 3$ component of the electron density at the rare earth ion).

The LDA Fermi surface (FS) is displayed in Fig. 3. It consists of a closed hole surface centered at Γ and two sets of (100) hole tubes connecting at Γ as well, from which we expect a long range ($\sim 1/r^2$) Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. The renormalization of the SK parameters ($pf\sigma$), ($pf\pi$) and ($df\sigma$) lowers the Fermi energy by 10 mRy but leaves the FS topology and n_f^{TB} unchanged. The corrections to extremal areas and effective masses are listed in Table 1. The mass enhancements are small, as expected from the value of q. The same applies to the specific heat mass, which is almost an order of magnitude smaller than what is obtained by linearly extrapolating the results of Fig. 2 to zero temperature.

Conclusion

We have shown that a single site treatment is capable of accounting for the specific anomaly found around 5K in YbAs. A (admitedly primitive) renormalization of the LDA bandstructure leads to a quasiparticle mass enhancement much smaller than in the classical heavy Fermion systems, while preserving a FS topology with strong nesting features, which should favor magnetic ordering. Clearly dHvA experiments are urgently needed to clarify the nature of the quasiparticles in this compound.

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Table 1: **Fermi surface parameters for YbAs**

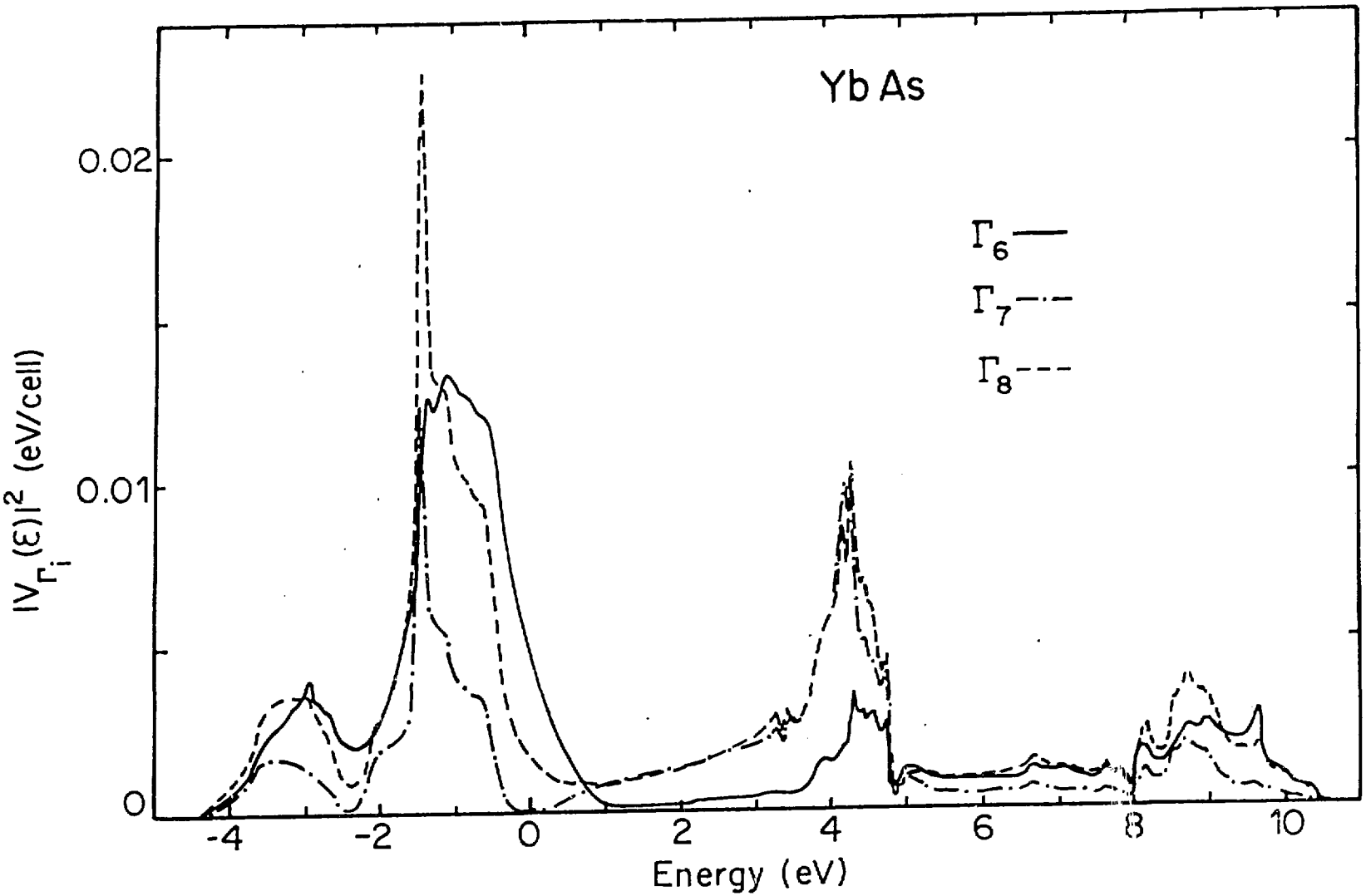
Extremal areas		area (a.u.)		effective mass (m_{el})	
H	origin	LDA	renorm.	LDA	renorm.
(100)	(000)	0.08841	0.7499	- 1.09	- 1.73
(110)	(000)	0.08872	0.7648	- 1.02	- 1.62
(111)	(000)	0.09147	0.7855	- 1.07	- 1.69
(100)	(100)	0.00569	0.00584	- 0.18	- 0.30
(111)	(000)	0.2059	0.1964	- 1.86	- 3.16
(100)	(100)	0.07091	0.05713	- 1.78	- 3.39
(111)	(000)	0.2752	0.2584	- 3.21	- 5.36

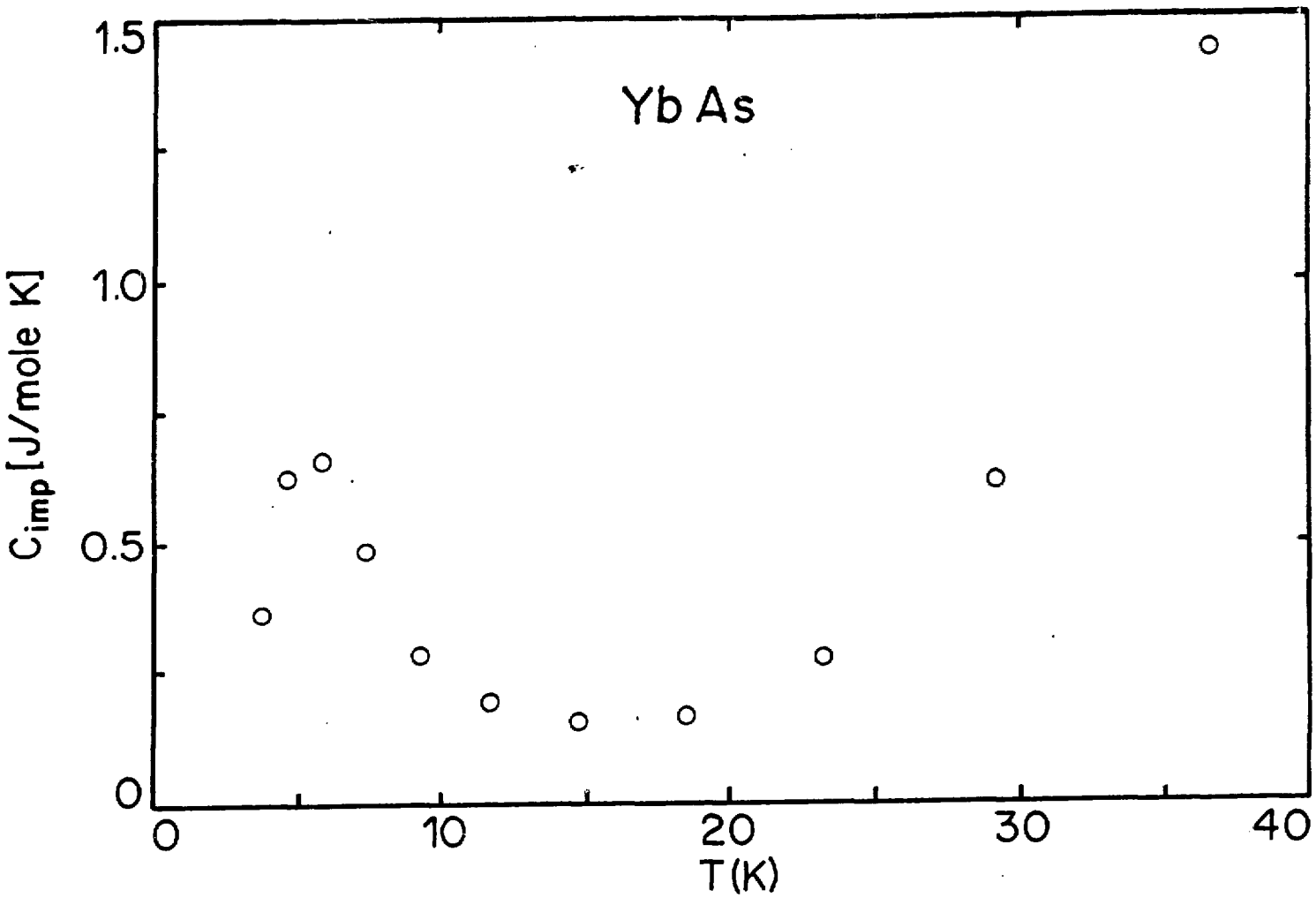
Figure Captions

Figure 1 Energy dependent coupling functions $|V_{\Gamma_i}(\varepsilon)|^2$ for the three crystal field levels Γ_6, Γ_8 and Γ_7 of a 'f hole on the ytterbium ion in YbAs.

Figure 2 Calculated specific heat of YbAs in the NCA to the selfconsistent large-N expansion approach to the degenerate Anderson impurity model.

Figure 3 LDA Fermi surface of YbAs.


Yb As
Γ_6
Γ_7
Γ_8
$|V_{\Gamma_i}(\varepsilon)|^2$ (eV/cell)
0.02
0.01
0
-4
-2
0
2
4
6
8
10
Energy (eV)


Yb As
C_{imp} [J/mole K]
1.5
1.0
0.5
0
0
10
20
30
40
T(K)

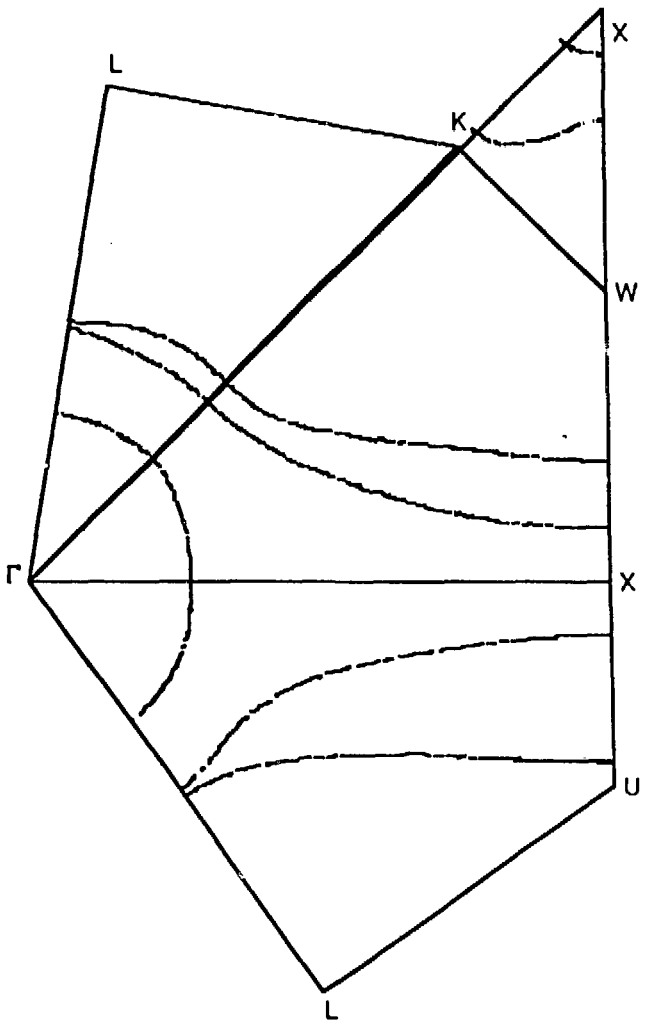


Fig. 3