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The electronic band structure and Fermi surface of YbBiPt

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Abstract. The local density band structure of the heavy-fermion compound YbBiPt is calculated using the linear-muffin-tin-orbital method. The topology of the resulting Fermi surface is investigated and found to be remarkably simple. In order to explain the observed low-field linear coefficient of the specific heat in terms of single particle excitations an enhancement of the band-structure density of states at the Fermi level by a factor of 750 is required. A corresponding enhancement of the calculated cyclotron masses would predict the existence of fermion quasiparticles with masses several thousand times that of the bare electron. The feasibility of observing such highly renormalized particles by means of the de Haas–van Alphen effect is considered.

In this paper we present a conventional one-particle electronic band-structure calculation for YbBiPt and detailed analysis of the resulting Fermi surface. This material is of interest because of its very large low-temperature linear specific heat coefficient (γ) of 8 J K^{-2} (mol Yb)$^{-1}$ (Fisk *et al* 1991), which is an order of magnitude greater than that found in the archetypal heavy fermion, UPt_3.

An important question in any system with a very large γ is whether a Fermi liquid description is valid—in particular whether the observed γ can be associated entirely with the existence of massive fermion quasiparticles. As calculations of the type presented here only use a static potential they cannot be expected to predict the dynamical mass renormalization seen in heavy fermions. They do, however, provide a starting point from which to try and understand a given material, especially as the calculated Fermi surface topology appears to provide a good description of the Fermi surface as inferred from quantum oscillatory experiments such as those using the de Haas–van Alphen (DHVA) or Shubnikov–de Haas effects. For example in UPt_3 Norman *et al* (1988) claim good agreement between their calculated Fermi surface topology and that observed by Taillefer *et al* (1987). Moreover, by noting that the average enhancement of observed cyclotron masses over the corresponding values calculated by Wang *et al* (1987) was comparable to the ratio of the measured to calculated values of γ, Taillefer and Lonzarich (1988) were able account for the observed γ entirely in terms of the quasiparticle contribution.

YbBiPt crystallizes in the cubic MgAgAs structure (Canfield *et al* 1991). This structure does not have inversion symmetry but contains only one formula unit per cell. The different atoms lie on interpenetrating face-centred-cubic lattices placed on along the body diagonal at $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, $(0,0,0)$, and $(\frac{3}{4},\frac{3}{4},\frac{3}{4})$, with a similar lattice of vacant sites at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The $(0,0,0)$ position is unique, having nearest neighbours on each side, and occupied by the Bi atoms in YbBiPt (Fisk *et al* 1991).

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Band-structure calculations on other systems having the same crystal structure as YbBiPt have be carried out previously for NiMnSb by de Groot *et al* (1983), for NiUSn by Albers *et al* (1987) and for PtMnSb by Ebert and Schütz (1991). The band structure presented here for YbBiPt was calculated using the linear-muffin-tin-orbital (LMTO) method in the atomic sphere approximation (ASA) (Andersen 1975, Skriver 1984). The local-density approximation (LDA) employing the parametrization of the exchange–correlation potential given by von Barth and Hedin (1972) was used. The LMTO basis set included s, p, d and f partial waves on each site and, because of the open nature of the crystal structure, an empty sphere was included on the vacant $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ site. A lattice constant of 6.60 Å (Canfield *et al* 1991) was used and for simplicity all the Wigner–Seitz radii were taken to be equal. The Yb f electrons were treated as valence electrons and because of the narrowness of the associated bands we found it useful to follow the approach used by Temmerman and Sterne (1990) in studying Gd and calculate the charge density directly from the wave-function coefficients rather than using the more common moment expansion. The densities of states was calculated using the variation of the linear tetrahedral method prescribed by Jepsen and Andersen (1984) and the final self-consistency cycles carried out using a dense, uniform mesh having 1664 k-points in the irreducible zone.

The spin–orbit interaction was included by adding the $L \cdot S$ coupling term to the variational Hamiltonian. As the MgAgAs structure does not have inversion symmetry Kramers' degeneracy is lifted and, given the relatively heavy atoms making up YbBiPt, the resulting splittings should be readily observable in the topology of the Fermi surface.

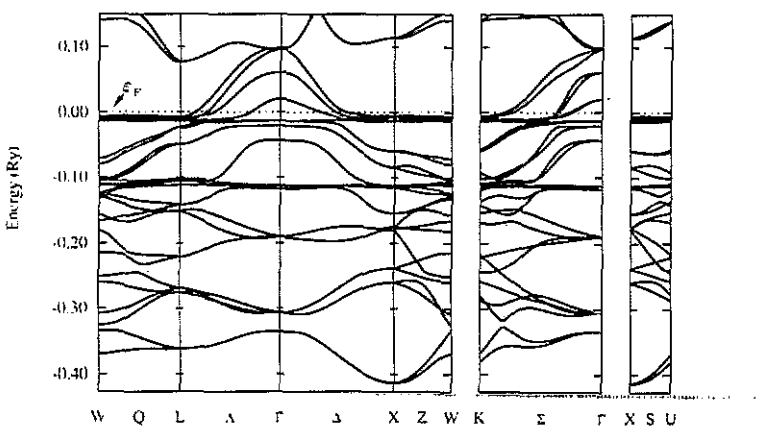

Figure 1. Energy bands along the major symmetry directions plotted relative to the Fermi level (ε_F) which is indicated by the dotted line. Two lower-energy bands of mainly Bi s character are not shown. The Yb f bands can be seen to be split into two narrow branches corresponding to $j=7/2$ and 5/2 which are respectively at 0.15 and 1.53 eV below the Fermi level.

The calculated bands along the major symmetry directions are shown in figure 1. Two lower bands of mainly Bi s-character are not shown. The Yb f-bands can be seen to split, as found in pure Yb by Min *et al* (1986), into two narrow branches corresponding to $j=5/2$ and $j=7/2$ states. These are separated by 1.38 eV with the peak of the upper $j=7/2$ branch lying just 0.15 eV below the Fermi level (ε_F). The corresponding densities of states is given in figure 2, showing clearly the two narrow

Yb f branches. The Fermi level lies on the upper shoulder of the Yb $j=7/2$ branch. The total density of states at the Fermi level, $N(\varepsilon_F)$, is 61.4 states cell Ryd^{-1} of which 60% is of Yb f character.

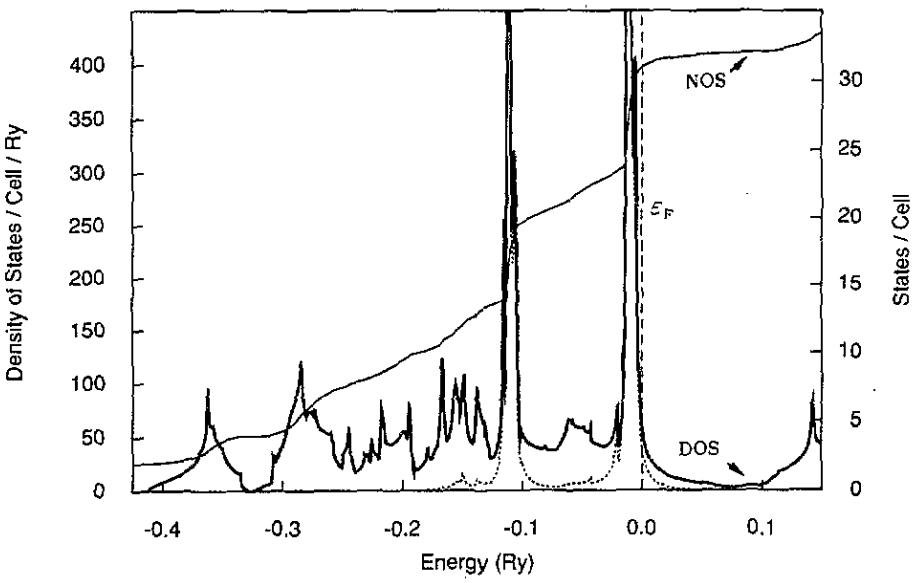

Figure 2. Calculated density of states (DOS) and number of states (NOS) over the same energy range in which the bands are given in figure 1. The Yb f contribution to the density of states is indicated by the dotted line.

The predicted Fermi surface is remarkably simple: consisting of six Γ-centred hole pockets associated with bands 27 to 32. The packing of these into the Brillouin zone is shown in figure 3, while the cross-sections of the Fermi surface in the [001], [110] and [111] directions are given in figure 4. Because of the lack of inversion symmetry the six sheets are non-degenerate and should actually be viewed as three pairs of split pseudo-spin sheets, a point that is emphasized in figures 3 and 4 by shading together the pseudo-spin pairs. In this respect the Fermi surface YbBiPt resembles that of a weak ferromagnet such as Ni_3Al (Sigfusson *et al* 1984). Note, however, that the splitting between the pseudo-spin sheets, unlike the case in weak ferromagnets, is predicted to vanish along Γ–X. As a consequence, even if a small splitting is introduced by an applied field, there still should be strong magnetic breakdown between the pseudo-spin sheets when an applied magnetic field is in the (010) plane.

The orientation dependence of the DHVA frequencies corresponding to extremal cross-sections of the predicted Fermi surface is shown in figure 5, while table 1 contains a summary of the the predicted frequencies and cyclotron masses along the major symmetry directions. In figure 5 only the breakdown orbits expected between the split pseudo-spin surfaces from bands 31 and 32 are indicated but similar orbits would also be expected between the other two pairs. As breakdown orbits are not expected when the field is in the [111] direction this orientation should be the simplest to look at experimentally.

It is well known that LDA calculations fail to predict the experimentally observed cyclotron masses; however, an estimate of the expected values can be obtained by scaling the calculated masses by the ratio of the observed γ to that calculated using

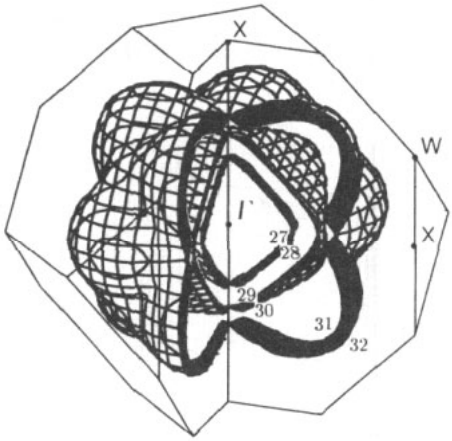

Figure 3. Packing of the sheets of the Fermi surface into the Brillouin zone. The Fermi surface consists of three pairs of of relatively simple Γ-centred hole surfaces. The splitting of the surfaces resulting from the breaking of Kramers' degeneracy, due to the combination of spin–orbit and lack of inversion symmetry, is indicated by the shading.

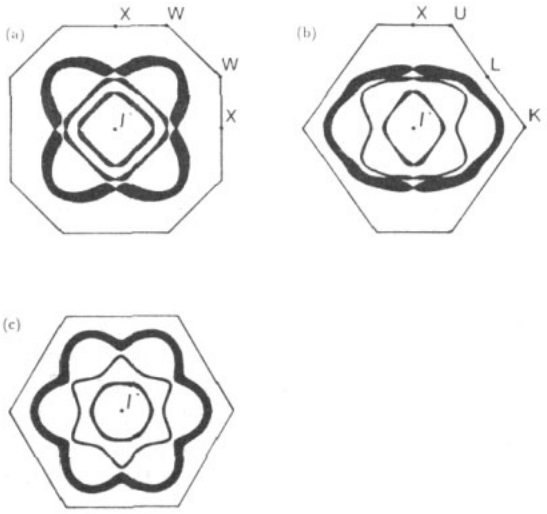

Figure 4. Calculated Γ-centred Fermi surface cross-sections perpendicular to the [100], [110] and [111] directions in (*a*), (*b*) and (*c*) respectively. The three pairs of surfaces associated with bands 27 and 28 (inner), 29 and 30 (middle) and 31 and 32 (outer) are clearly visible. As in figure 3, the splitting resulting from the breaking of Kramers' degeneracy is indicated by shading. Note that this splitting vanishes along Γ–X.

$\gamma_{\text{calc}} = \frac{1}{3}\pi^2 k_B^2 N(\varepsilon_F)$. In the present calculation $\gamma_{\text{calc}} = 10.6$ mJ K^{-2} (mol Yb)$^{-1}$ and so the estimated enhancement factor is ~ 750. The enhanced quasiparticle masses obtained by multiplying the calculated values, as given in table 1, by this factor are therefore extremely heavy. In particular the masses of the quasiparticles on orbits associated with band 32 are $\sim 4000\, m_0$. It has to be stressed that this is for zero applied field since a field of 5 T is sufficient to reduce γ, and hence the expected mass enhancement, by a factor of 5 (Fisk *et al* 1991). A DHVA study carried out in a field $\sim$ 15 T would therefore be expected to see much smaller mass enhancements—but note that even a reduction of the zero-field enhancement by a factor of 10 would still leave expected masses from band 32 over over $400\, m_0$. Observing such heavy masses will obviously pose severe experimental difficulties.

In the conventional theory of the DHVA effect (see e.g. Shoenberg *et al* 1984) the signal strength at temperature T and applied field H is proportional to $\exp(-\alpha r_0/\ell_0)/\sinh(\lambda m^* T/H)$ in which α and λ are temperature- and field-

Table 1. Summary of the theoretical de Haas–van Alphen frequencies and cyclotron masses at zero field on the major symmetry directions. All frequencies are associated with hole-type, Γ-centred orbits. As explained in the text, a crude estimate of the zero field enhanced masses can be obtained by multiplying the calculated cyclotron masses by ~ 750.

	[001]		[110]		[111]	
Band	Frequency (MG)	Cyclotron mass (m_0)	Frequency (MG)	Cyclotron mass (m_0)	Frequency (MG)	Cyclotron mass (m_0)
27	26.7	2.1	23.4	1.7	21.5	1.6
28	32.6	2.9	26.3	2.0	24.8	1.8
29	54.2	1.6	75.7	2.3	60.1	1.8
30	60.8	1.5	79.4	2.6	63.6	1.9
31	125.5	4.6	121.1	3.9	150.6	4.7
32	164.3	6.5	152.5	4.6	183.2	5.7

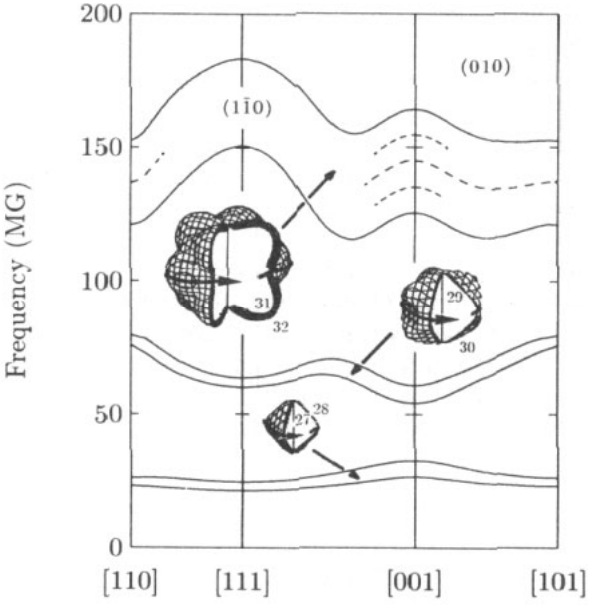

Figure 5. Calculated de Haas–van Alphen spectra at zero field indicating the origins of the various branches. The dashed lines indicate probable breakdown orbits, of which only those associated with bands 31 and 32 are shown.

independent coefficients while m^*, ℓ_0 and r_0 are the quasiparticle mass, an effective mean free path and cyclotron radius of an orbit. In general it is not possible to give an *a priori* estimate for ℓ_0 and hence the expected DHVA signal strength; but obviously the better the sample and the larger the applied field the stronger the signals will be. Provided samples of comparable quality can be grown the the results obtained with one material can be used in order to estimate the conditions required for another. For example, to see masses $\sim 100 m_0$ at 11 Tin UPt_3 Taillefer *et al* (1987) required temperatures below 40 mK and so to obtain the same signal strength with masses $\sim 1000\, m_0$ at the same field will require temperatures below 4 mK. As higher fields and greater sensitivity are now available, higher temperatures may actually suffice. Note, however, that in order to see the very high masses the suppression of the

mass enhancement resulting from the applied field will have to be minimised and consequently temperatures of only a few millikelvin will be essential.

Though the uniform scaling of calculated masses to obtain the experimental values works for many materials it fails in others. For example in $CeRu_2Si_2$ both highly and weakly enhanced branches are found to co exist (Howard 1989, Lonzarich 1988). In this case some progress has been made by the the renormalized band calculations of Zwicknagl *et al* (1990) but as yet similar calculations have not been carried out for YbBiPt.

We have also carried out a number of variations on the band-structure calculation as described above. Calculations carried out using the combined correction terms, with different Wigner–Seitz radii on the different sites and omitting the empty sphere, all lead to only minor changes in the predicted Fermi surface. The calculated density of states at the Fermi energy, and hence estimate of the mass enhancement, varied more markedly between calculations. For example inclusion of the combined correction terms positioned the Fermi level further down the shoulder of the Yb f peak in the density of states leading to a decrease in the total density of states by 30%.

There is some question about how the Yb f electrons should actually be treated in a LDA calculation in order to make comparison with experiment. Because of this we also looked at the effects on the Fermi surface of freezing varying numbers of Yb f electrons in core. With 14 f electrons in core the Fermi surface was found to consist of only two pairs of pseudo-spin Γ-centred hole surfaces, the larger of which came very close to forming Cu-like necks at W. On the other hand, freezing 13 f electrons in the Yb core leads to a semi-metal with a Fermi surface consisting of small pockets around Γ, L and between Γ and X. Because of the differences in the calculated topologies an experimental Fermi surface study should be able to determine the correct way to treat the Yb f electrons unambiguously.

The simplicity of the predicted Fermi surface together with the expected large quasiparticle masses single out YbBiPt as a material well worth investigating using the de Haas–van Alphen effect. The large expected masses mean, however, that the success of any such study will depend crucially on the experimental conditions. In particular high-quality samples and temperatures of a few millikelvin will be required.

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