The Hall Number in YbRh$_2$Si$_2$

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Recent experimental studies have revealed an abrupt change in the Hall number at a field tuned quantum critical point in the heavy fermion magnet YbRh$_2$Si$_2$. We investigate this by calculating the local density band structure for this metal and the appropriate transport integrals. We find the Fermi surface to be multi-sheeted with the two largest sheets having opposite sign contributions to the Hall number. Small changes in the f electron occupation are sufficient to reproduce the observed large change in the Hall number. This suggests that YbRh$_2$Si$_2$ may be the first example of a quantum critical valence fluctuator.

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The nature of the magnetic quantum critical point and the associated non Fermi liquid behavior in heavy fermion metals is a subject of active debate [1,2]. One of the most interesting suggestions is that at the quantum critical point, the Fermi surface would transform from a large surface on the paramagnetic side (with the f electrons participating in the Fermi surface) to a small Fermi surface on the magnetic side (with the f electrons decoupled from the Fermi surface) [3]. These authors suggested that the Hall number would be a good test for this scenario.

YbRh$_2$Si$_2$ has emerged as the classic example of a heavy fermion quantum critical point. An advantage is that it is stochiometric, and the crystal structure is relatively simple. This metal shows pronounced non Fermi liquid behavior in the vicinity of a field induced quantum critical point, including a log T divergence of the specific heat coefficient which turns into a power law divergence at sufficiently low temperatures, and a linear T behavior of the resistivity [4]. Recently, it has been shown that the Hall number goes through a significant change at the critical point, suggesting a Fermi surface topology change as discussed above [5].

The Hall number in the magnetic phase is observed to be around 2 carriers, and in the paramagnetic phase around 3 carriers. This large change (1 carrier per formula unit) seems to imply that indeed, the f electrons might be decoupling from the Fermi surface. But there are a number of puzzling issues to address if this is the case. First, the ordered magnetic moment is only about 0.002 $\mu_B$ [6], which would seem to be inconsistent with localized Yb moments. Unlike another small moment case, URu$_2$Si$_2$, there is no evidence for any hidden order. In particular, the observed specific heat anomaly at the magnetic transition is consistent with the small moment. Moreover, the specific heat coefficient remains large in the ordered state, which would argue for the existence of heavy fermions in this phase as well.

In the case of vanadium doped chromium, there is also a large change in the Hall number at its quantum critical point [6], which can be simply explained by the removal of flat parts of the Fermi surface due to magnetic ordering [7]. As the authors in Ref. [6] remark, the problem with such a scenario for YbRh$_2$Si$_2$ is the smallness of the ordered moment. It is difficult to understand how such a small moment could drive such a large Hall number change.

In fact, very little is known about the ordered phase in YbRh$_2$Si$_2$, except that it is probably antiferromagnetic in nature. In particular, the ordering vector is unknown at this point. So, as a first step, we will simply consider the behavior of the Hall number in a paramagnetic calculation. Surprisingly, we find that unlike paramagnetic chromium, the Hall number in YbRh$_2$Si$_2$ is a strong function of the position of the Fermi level. We then perform a series of calculations as a function of the position of the f levels. We find that a small change in the f level position is sufficient to reproduce the Hall number change. The topology of the two Fermi surfaces corresponding to Hall numbers of 2 and 3 are quite similar, and the f electron occupation in the two cases only differs by 0.03. This value is remarkably similar to the 0.03 Rh2 value seen in the entropy associated with the phase transition on the ordered side [7]. This implies that the quantum critical behavior might be associated with a small change in valence. That is, YbRh$_2$Si$_2$ may be the first example of a quantum critical valence fluctuator. This scenario has some similarities to a recent theoretical proposal by Pépin [8].

The calculations in this paper were performed using the local density approximation within a linear muffin tin orbital scheme [9]. The exchange-correlation potential used was that of Hedin and Lundqvist [10], but our experience has been that the choice of this potential is not very critical for f electron systems, as the large Hartree potential of the f electrons dominates the calculation. Calculations were performed assuming two choices of muffin tin sphere radii, and the results were similar. The results presented in this paper used a sphere radius of 3.886 a.u. for Yb, 2.748 a.u. for Rh, and 2.390 a.u. for Si (the body centered tetragonal lattice has an a axis of 4.007Å and a c axis of 9.858Å [11]). These radii were
orations (by shifting the f levels about). In all cases, the
spin-orbit is fully accounted for in the calculation.

The zone was broken down into 48
irreducible wedge. The eigenvalues were then fit using a
Fourier spline series [13] with 3208 tight binding func-
tions. Other zone notation as in Fig. 1. 3D Fermi surface plot of (b) band 3 and (c) band 4. The black lines are the BCT zone.

First, we would like to make some general remarks about the electronic structure of YbRh$_2$Si$_2$. The spin-orbit splitting is very large (around 1.3 eV), so the f electron states near the Fermi energy are almost purely of J=7/2 character. The J=7/2 electron occupation is 7.875. Some of this charge is due to reanalysis from other sites (the muffin tin spheres overlap). To estimate this, we calculate the total J=7/2 occupation for the lowest 25 bands, and find a value of 8.478. This implies an f hole value of 0.603, indicating that YbRh$_2$Si$_2$ is in the mixed valent regime. This is a bit of a surprise, given the heavy fermion nature of this metal.

In Figure 1a, the density of states in the near vicinity of the Fermi energy is shown. Note the presence of two very sharp peaks below the Fermi energy. These are the local J=7/2 f states which are most flat near the P (111) points of the zone, as can be seen from Figure 1b. In the notation of this paper, these states correspond to bands 1-4. Bands 1 and 2 form small hole ellipsoids around the Z point, as can be seen in Figure 2a. Band 3 forms a much larger hole surface centered at the Z point, which resembles a flying saucer (Figure 2b). For band 4, the hole surface surrounding the Z point becomes so large, it forms an interconnected network (Figure 2c). These two bands have roughly equal density of states and account for over 97% of the total density of states. The J=7/2 average weight is 62% for the band 3 Fermi surface, and 50% for the band 4 Fermi surface (with an average value of 56%). But the total density of states at EF only corresponds to 8 mJ/mol K$^2$, a rather small value. Again, this implies the band result is in the mixed valent regime.

In Figure 3, we plot $\sigma_{xx}$, $\sigma_{zz}$, $\sigma_{xyz}$, and $R_H^{-1}$ as a function of the Fermi energy. Unlike the case of paramagnetic
chromium, these quantities are all strong functions of the doping. In particular, as the Fermi energy approaches the local f bands, the various \( \sigma \) become very small, and the Hall number diverges rapidly before changing sign. Interestingly, the Hall number also changes sign for strong electron doping. At the Fermi energy, the calculated Hall number is about 1.5, which is not too far from the zero field value of 2.0 reported in Ref. 4. On the other hand, the \( \sigma_{ii} \) integrals at \( E_F \) indicate that the residual resistance along the c-axis should be about half that along the a axis. Experimentally, this ratio is about 0.9 [8]. Despite this discrepancy (which could be due to anisotropy of \( 1/\gamma \)), this result along with the experimental resistivity indicates the strong three dimensionality of YbRh\(_2\)Si\(_2\), which is also consistent with the Fermi surface shown in Figure 2.

Rather than adjusting the Fermi energy (i.e., doping), one can surmise from Figure 3 that changes of the f level positions will also invoke strong changes in the transport quantities. From this figure, it is obvious that significant changes can be made by moving the f levels either towards or further away from the Fermi energy. We have verified in both cases that this occurs. For the purposes of this paper, though, we only show results where the f levels are moved towards the Fermi energy. This would seem to be more consistent with the observed heavy fermion behavior. Such f level shifts are not unexpected, as they are often needed to fit deHaas-vanAlphen data on f electron systems, and simply represent the need to compensate for deficiencies of the local density approximation when applied to such localized systems.

In Figure 4a, we plot the variation of \( \sigma_{xyz} \) with respect to the f level shift. On this plot are dotted lines corresponding to the Hall number values of 2 and 3 found for the magnetic and paramagnetic phases in Ref. 4. As seen here, bands 1-3 have a positive Hall response as expected (they are hole sheets). But the interconnected sheet, band 4, has a negative Hall response (as does band 5, which appears at higher shifts, and corresponds to a small electron ellipsoid around the \( \Gamma \) point). This competition between a large positive sheet (band 3) and a large negative sheet (band 4) is reminiscent of chromium Si\(_2\). We note that a shift of the f levels by 2.7 mRyd (37 meV) is sufficient to reproduce the observed Hall number change. To further quantify this, we show in Figure 4b the density of states for these two cases.

![Figure 3](image1.png)

**FIG. 3:** (a) \( \sigma_{II} \), (b) \( \sigma_{xyz} \), (c) \( R^{-1}_{H} \) and (d) density of states as a function of Fermi level position relative to \( E_F \) (0).

![Figure 4](image2.png)

**FIG. 4:** (a) Band decomposed \( \sigma_{xyz} \) and its sum versus f level energy shift. The dotted lines mark values where the Hall number is either 2 or 3. (b) Density of states plots for a shift of 7.2 mRyd (Hall number of 2) and 9.9 mRyd (Hall number of 3). 0 is \( E_F \).
FIG. 5: Fermi surface in symmetry planes of the BCT zone for (a) a Hall number of 2 and (b) a Hall number of 3. Zone notation as in Fig. 2.

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