Lifshitz transitions and quasiparticle de-renormalization in YbRh$_2$Si$_2$

H R Naren$^{1,5}$, S Friedemann$^2$, G Zwicknagl$^3$, C Krellner$^4$, C Geibel$^1$, F Steglich$^1$ and S Wirth$^{1,6}$

$^1$ Max Planck Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, D-01187 Dresden, Germany
$^2$ Cavendish Laboratory, University of Cambridge, Cambridge CB3 OHE, UK
$^3$ Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstrasse 3, D-38106 Braunschweig, Germany
$^4$ Physikalisches Institut, Goethe-Universität Frankfurt, D-60438 Frankfurt/Main, Germany
E-mail: wirth@cpfs.mpg.de

New Journal of Physics 15 (2013) 093032 (13pp)
Received 8 April 2013
Published 23 September 2013
Online at http://www.njp.org/
doi:10.1088/1367-2630/15/9/093032

Abstract. We study the effect of magnetic fields up to 15 T on the heavy fermion state of YbRh$_2$Si$_2$ via Hall effect and magnetoresistivity measurements down to 50 mK. Our data show anomalies at three different characteristic fields. We compare our data to renormalized band structure calculations through which we identify Lifshitz transitions associated with the heavy fermion bands. The Hall measurements indicate that the de-renormalization of the quasiparticles, i.e. the destruction of the local Kondo singlets, occurs smoothly while the Lifshitz transitions occur within rather confined regions of the magnetic field.

$^5$ Present address: Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel.
$^6$ Author to whom any correspondence should be addressed.

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
1. Introduction

YbRh$_2$Si$_2$ is a well-studied heavy fermion compound [1] which has an antiferromagnetic (AFM) ground state below $T_N = 70$ mK. The corresponding AFM transition can be suppressed to zero temperature by the application of a small magnetic field $B_N = 60$ mT (660 mT) perpendicular (parallel) to the crystallographic $c$ direction of the tetragonal lattice structure. Right at $B_N$ indications for the existence of a quantum critical point (QCP) have been observed [2]. At fields higher than $B_N$, the system resides in a heavy Fermi liquid state below a crossover temperature $T_{FL}$. There is an extended regime of non-Fermi liquid behavior fanning out above the QCP in the $B-T$ phase space. This QCP is believed to be unconventional, in that it involves the breakup of Kondo singlets at fields below a certain field $B_{Hall}(T)$ which coincides with the QCP at zero temperature, and can be traced up to much higher temperatures [3].

The $J = 7/2$ multiplet state of the Yb$^{3+}$ ions is split into four Kramer’s doublets by the crystalline electric field (CEF) within the tetragonal structure of YbRh$_2$Si$_2$. Kondo scattering over the entire $J = 7/2$ multiplet gives a Kondo temperature estimate of $T_K^{high} \approx 80$ K from the minimum observed in thermopower measurements [4] (in our notation of a high Kondo temperature, $T_K^{high}$, and a lower one, $T_K^{low}$, we rely on [5]). However, since the separation between the ground state doublet and the first excited CEF state is large [6] ($\sim$200 K), the ground state doublet dominates the Kondo scattering at low temperatures. The single-ion Kondo temperature of the ground state doublet, $T_K^{low} \equiv T_K$, has been estimated from entropy considerations via specific heat measurements [7] to $T_K \approx 25$ K. Moreover, thermopower measurements [4] on magnetically diluted Lu$_{1-x}$Yb$_x$Rh$_2$Si$_2$ yielded $T_K \approx 29$ K for YbRh$_2$Si$_2$. In general, there is a third energy scale, $T_{coh}$, which denotes the temperature below which Kondo-lattice coherence sets in and hybridized heavy fermion bands start to form. However, at least in the case of YbRh$_2$Si$_2$, scanning tunneling microscopy measurements [8] provided evidence that the Kondo-lattice coherence develops once the 4f electrons have sufficiently condensed into the CEF ground state, i.e. that $T_K \approx T_{coh}$. Therefore, we will use $T_K$ for this scale henceforth. One focus here is to study the fate of the heavy quasiparticles in the Kondo system YbRh$_2$Si$_2$ in high magnetic fields.

Applying a magnetic field to a heavy fermion system can cause several effects: one is similar to increasing the temperature in that the single-ion Kondo effect is increasingly weakened. Another is Zeeman splitting which may become significant by inducing Lifshitz transitions (LTs), i.e. a band may get spin-split beyond the Fermi energy $E_F$, or the Fermi surface...
topology may change drastically. Zeeman splitting is practically insignificant in normal metals since the relevant energy scale $E_F$ is of the order of a few eV which corresponds to magnetic fields of about $10^4$ T. In heavy fermion metals, however, this scale is greatly reduced due to the hybridization of conduction and localized f electrons via the Kondo effect.

A further effect can be a metamagnetic transition which many heavy fermion compounds undergo at a characteristic magnetic field $\hat{B}$ applied along the easy direction of magnetization. A few examples are CeRu$_2$Si$_2$ ($\hat{B} \approx 7.8$ T, [9, 10]), CeTiGe (12 T, [11]), UPt$_3$ (20 T, [12]) and CeCu$_6$ (4 T, [13]). The former three compounds show a sharp jump in the field-dependent magnetization at $\hat{B}$ whereas the latter one only exhibits a kink at $\hat{B}$. Moreover, in CeTiGe there are indications [11] for a first order phase transition at $\hat{B}$. The metamagnetic transition in CeRu$_2$Si$_2$, which has extensively been investigated with respect to this issue, was initially attributed to a destruction of the Kondo effect resulting in the increase of magnetization [10]. The field scale $\hat{B} = 7.8$ T was believed to correspond to the Kondo energy scale of $\sim 20$ K in this system beyond which the f electrons were thought to become localized. However, the metamagnetic transition was later argued [14] to result from a LT, a conclusion based on transport measurements, model calculations and a re-interpretation of de Haas–van Alphen (dHvA) results.

A corresponding scale $\hat{B} \approx 10$ T for YbRh$_2$Si$_2$ along its crystallographic $ab$ plane (which is the easy plane of magnetization) was estimated from a kink in magnetization [7]. Moreover, the quantities depending on the density of states (DOS), like the magnetic susceptibility, the Sommerfeld coefficient of the electronic specific heat $\gamma$, the $A$-coefficient of the resistivity $\varrho$ (within Fermi liquid theory $\varrho = \varrho_0 + AT^2$ where $\varrho_0$ is the residual resistivity) and the linear magnetostriction coefficient all decrease in a pronounced fashion around this field. The decrease in DOS, cf figure 1(b), was interpreted as a destruction of the heavy fermion state [15, 16] and $\hat{B} \approx 10$ T could experimentally be related to the Kondo energy scale via $k_B T_K \approx g \mu_B \hat{B}$ ($k_B$ and $\mu_B$ are the Boltzmann constant and the Bohr magneton, respectively; $g \sim 3.5$ is the $g$ factor [17]). Another reasoning for the association of $\hat{B}$ and $T_K$ was based on the identical pressure dependence of the two quantities [7].

A dHvA study of YbRh$_2$Si$_2$ revealed [18] a gradual reduction of the dHvA frequency across $\hat{B}$. This was interpreted in terms of a LT, i.e. at $\hat{B}$ one of the spin-split components of a heavy band is shifted beyond the Fermi level. Calculations based on static [19] and dynamic mean field theory [20] endorsed the LT scenario to be responsible for the anomaly at $\hat{B}$. Another argument against an alternative explanation, namely the destruction of the heavy fermion state, would be the sizeable value of $\gamma$ of around 100 mJ mol$^{-1}$ K$^{-2}$ even beyond 10 T. This value is much larger than the one reported [21] for the local moment analogue LuRh$_2$Si$_2$ (6.5 mJ mol$^{-1}$ K$^{-2}$). Finally, the differences in the observed quantum-oscillation frequencies of YbRh$_2$Si$_2$ and LuRh$_2$Si$_2$ rule out the occurrence of a small Fermi surface at these fields that would arise in YbRh$_2$Si$_2$ if the Kondo effect was already destructed [22].

In this work, we report on a high-resolution study of magnetotransport (Hall effect and magnetoresistivity) on high-quality single crystals of YbRh$_2$Si$_2$ and concentrate on high magnetic fields (up to 15 T, in contrast to earlier reports [3, 23] which focused on the QCP at small fields) in order to shed light on these transitions. These measurements are facilitated by renormalized band structure calculations to support our assertions (for the ease of discussion we start off with presenting these results first). While topological changes of the Fermi surface may not necessarily reflect a significant change of the DOS, they can create new open or closed orbits. Thus, transport measurements can be a very sensitive tool to study such changes.

New Journal of Physics 15 (2013) 093032 (http://www.njp.org/)
Figure 1. Renormalized band structure calculations on YbRh$_2$Si$_2$. (a) Energies close to $E_F$ displaying the van Hove singularity and the division into four regions (marked I–IV) separated by LT (marked by dashed lines). Inset shows major symmetry directions in the first Brillouin zone. (b) Variation of the renormalized DOS with magnetic field. Insets: DOS($E$) at different magnetic fields clearly showing a Zeeman splitting of the van Hove singularity (for comparison, the zero-field DOS is shown in gray in the background, same scales are used for all insets). (c) Calculated Fermi surfaces for the two main bands 35 and 37. Colors indicate the Fermi velocity. (d) Fermi surfaces at 15 T for the same two bands and for majority and minority spin direction.

2. Renormalized band calculations with applied magnetic field

The renormalized band calculations for YbRh$_2$Si$_2$ have also been extended to study the magnetic field evolution of the DOS [24]. The influence of the magnetic field is accounted for by
field-dependent values for the centers-of-gravity $\tilde{\epsilon}_{fm}(B)$ and effective widths $\tilde{\Delta}_{fm}(B)$ of the renormalized f-bands which are obtained from fits to the field-dependent quasiparticle DOS of the single-impurity Anderson model [25–28]. The latter are calculated by means of the numerical renormalization group (NRG).

The quasiparticle bands arise from the hybridization between broad conduction bands and narrow, renormalized f-states. Since the energies associated with the magnetic field are small compared to the width of the conduction bands and the CEF excitations, the topology of the surfaces of constant energy in momentum ($k$-) space will remain (almost) unaffected. As a result, the Fermi surfaces for the majority and minority states can be related to isoenergy surfaces of the field-free system even though the height of the DOS in general, and of the van Hove singularity in particular, decrease with field (see insets to figure 1(b)). The Kondo correlations, however, imply a nonlinear variation of the chemical potentials $\mu_{\uparrow}(B)$ and $\mu_{\downarrow}(B)$ with magnetic field for the majority and minority states, respectively. Figure 1(d) displays the Fermi surface sheets for the majority and minority spin states at 15 T.

Figure 1(a) displays the zero-field DOS from which the partially developed hybridization gap and a van Hove singularity can be recognized. These features are found below $E_F$ as expected for a hole (Yb-based) system. Four regions can be identified within the investigated energy range within which the isoenergy surfaces mainly keep their topology and which are labeled I–IV in figure 1(a) [29]. The transitions between these regions are marked by LTs, dashed lines in figure 1(a).

With increasing field, the calculated DOS exhibits a progressive reduction, with a marked jump at 10 T (see figure 1(b)). These calculations indicated that the quasiparticle de-renormalization, i.e. the field-induced suppression of the Kondo effect, takes over rather smoothly and hence, by itself cannot create the anomaly at 10 T [24]. The field evolution of the DOS as depicted in the insets of figure 1(b) involves the Zeeman splitting of the zero-field DOS. With increasing magnetic field the majority spin van Hove singularity sweeps rapidly away from the Fermi level while the minority spin van Hove singularity crosses $E_F$ at around 10 T (see insets). In addition, the peak height of the van Hove singularity reduces with increasing field owing to the de-renormalization of the quasiparticles. Clearly, it takes the renormalized band calculation including both the above-mentioned effects as well as the quasiparticle interactions to reproduce a field evolution of the DOS which conforms to the variation of the Sommerfeld coefficient and thermopower [29].

Fermi surfaces have been calculated for the two bands predominantly contributing to the DOS. These two bands, band 35 and 37, give rise to the so-called ‘pillow’ (upper picture in figure 1(c)) and ‘jungle-gym’ (lower picture), respectively. The color code in figure 1(c) indicates the Fermi velocity. Upon shifting the majority spin DOS($B$) to lower energies by increasing the magnetic field the topology of its Fermi surfaces remains largely unchanged, right column in figure 1(d), since $E_F$ stays within region I of the DOS. In contrast, the minority spin Fermi surfaces strongly change when the minority spin DOS($B$) moves up in energy and its corresponding $E_F$ travels through regions I–IV [29]. Consequently, LTs are encountered in the minority spin DOS($B$). The prominent one within band 35 is the formation of a single, connected surface upon crossing from region II to III, figure 1(d). The isoenergy surfaces of band 37 within the four regions I–IV are depicted in figure 2. In contrast to band 35, several transitions can be inferred: a ‘neck-forming’ LT in the crystallographic direction $\Gamma \rightarrow X$ between regions I and II (for directions see inset to figure 1(a)), followed by a ‘neck-disrupting’
LT at an angle between $\Gamma \rightarrow X$ and $\Gamma \rightarrow s$ and a ‘pocket-disappearing’ LT of the pocket along $X \rightarrow P \rightarrow u$ upon entering region IV.

As is obvious from the insets to figure 1(b), the dominant peak of the minority spin van Hove singularity is shifted beyond $E_F$ at around 10 T. Since the width of this peak is supposed [30] to be the same as $T_K$, this again indicates that the magnetic field scale of 10 T is indeed the equivalent of $T_K$. From the magnitude of the shift of the minority van Hove singularity, we can assign magnetic field values to the transitions between the different regions: the corresponding LTs are calculated to take place at $B_1 = 2.5 \pm 1$ T (region I to II), at $B_2 = 9 \pm 1$ T (region II to III) and from region III to IV at $B_3 = 11 \pm 1$ T.

Depending on the extent of contribution of a specific band to the DOS, the corresponding LTs are expected to cause changes in the DOS($B$), figure 1(b). A kink is seen at around $B_1$, a drop at $B_2$ and a small maximum at $B_3$. However, the kink at $B_1$ is, to some extent, already visible in the DOS($B$) just due to the de-renormalization of the quasiparticles [24]. Thus, the LT at $B_1$ seems to have a very minor effect on the DOS. This can be understood [24] from the fact that the dominant contribution to the zero-field DOS stems from the ‘pillow’ Fermi surface while it is the ‘jungle-gym’ one that undergoes a LT at $B_1$. The comparatively large jump at $B_2$ is likely caused by both, the ‘pillow’ and the ‘jungle-gym’, sheets being subject to LTs. In contrast, the faint feature at $B_3$ is solely due to the LT of the erstwhile ‘jungle-gym’ sheet whose contribution appears to be more significant at high fields, perhaps due to a reduced contribution from the erstwhile ‘pillow’ sheet. We note that the features at $B_1$ and $B_3$ were not obvious in magnetization or heat capacity measurements [7], but could be resolved in thermopower [29, 31]. In our magnetotransport measurements, we clearly observe all these features as well as indications related to the de-renormalization of quasiparticles.

3. Experimental

We performed simultaneous isothermal magnetoresistivity (MR) and Hall effect measurements down to $T \geq 50$ mK and in magnetic fields up to $B \leq 15$ T. To facilitate direct comparison, current $j$ and $B$ were applied perpendicular to the crystallographic $c$ direction for both, MR ($j \parallel B$) and Hall measurements. Consequently, the Hall voltage $V_H$ was to be measured along the $c$ direction. Since YbRh$_2$Si$_2$ cleaves perpendicular to the $c$-axis, we used two different crystals (from the same batch, also same batch as in [32]) with optimized geometries for the respective measurements. Note that these are among the highest-quality crystals of YbRh$_2$Si$_2$ (residual resistivity $\sim 0.5 \times 10^{-8}$ $\Omega$ m). For optimized sensitivity the sample for Hall measurements was...
thinned down to 70 µm, and the signals were consecutively amplified by low-temperature transformers, low-noise amplifiers and lock-in amplifiers for both types of measurements. The actual Hall voltage was taken as the antisymmetric component of the measured Hall voltage under field reversal [33].

4. Magnetoresistivity

Figure 3 exhibits the field-dependent resistivity \( \rho_{xx}(B) \), the magnetoresistivity \( MR = \frac{\rho_{xx}(B) - \rho_{xx}(B=0)}{\rho_{xx}(B=0)} \) and the field derivative of MR. The MR is positive at lowest temperatures, as expected for the coherent state. At 50 mK and 15 T, the resistivity enhancement over the zero-field value is close to 90%. At very low fields, a step-like transition is visible (marked

\[ \text{Figure 3.} \] (a) Resistivity \( \rho_{xx}(B) \), (b) magnetoresistivity \( \frac{\rho_{xx}(B) - \rho_{xx}(B=0)}{\rho_{xx}(B=0)} \) and (c) field derivative of the MR as functions of magnetic field. All panels exhibit results at the same selected temperatures, \( 0.05 \leq T \leq 2.25 \text{ K} \), and the same color code. Black dashed lines: results of the nonmagnetic reference compound LuRh\(_2\)Si\(_2\) at \( T = 2 \text{ K} \).
by an upward arrow in figure 3(b)) at lowest temperatures which gets smeared out quickly as temperature increases. This has been reported to be a signature of the Fermi surface reconstruction related to the unconventional QCP in this compound [23]. With increasing $T$, $Q_{xx}$ at low fields increases due to progressive inelastic scattering of conduction electrons. The negative MR at higher $T$ is then a result of the magnetic-field suppression of the spin-flip scattering.

At fields above 3 T, a small kink in the MR is observed that is clearly reflected as a step in its derivative, marked by an arrow in figure 3(c). A feature at this field scale has not been observed in previous measurements even though it should be expected from the kink seen in the DOS($B$) [24]. The anomaly observed at 10 T in [7] appears as a double kink in our MR data, again marked by arrows in figure 3(c). The two kinks are roughly at 9 and 11 T and are most sharply visible at lowest $T = 50$ mK. Although these kinks get smeared out at higher temperatures their positions in field remain roughly the same. Thus, we indeed observe signatures of all the three predicted LTs in our MR data.

At fields beyond 12 T, i.e. beyond the high field anomaly, the MR appears to become linear in field, at least at low temperature. In fact, the linear regions in the low-temperature $Q_{xx}(B)$-curves nicely overlap implying a temperature independent high-field state. This point of view is further supported by results obtained on the nonmagnetic reference compound LuRh$_2$Si$_2$ which exhibits a featureless MR throughout the measured field range (up to 12 T) with a slope very similar to the high-field MR in YbRh$_2$Si$_2$. Such an increase of the MR is in line with the existence of open orbits in the Fermi surface of YbRh$_2$Si$_2$ at higher fields, figure 1(d): the vertical sheets present in both the minority Fermi surface of band 35 and the majority Fermi surface of band 37 form continuous pillars in an extended zone scheme and perpendicular to the applied field. Nonetheless, it should be noted here that further modeling would be required to straightforwardly link the different features observed in the MR to the nature of the corresponding LT.

5. Hall measurements

We now focus on the results of our Hall measurements presented in figure 4. It has been shown that in YbRh$_2$Si$_2$ at temperatures below 1 K the anomalous contribution to the Hall effect data is less than a few per cent [34]. In both models considered in [34], the anomalous Hall contribution is proportional to the magnetic susceptibility $\chi$. Since $\chi(B)$ goes down for increasing fields $B$, the anomalous contribution to the Hall effect is expected to continue to be insignificant even at the high fields we have measured in. In contrast, at higher temperatures the anomalous Hall contribution becomes dominant. For example, the Hall resistivity $Q_{xy}$ at $T = 2.25$ K in figure 4(a) appears to largely resemble the magnetization curve measured earlier [7]. We note here that, unfortunately, a comparison to Hall measurements on the nonmagnetic reference compound LuRh$_2$Si$_2$ was defiled by the extremely small size of the LuRh$_2$Si$_2$ single crystals.

The most intriguing result is the collapse of all measured curves $Q_{xy}(T, B)$ at high fields into a single, linear-in-field curve, i.e. $Q_{xy}(T, B)$ appears to be independent of temperature, see dashed line in figure 4(a). The field value beyond which this collapse occurs increases with temperature. Since the anomalous Hall contribution is small at lowest temperature (see above), the temperature independence of $Q_{xy}(T, B \gtrsim 12$ T) at high fields also implies that the anomalous contribution becomes very small for all measured temperatures at high fields. In turn, this implies that the system at sufficiently high fields behaves largely like an ordinary
paramagnetic metal, even though it is polarized. This view is corroborated by the fact that the field-derived energy scale at which these ordinary metallic properties occur corresponds to the energy scale $T_K$ relevant at the low temperatures investigated in the present study.

At low temperature (below 0.5 K), the isothermal $\rho_{xy}(T, B)$ curves appear almost linear in $B$. However, there are subtle changes of slope that become apparent if a (large) linear ‘background’ is subtracted. In figure 4(b), we plot $\rho_{xy}(T, B) - \alpha \cdot B$, where the constant $\alpha$ corresponds to the $T$-independent high-field slope of $\approx 4.7 \times 10^{-11} \text{Ω m}^{-1}$. For clarity, an increasing offset (by $0.5 \times 10^{-10} \text{Ω m}$) was added to the $\rho_{xy}(T, B)$-curves above 50 mK. There is a clear inflection point at around 3 T (marked by a vertical dashed line) which corresponds to the inflection seen in the DOS($B$), figure 1(b). This feature develops into a maximum at higher temperatures, likely as a result of the additional anomalous contribution to $\rho_{xy}(T, B)$. Moreover, $\rho_{xy}(T, B)$ at lower temperatures exhibits a step-like decrease at around 11 T (dotted line cutting through low-$T$ curves only) which gets smeared out at higher temperatures. This decrease, which seems to appear at constant fields at different temperatures, is likely related to the third LT at $B_3$.

New Journal of Physics 15 (2013) 093032 (http://www.njp.org/)
To gain insight into the evolution of the Fermi surface we now consider the Hall coefficient $R_H$ (same temperatures and symbols as in figures 3 and 4). The most prominent feature in figure 5(a) is the minimum in $R_H$ at fields of roughly 9 T. This minimum strongly develops with increasing temperature (above 0.5 K) and shifts its position towards higher field indicating that it is not related to the DOS [35]. Rather, it appears to be caused by fluctuations evolving upon leaving the Fermi liquid regime with increasing $T$. Such behavior is in line with a model [36] which describes the temperature evolution of $R_H$ by skew scattering related to the on-site Kondo effect, rather than coherent effects. This temperature evolution of $R_H$ (as measured at 0.5 T) is presented in figure 6 and resembles the one obtained [3] for $B||c$. It confirms our conjecture above that $R_H$ is dominated by the normal contribution, i.e. it is related to the DOS, only at lowest temperatures or at high fields $B \gtrsim 12$ T. Inspecting the low-$T$ curves of $R_H$, figure 5(b), an anomalous Hall contribution appears to set in at $T = 0.75$ K as signaled by the dent observed around 9 T. We therefore concentrate on the lowest measured temperatures in the following, figure 5(b).

At $T \lesssim 0.2$ K, a maximum in $R_H$ is observed around 3 T (dashed line in figure 5(b)). In all likelihood this feature is related to the LT at $B_1$, i.e. the inflection in DOS$(B)$ and above-mentioned neck formation along the $\Gamma \to X$ direction. Interestingly, among the three transitions,
Figure 6. Temperature dependence of the Hall coefficient $R_H$ at 0.5 T. Data marked by crosses (×) were obtained on the same sample but using a physical properties measurement system.

the one at $B_1$ appears to have the most pronounced effect on $R_H$ resulting in the corresponding maximum.

Upon increasing field there is a clear minimum in $R_H$ visible at around 11.5 T and for $T \leq 0.4$ K, without apparent shift for different temperatures (as indicated by the dotted line). One may therefore speculate that this feature is related to the LT at $B_1$. At this field, there is a maximum in DOS$(B)$, see figure 1(b), along with severe changes in the topology of the Fermi surfaces at these fields. The combination of these two effects may account for the somewhat higher field values at which the transitions are observed in $R_H$ compared to the calculations. On the other hand, there is no clear feature seen in $R_H$ in the field range around 9 T. As noted above (cf figure 1) there are two major bands at $E_F$, both undergoing LTs. We speculate that the transitions in these two bands compensate each other such that the net change in $R_H$ is weak. We note here that thermopower measurements [29] on a sample of the same batch and for identical orientation also showed a maximum–minimum feature at fields around 11 T, but an additional, second maximum at around 9.5 T. While this nicely corroborates our Hall data the occurrence of an additional maximum also hints at the fact that electrical and thermal transport measurements could be differently sensitive to these phenomena.

At low $T$ an increasing background is visible in $R_H$ upon increasing $B$, best seen in figure 5(b). This background is even obvious in $R_H$ measured at 70 K (obtained on the same sample but in a different measurement system limiting the absolute quantitative comparison). Such an increase suggests a reduction in the number of charge carriers (in the simplest model, $R_H = -1/e n_{\text{eff}}$ where $n_{\text{eff}}$ is the effective charge carrier concentration and $e$ is the charge of an electron). This may be taken as another indication for the progressive de-renormalization of quasiparticles at high magnetic fields, i.e. of the on-site Kondo interaction. In other words, the f-electrons seem to be gradually driven out of the Fermi volume with increasing magnetic field. It nicely confirms the evolution of the Kondo effect with decreasing temperature as discussed in the introduction: the fact that the increase of $R_H$ with field is still seen at 70 K, i.e. below $T_K^{\text{high}}$ but well above $T_K$, clearly points towards the single-ion nature of this effect.

Our measurements indicate a rather smooth delocalization–localization transition at high fields. These observations are in line with the already mentioned fact [7] that the Sommerfeld coefficient remains as large as $\sim 100$ mJ mol$^{-1}$ K$^{-2}$ beyond 10 T and is much larger than
the value of LuRh$_2$Si$_2$. In contrast, there is clear evidence from renormalized bandstructure calculations that the observed features at the different fields $B_1$, $B_2$ and $B_3$ could be due to LTs which appear more abrupt in field.

A generic low-field LT was predicted [37] via dynamical mean field theory (DMFT) calculations on the Kondo lattice model. Indeed, we do observe such a transition in YbRh$_2$Si$_2$ in our measurements. In addition, LTs have been predicted to occur at high fields in heavy fermion systems [19, 20], at the scale given [37] by $T_K$. However, we find two closely spaced LT near 10 T. This could be due to a slight difference in the coupling of the two bands to the magnetic field.

6. Conclusion

We have found evidence for several LTs in YbRh$_2$Si$_2$, by severe changes of the Fermi surface topology of the dominating bands vis-à-vis the shifting of the Zeeman-split Kondo resonance through $E_F$. While these transitions occur rather abruptly, the de-renormalization of the quasiparticles takes place comparatively smoothly. This phenomenology could be generic among heavy fermion compounds, and magnetotransport seems to be a useful tool in addressing such issues.

Acknowledgments

We thank H Pfau and M Brando for insightful discussions. This work is partly supported by the German Research Foundation through DFG Forschergruppe 960. SF acknowledges support by the Alexander von Humboldt foundation and the European research council.

References

[1] Trovarelli O, Geibel C, Mederle S, Langhammer C, Grosche F M, Gegenwart P, Lang M, Sparn G and Steglich F 2000 Phys. Rev. Lett. 85 626
[2] Gegenwart P, Custers J, Geibel C, Neumaier K, Tayama T, Tenya K, Trovarelli O and Steglich F 2002 Phys. Rev. Lett. 89 056402
[3] Paschen S, L¨uhmann T, Wirth S, Gegenwart P, Trovarelli O, Geibel C, Steglich F, Coleman P and Si Q 2004 Nature 432 881
[4] K¨ohler U, Oeschler N, Steglich F, Maquilon S and Fisk Z 2008 Phys. Rev. B 77 104412
[5] Cornut B and Coqblin B 1972 Phys. Rev. B 5 4541
[6] Stockert O, Koza M M, Ferstl J, Murani A P, Geibel C and Steglich F 2006 Physica B 378–80 157
[7] Gegenwart P et al 2006 New J. Phys. 8 171
[8] Ernst S, Kirchner S, Krellner C, Geibel C, Zwicknagl G, Steglich F and Wirth S 2011 Nature 474 362
[9] Flouquet J, Kambe S, Regnault L P, Haen P, Brison J P, Lapierre F and Lejay P 1995 Physica B 215 77
[10] Flouquet J, Haen P, Raymond S, Aoki D and Knebel G 2002 Physica B 319 251
[11] Deppe M, Lausberg S, Weickert F, Brando M, Skourski Y, Caroca-Canales N, Geibel C and Steglich F 2012 Phys. Rev. B 85 060401
[12] Sugiyama K et al 1999 Phys. Rev. B 60 9248
[13] Sakakibara T, Goto T, Ônuki Y and Komatsubara T 1987 J. Magn. Magn. Mater. 70 375
[14] Daou R, Bergemann C and Julian S R 2006 Phys. Rev. Lett. 96 114709
[15] Tokiwa Y, Gegenwart P, Radu T, Ferstl J, Sparn G, Geibel C and Steglich F 2005 Phys. Rev. Lett. 94 226402
[16] Knebel G et al 2006 J. Phys. Soc. Japan 75 114709
[17] Schaufuß U, Kataev V, Zvyagin A A, Büchner B, Sichelschmidt J, Wykhoff J, Krellner C, Geibel C and Steglich F 2009 Phys. Rev. Lett. 102 076405
[18] Rourke P M C, McCollam A, Lapertot G, Knebel G, Flouquet J and Julian S R 2008 Phys. Rev. Lett. 101 237205
[19] Kusminskiy S V, Beach K S D, Castro Neto A H and Campbell D K 2008 Phys. Rev. B 77 094419
[20] Beach K S D and Assaad F F 2008 Phys. Rev. B 77 205123
[21] Friedemann S, Wirth S, Oeschler N, Krellner C, Geibel C, Steglich F, MaQuilon S, Fisk Z, Paschen S and Zwicknagl G 2010 Phys. Rev. B 82 035103
[22] Friedemann S, Goh S K, Rourke P M C, Reiss P, Sutherland M L, Grosche F M, Zwicknagl G and Fisk Z 2013 New J. Phys. 15 093014
[23] Friedemann S, Oeschler N, Wirth S, Krellner C, Geibel C, Steglich F, Paschen S, Kirchner S and Si Q 2010 Proc. Natl Acad. Sci. USA 107 14547
[24] Zwicknagl G 2011 J. Phys.: Condens. Matter 23 094215
[25] Hewson A C, Oguri A and Meyer D 2004 Eur. Phys. J. B 40 177
[26] Hewson A C, Bauer J and Koller W 2006 Phys. Rev. B 73 045117
[27] Bauer J and Hewson A C 2007 Phys. Rev. B 76 035119
[28] Peters R, Pruschke T and Anders F B 2006 Phys. Rev. B 74 245114
[29] Pfau H et al 2013 Phys. Rev. Lett. 110 256403
[30] Costi T A and Manini N 2002 J. Low Temp. Phys. 126 835
[31] Pourret A, Knebel G, Lapertot G, Matsuda T D and Flouquet J 2013 J. Phys. Soc. Japan 82 053704
[32] Oeschler N, Hartmann S, Pikul A P, Krellner C, Geibel C and Steglich F 2008 Physica B 403 1254
[33] Nair S, Wirth S, Nicklas M, Sarrao J L, Thompson J D, Fisk Z and Steglich F 2008 Phys. Rev. Lett. 100 137003
[34] Paschen S, Lühmann T, Wirth S, Trovarelli O, Geibel C and Steglich F 2005 Physica B 359 44
[35] Fert A and Levy P M 1987 Phys. Rev. B 36 1907
[36] Coleman P, Anderson P W and Ramakrishnan T V 1985 Phys. Rev. Lett. 55 414
[37] Bercx M and Assaad F F 2012 Phys. Rev. B 86 075108