Fractionalization and Fermi surface volume in heavy fermion compounds: the case of YbRh$_2$Si$_2$.

Catherine Pépin

SPhT, L’Orme des Merisiers, CEA-Saclay, 91191 Gif-sur-Yvette, France

We establish an effective theory for heavy fermion compounds close to a zero temperature Antiferromagnetic (AF) transition. Coming from the heavy Fermi liquid phase across to the AF phase, the heavy electron fractionalizes into a light electron, a bosonic spinon and a new excitation: a spinless fermionic field. Assuming this field acquires dynamics and dispersion when one integrates out the high energy degrees of freedom, we give a scenario for the volume of its Fermi surface through the phase diagram. We apply our theory to the special case of YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ where we recover, within experimental resolution, several low temperature exponents for transport and thermodynamics.

In some heavy fermion compounds, pronounced deviations from the conventional Landau Fermi liquid behavior have been reported when the compounds are tuned through an antiferromagnetic (AF) quantum critical point (QCP) [1]. Generically, the specific heat coefficient is seen to diverge at the QCP, showing at least logarithmic increase [2–5] as the temperature is decreased. The resistivity is quasi-linear in temperature [6–9]. NMR and μ-SR studies, as well as neutron scattering measurements for one compound [4] show that the spin susceptibility acquires some anomalous exponent [6,7]. Here we focus on the special case of YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ doped with Ge to reach a QCP at $x = 0.05$. In this compound, linear resistivity is observed, at the QCP, over three decades of temperature, from 10 K to 10 mK [10]. At the same time, the specific heat coefficient shows an upturn below 300 mK from its original logarithmic increase, $C/T \sim T^{-\alpha}$ with $\alpha \approx 0.33$ [7,11]. The entropy associated with the upturn is of the order of 5 % of the total spin entropy of the Yb atom. Curiously, the upturn in specific heat is un-correlated with transport, since one doesn’t see any kink at 300 mK, or any deviation from the linear slope in the resistivity. An NMR study on the pure compound [12] shows that the relaxation time on Si $1/T_1 T \sim T^{-1/2}$ when the system is driven close to the QCP with applied magnetic field, suggesting that $\sum_q \chi' (q,\omega) / \omega \sim T^{-0.5}$. The Grüneisen parameter, ratio of the thermal expansion coefficient and the specific heat is seen to diverge with an unusual exponent, i.e. $\Gamma = \beta/C \sim T^{-0.7}$, compared to the case of CeNi$_2$Ge$_2$, well understood within a Spin Density Wave(SDW) scenario [13]. Latest measurements of the Hall constant [14] suggest that the Fermi surface volume is increasing, when one goes from the AF to the field induced heavy Fermi liquid phase. A recent study of the heavy Fermi liquid phase shows a generic scaling in $B/T$ in the transport and specific heat [11]. One also observes that the Kadowaki-Woods ratio $K = A/\gamma^2$ where $A$ is the $T^2$ coefficient of the resistivity and $\gamma = C/T |_{T \to 0}$ is the specific heat coefficient– increases in approaching the QCP. Likewise the Wilson ratio $W = \chi/\gamma |_{T \to 0}$ where $\chi$ is the bulk susceptibility– shows a dramatic increase. In contrast, the ratio of $A/\chi^2$ stays constant over the whole magnetic field range. We deduce from the fact that the $A$ coefficient doesn’t feel the upturn in specific heat, that the bulk susceptibility $\chi$ doesn’t feel it either—their ratio being constant [15]. In other words, the excitations responsible for the upturn seen in $C/T$ don’t couple to the bulk susceptibility.

In this paper we introduce an effective theory for heavy fermion compounds, which, in the particular case of YbRh$_2$Si$_2$, accounts for the whole set of experimental evidence quoted above.

Our starting point is the Kondo-Heisenberg lattice model, where we use a Schwinger representation for the spin of the impurities, which we refer to as the bosonic Kondo-Heisenberg (BKH) model. The BKH lattice Hamiltonian

\[ H = H_c + H_K + H_H, \]

where

\[ H_c = \sum_{k\sigma} \varepsilon_k f_{k\sigma}^\dagger f_{k\sigma}, \]

\[ H_K = J_K \sum_{i\sigma} b_{i\sigma}^\dagger b_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma}, \]

\[ H_H = J_H \sum_{(i,j)\sigma\sigma'} b_{i\sigma}^\dagger b_{j\sigma'}^\dagger b_{j\sigma}^\dagger b_{i\sigma} \]

(1)

describes the conduction band ($H_c$), the Kondo coupling between local moments and the conduction electrons at site $i$ ($H_K$), and the super-exchange between neighboring spins ($H_H$). When we formulate the BKH model as a functional integral, we can decouple the fields as follows

\[ H_K \to H_K' = \sum_{i\sigma} \left[ b_{i\sigma}^\dagger \chi_i^\dagger h.c. + h.c. \right] - \frac{\chi_i^\dagger \chi_i}{B_K} \]

(2)
where the on-site bond variable in the first term is a Grassman field which doesn’t carry a spin and the bond variable in the second term has been chosen following an SP(2) decomposition of the interaction [16].

We believe the fermion field $\chi$ is a good decoupling of the Kondo interaction in the sense that it describes the set of elementary excitations close to the QCP [17]. Through coupling to the spinons ($b_{i\sigma}$) and the itinerant electrons ($f_{j\sigma}$) the $\chi$-fermion Kondo bond states acquire some dynamics, damping and dispersion. Within this set of variables, the formation of the Kondo heavy quasiparticle is described with the formation of a “band” for the $\chi$-fermion bound state. To see how this happens it is instructive to step back to the impurity case.

Magnetism in the bosonic Kondo impurity model has been investigated in the past [18,19], but here we focus on the fate of the $\chi$-fermion chemical potential [20]. From (2), one notices that, for the antiferromagnetic Kondo effect ($J_K > 0$), the energy level is negative, thus full, and the chemical potential $\mu = -1/J_K$ flows to zero at strong coupling. The $\chi$-fermion becomes massless. This singularity accounts for the increase of the Fermi surface volume by one. Oppositely, in the ferromagnetic case ($J_K < 0$), the energy level is positive, thus empty, and the chemical potential $\mu = -1/J_K$ flows to infinity at low energies, leaving the Fermi surface volume unchanged.

In the Kondo lattice, the $\chi$-fermion acquires some dynamics, damping and dispersion. The competition between AF fluctuations and the Kondo screening affects the formation of the $\chi$-band. Moreover, one can imagine that the lattice accommodates partial screening of the impurity spin through the $\chi$-dispersion: the “unscreened” part of the spin – by analogy with ferromagnetic Kondo – has positive energies, while the screened part of the spin has negative ones. Deep inside the AF phase (diagram a in Fig. 1), the spin of the impurities are partially screened and the $\chi$-fermion bandwidth is large – partially filled band, with a rather “small” Fermi surface. As the strength of AF fluctuations is decreased, the number of empty energy levels decrease compared to full energy levels, the $\chi$-band becomes flatter and the Fermi surface is bigger (diagram b in Fig. 1). Deep inside the heavy Fermi liquid phase, the Kondo effect is dominant, and one expects a situation similar to the one impurity case, with a totally flat $\chi$-band and a large Fermi surface; in this phase the $\chi$-fermion is no longer a good elementary excitation and, $\chi$ being a flat massless mode, the theory is ill defined. Just at the brink of the Fermi liquid phase, the $\chi$-band is “almost” flat (diagram c in Fig. 1). One can thus expect that the velocity vanishes for part of the Fermi surface, producing a singularity.

To summarize, our scenario predicts a new excitation close to the QCP, which is fermionic in nature and doesn’t carry a spin. As one integrates out the high energy degree of freedom, this new fermion forms a “band”: its dispersion has positive and negative energy levels. The band structure at the QCP is not universal, it depends on the relative strengths of the Kondo effect and AF interactions (Fig. 2). If the AF interaction is small compared to the Kondo interaction, the QCP lies inside the heavy Fermi liquid phase, which is expected to be the case for CeNi$_2$Ge$_2$ (diagram a in Fig. 2). In the opposite limit, when the AF fluctuations are strong compared to the Kondo effect, the Fermi liquid phase can lie outside the AF phase, and one can expect singularities at the QCP (diagram b in Fig. 2). This is the case for the YbRh$_2$Si$_2$ compound. The evolution of the $\chi$-band structure accounts for the variation of the total Fermi surface volume, with a smooth cross-over from a rather small Fermi surface inside the AF phase to a big Fermi surface inside the Fermi liquid phase.

We now turn to the specific case of YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ doped to criticality for $x = 0.05$. We assume that, at the QCP, the $\chi$-band is well formed, but the velocity vanishes at the hot lines. The effective Lagrangian comprises four terms: a conduction electron term $S_f$, a boson term $S_b$ which describes the critical spinons, the $\chi$-fermion term $S_{\chi}$, and the interaction $S_{int}$ between those modes. Both the $f$ and $\chi$-fermion’s Fermi surface have hot lines related by the ordering wave vector $Q^*$ (Fig.3).

\[
S = S_f + S_{\chi} + S_b + S_{int}
\]

\[
S_f = \int \frac{d\omega}{(2\pi)^{3}} \frac{d^3k}{(2\pi)^3} \sum_{\sigma} f_{k\sigma}^+ (i\omega - v_F \cdot k) f_{k\sigma}
\]

\[
S_{\chi} = \int \frac{d\omega}{(2\pi)^{3}} \lambda_k^+ (i\Sigma_{\chi} - v_{\chi} \cdot k + a \cdot k^3) \chi_k
\]
The free energy of the heavy $f$-fermions, $F_x$ is the contribution from the $\chi$ fermions and $F_{bos}$ from the boson modes. Any of these individual contributions is extensive and proportional to the phase space volume $F \sim T \prod \Delta q_i$, where $\Delta q_i$ is the momentum width in the $i$-direction. For the $\chi$-fermions, only two directions, perpendicular to the hot lines, reduce the phase space with $\Delta q_{1,2} \sim (T/a)^{1/3}$ leading to $F_x \sim T(T/a)^{2/3}$. The boson modes scale in all directions, leading to $F_{bos} \sim T (\Sigma_0(T)/\lambda)^3 \sim T^2$. The $f$-fermions scale in two directions, perpendicular to the hot lines, with $\Delta q_1 \sim (T/a)^{1/3}$ and $\Delta q_2 \sim \Sigma_f(T)/\nu_F$, leading to $F_{f,hot} \sim T^2$. Notice that the scaling exponents of the hot fermion’s and the boson’s entropy are the same, which is a property of spin-fermion models above their upper critical dimension [27]. At low temperatures, $F_x$ is the dominant contribution, leading to a specific heat coefficient which captures the upturn observed in the experiments:

$$\gamma = C/T \sim 6^{2/3}T^{-1/3}.$$  

We now turn to the behavior of the conductivity at criticality. The $f$-fermions are the sole contributors to electric transport because the velocity of the $\chi$-fermions vanishes on the hot lines. Assuming that the scattering processes from magnetic spinons dominate the transport, one distinguishes the contributions from the cold and hot regions $\sigma(T) = \sigma_{cold}(T) + \sigma_{hot}(T)$. Following [21], the conductivity is the sum of inverse scattering rates associated with the hot and cold regions, multiplied by the phase space allowed to these regions

$$\sigma_{cold} \sim \frac{1}{x + t^2}; \quad \sigma_{hot} \sim \frac{t^{1/3}}{x + t^{3/2}},$$

where $x$ is a dimensionless parameter which characterizes the residual resistivity— for example, the inverse of the Residual Resistivity Ratio (RRR), being the ratio of the resistivity at 100 K to the resistivity at 10 K. $t$ is a dimensionless parameter characteristic of the temperature—one can take for example $t = T/T_K$, where $T_K$ is the one impurity Kondo temperature of the compound. $t^{1/3}$ is the width of the hot lines, $t^2$ is the inverse scattering rate of the cold conduction electrons, and $t^{2/3}$ is the inverse scattering rate of the conduction electrons—up to logarithms—from the paramagnetic spinons around the hot lines. One sees three regimes in the conductivity:

$$t < x^{3/2}; \quad x^{3/2} < t < x^{1/2}; \quad x^{1/2} < t$$

$$\rho = x + t; \quad \text{cross-over}; \quad \Delta \rho \sim t^2.$$  

### FIG. 4. Feynman diagrams associated with a) the spinon self-energy b) the $f$-fermion self-energy c) the $\chi$-fermion self-energy. Solid, dashed and wavy lines are respectively $f$-fermion, $\chi$-fermion and boson propagators.
FIG. 5. Linear in \( T \) resistivity and variation of the temperature exponent as function of \( t = T/T_K \). \( x \) is the inverse Residual Resistivity Ratio.

With \( x \approx 0.1 \) and \( T_K \approx 30K \) for YbRh\(_2\)Si\(_2\), one sees that the resistivity is linear in \( T \), below \( T = 3K \) down to the lowest temperature (Fig.5), while the \( T^2 \) behavior would appear roughly above \( T = 10K \), corresponding to the experimental observation. To conclude the study of thermal observables, we focus on the Grüneisen parameter, defined as \( \Gamma = \alpha/C_p \) with \( \alpha \approx \partial \alpha/\partial T \) and \( C_p \approx \partial C_p/\partial T \). \( p \) is the hydrostatic pressure. Calling \( r = (p_p-p_e)/p_c \) the departure from the QCP, and noticing, from a small displacement of the \( \chi \)-fermion hot line that \( r \approx q_{\chi\psi} \approx T^{2/3} \), one finds \( T \approx T^{-2/3} \) close to the QCP. This exponent is in good agreement with the experiments [13].

Several theoretical descriptions have been advanced to account for the striking experimental results around the QCP of heavy fermions. Anisotropic (2D) spin density wave scenario [22,23] can explain the linear in \( T \) resistivity, as well as the logarithmic dependence of the specific heat coefficient. A theory with a “local” mode, as well as 2D spin fluctuations at criticality, has been advocated [23], which also captures the anomalous exponent of the spin susceptibility. None of those theories can account for the upturn in the specific heat coefficient, with the right exponent with temperature, as well as the linear resistivity at very low temperatures. The upturn in the specific heat coefficient doesn’t couple to transport, and couples only indirectly –via the spinons and \( f \)-fermions– to the bulk spin susceptibility. This explains the observation that the ratio \( A/\chi^2 \) is constant in the heavy Fermi liquid phase [15]. One also reproduces the variation of the Grüneisen parameter with the anomalous temperature exponent.

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[1] P. Coleman et al., J. Phys. Cond. Mat. 13 R723, (2001).
[2] H. von Löhneysen et al., J. Phys. Cond. Mat. 8 (1996) 9689.
[3] O. Trovarelli et al., Phys. Rev. Lett. 85 (2000) 626.
[4] A. Schröder et al. Nature 407 (2000) 351.
[5] A. Bianchi et al., Phys. Rev. Lett. 91, 257001 (2003).
[6] M. Grosche et al., J. Phys. Cond. Mat. 12 (2000), 533.
[7] P. Gegenwart et al., Phys. Rev. Lett. 89 (2002), 56402.
[8] S. R. Julian et al., J. Phys. Cond. Mat. 8 (1996), 9675.
[9] J-P. Paglione et al., Phys. Rev. Lett. 91 (2003), 246405.
[10] J. Custers Ph. D. Thesis, Dresden(2004), p. 35.
[11] J. Custers et al., Nature 424,524-527 (2003).
[12] K. Ishida et al., Phys. Rev. Lett. 89, 107202 (2002).
[13] R. Kuechler et al., Phys. Rev. Lett. 91, 066409 (2003).
[14] S. Pashen et al., Acta Phys. Pol. B 34, 359 (2002) and preprint to Nature.
[15] J. Custers Ph. D. Thesis, Dresden(2004), p. 72.
[16] N. Read and S. Sachdev Phys. Rev. Lett. 66, 1773 (1991).
[17] C. Pépin, cond-mat/0402447.
[18] P. Coleman et al.,Phys. Rev. B. 68, 220405 (2003).
[19] O. Parcollet et al.,Phys. Rev. Lett. 79, 4665 (1997).
[20] C. Pépin and I. Paul, in preparation.
[21] A. Rosch, Phys. Rev. Lett. 82 (1999) 4280.
[22] A. Rosch, Phys. Rev. Lett. 79 (1997) 159.
[23] Q. Si et al., Nature 413 (2001) 804.
[24] T. Senthil et al., Phys. Rev. Lett. 90, 216403 (2003).
[25] T. Senthil et al., Science 30, 1490 (2004).
[26] S. Nakatsuji , Phys. Rev. Lett. 92, 16401 (2004).
[27] Ar. Abanov et al. Adv. in Phys. 52, 119 (2003).