Recent trends in heavy-fermion physics

F. Steglich[a,*], N.K. Sato[b], N. Aso[c], P. Gegenwart[a], J. Custers[a], K. Neumaier[d], H. Wilhelm[a], C. Geibel[a], O. Trovarelli[a]

[a] *Max-Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany*
[b] *Department of Physics, Graduate School of Science, Nagoya University, Nagoya 464-8602, Japan*
[c] *Neutron Scattering Laboratory, Institute for Solid State Physics, University of Tokyo, Ibaraki 319-1106, Japan*
[d] *Walther Meissner Institute for Low Temperature Research of the Bavarian Academy of Sciences, Walther-Meissner-Str. 8, D-85748 Garching, Germany*

Abstract

We discuss recent results obtained for the heavy-fermion metals UPd_2Al_3 and $YbRh_2Si_2$. UPd_2Al_3 is the first among all superconductors for which tunneling and inelastic neutron-scattering data highlight a non-phononic, i.e., magnetic-exciton mediated, pair state. $YbRh_2Si_2$ represents a model system exhibiting pronounced non-Fermi liquid effects above a weak antiferromagnetic phase transition at $T_N = 70$ mK. Upon approaching the quantum critical point ($T_N \rightarrow 0$), by low doping with Ge, one observes for $T < 0.3$ K disparate behavior in the temperature dependences of both the electrical resistivity and the electronic specific heat as well as a Curie–Weiss law in the uniform magnetic susceptibility, implying uncompensated large 4f moments. These observations indicate a break up of the composite quasiparticles into their local f-spin and itinerant conduction-electron parts.

Keywords: Heavy-fermion; Superconductivity; Quantum critical point

1. Heavy-fermion metals

Certain lantanide- and actinide-based intermetallics, commonly known as heavy-fermion metals, are ideally suited to study strongly correlated electron systems. At high temperatures, these materials contain a periodic arrangement of localized 4f/5f shells with local magnetic moments that are only weakly coupled to the sea of itinerant (s, p, d) conduction electrons. Upon cooling to below a characteristic temperature T^* (10–100 K), the mixing between the f electrons and the conduction electrons becomes progressively stronger. This causes, along with the large Coulomb forces between f electrons, the magnetic moments to become progressively reduced and, simultaneously, new quasiparticles to be formed. These so-called “heavy fermions” (HF) resemble the conduction electrons of a simple metal, albeit with a much larger effective mass m^*, i.e., $(100-1000)m_{el}$. Heavy fermions might be called “composite fermions” which consist of a dominating local f part and some admixture of itinerant conduction-electron contributions, the “heavy” and “light” components that might be loosely assigned to the spin and charge degrees of freedom, respectively. For some of the HF metals a heavy Landau–Fermi Liquid (LFL) state forms well below $T = T^*$. However, a true LFL ground state appears to be the exception rather than the rule. Interactions between incompletely compensated local moments do still exist at low temperatures and may cause either an (antiferro-) magnetic phase transition at T_N or a complex “non-Fermi-liquid” (NFL) behavior. This hints at the vicinity of a magnetic “quantum critical point” (QCP), at which $T_N \rightarrow 0$ continuously as a function of the strength of the f-conduction electron mixing.

---

*Corresponding author. Tel.: +49-351-4646-3900; fax: +49-351-4646-3901.

E-mail address: steglich@cpfs.mpg.de (F. Steglich).

In this paper we first address UPd_2Al_3 [1], one of the HF metals that show coexistence of long-range antiferromagnetic order with a LFL state above T_c ($<T_N$) and with HF superconductivity below T_c (Section 2). Section 3 deals with the prototypical NFL system $YbRh_2Si_2$ [2]. An outlook is given in Section 4.

2. Magnetic Cooper pairing in UPd_2Al_3

The hexagonal compound UPd_2Al_3 is unique amongst those Uranium-based HF superconductors that show coexistence between superconductivity and long-range AF order. While the other members of this group like UPt_3 and UNi_2Al_3 exhibit relatively small ordered moments $\mu_s \approx (0.01 - 0.1)\mu_B$, for UPd_2Al_3 $\mu_s \approx 0.85\mu_B$ [3]. This points to the existence of quasi-localized 5f electrons. On the other hand, an enhanced Sommerfeld coefficient, $\gamma = 140\ \mathrm{mJ/K^2mol}$, of the electronic specific heat determined slightly above $T_c \approx 2$ K indicates moderate HF behavior due to a strong hybridization of less localized 5f states with the ligand states. Superconductivity below T_c is carried by massive Cooper pairs formed by these HFs, and is coexisting with local AF order [3]. The two-component nature of the Uranium 5f shell, including both "localized" and "itinerant" 5f states is evident [3] in bulk properties, e.g., susceptibility and specific heat as well as in μSR.

Tunneling [4] and inelastic neutron-scattering (INS) [3] experiments have revealed a strong coupling between these two different kinds of 5f states. In the tunneling density of states (DOS) of UPd_2Al_3 as registered well below T_c a modulation, i.e., a shallow minimum followed by a shallow maximum, has been observed in the energy range 0.5–1.5 meV above the superconducting gap [4]. These anomalies resemble those detected in the tunneling DOS of classical strong-coupling superconducters which, by comparison with INS spectra, could be ascribed to phonon modes and further on, with the aid of the Eliasberg theory, to the "exchange bosons" mediating the Cooper pair formation [5]. Because of the low energy of the tunneling DOS structure found for UPd_2Al_3, phonons can be safely discarded as exchange bosons. In Ref. [4], this compound was assumed to be a spinfluctuation-mediated superconductor in which overdamped AF paramagnons of the Fermi sea provide the effective attractive interaction between the itinerant quasiparticles.

Owing to the relatively low energy of ≈ 1 meV, the role of AF paramagnons in forming Cooper pairs must, however, be questioned. For, the latter would require paramagnon frequencies above a substantial threshold, while low-frequency paramagnons should rather break Cooper pairs [6]. To identify the excitation causing the unique structure in the tunneling DOS, we have reanalyzed published INS results [3]. As argued in Ref. [3], earlier susceptibility results for $T > T_N$ highlight the existence of two quasi-localized 5f electrons and of another "itinerant" one. The interaction of the localized $5f^2$ configuration with the crystal electric field (CF) separates a singlet ground state from the first excited state (perhaps a doublet), about 7 meV above the ground state. Intersite interactions allow this local CF excitation to propagate through the crystal, forming a band of "magnetic excitons" which manifests itself, in the INS spectra, in a q-dependent broad peak. At the center of the AF Brillouin zone, $\boldsymbol{Q}_0 = (0, 0, q_L = 1/2)$, the latter occurs for $T = 2.5\ \mathrm{K} \gtrsim T_c$ around $\hbar\omega \approx 1.5$ meV (Fig. 1). This magnetic-exciton-derived maximum is well separated from a quasielastic contribution which reflects the influence of the itinerant quasiparticles. Because of the singlet ground state the large ordered moment $\mu_s = 0.85\mu_B$ must be induced by the excited magnetic CF states below $T_N = 14.3$ K, where magnetic order forms due to the same intersite interactions that cause the band of magnetic excitons to form already above T_N. In the antiferromagnetically

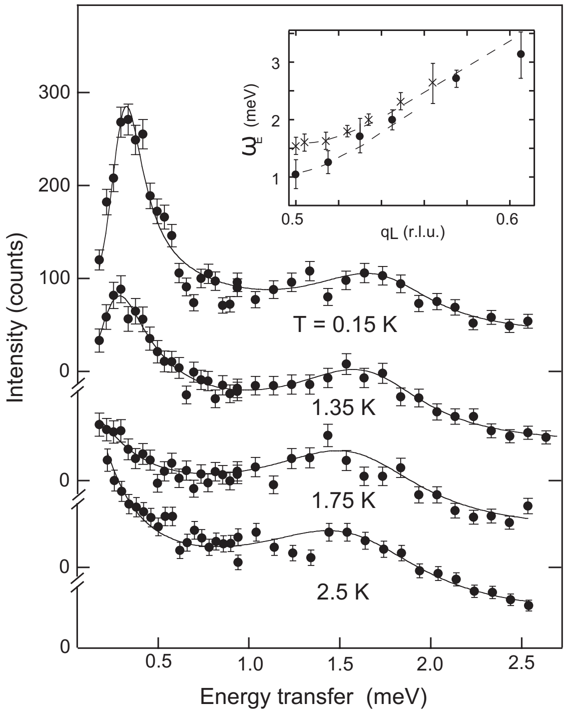

Fig. 1. Temperature evolution of the INS spectrum for a UPd_2Al_3 single crystal at $\boldsymbol{q} = (0, 0, q_L) = (0, 0, 0.5) = \boldsymbol{Q}_0$ through $T_c \approx 1.8$ K. Solid lines represent fits using the microscopic "two-component" model described in Ref. [3]. There is only one fit parameter at given values of temperature and $\boldsymbol{q}$: the magnetic-exciton energy $\omega_E(q)$, shown in the inset for $T =$ 2.5 K (crosses) and 0.15 K (circles).

ordered state, the latter play the role of acoustic magnons with a uniaxial anisotropy gap at the zone center. In the inset of Fig. 1, its dispersion $\omega_E(q_L)$ is displayed at both $T_c = 2.5$ K and $T = 0.15$ K, i.e., well below T_c (= 1.8 K for the single crystal studied in Ref. [3]). Note that the magnetic excitons can be regarded as bosons at $T \ll \hbar\omega_E/k_B$.

The zone-center exciton becomes softened by as much as 30% upon the onset of superconductivity, demonstrating that a strong coupling must exist between the heavy quasiparticles and the local magnetic moments. This is also inferred from the unique temperature dependence of the low-energy response which is changing from a quasielastic into an inelastic line below T_c. Although the neutron-scattering cross-section is dominated by the localized 5f states due to their large form factor, the observations that (i) the low-energy peak has high intensity and (ii) follows, upon cooling, the shift of the quasiparticles to the gap edge of the superconductor (Fig. 1) highlight a considerable interaction between the localized and the itinerant 5f states [3]. In fact, early NMR results [7] as well as the analysis of the INS data [3] reveal a superconducting energy gap (as $T \to 0$) $2\Delta_0 \approx 6k_BT_c$. In other words, $2\Delta_0$ is almost identical with the excitation energy of the boson that is mediating the Cooper pairing—a strong coupling scenario "par excellence" [3]. As is shown in Ref. [3], separating the spectrum of the magnetic excitons from the INS data and inserting it into Eliashberg theory enables one to reproduce well the minimum/maximum structure in the tunneling results [4].

In conclusion, UPd_2Al_3 is the first superconductor for which a magnetic pairing mechanism could be convincingly demonstrated experimentally, based upon tunneling and INS results. Here, a local CF excitation that is propagating through the lattice of U-ions is playing the same role as high-energy phonons do in classical strong-coupling superconductors.

3. Break up of the heavy-fermion quasiparticle at the antiferromagnetic quantum critical point in $YbRh_2Si_2$

The tetragonal compound $YbRh_2Si_2$ contains Yb^{3+} ions whose $J = 7/2$ Hund's rule multiplet splits into three Kramers doublets due to the CF. The ground-state doublet is well separated from the excited ones [8]. A single-ion Kondo temperature $T_K \approx 30$ K can be inferred from various experimental probes [2]. A quasilinear temperature dependence of the electrical resistivity, $\rho(T)$, and a logarithmic increase, upon cooling, of the Sommerfeld coefficient of the electronic specific heat, $\gamma(T) = C_{el}(T)/T$, clearly demonstrate NFL behavior pointing to the vicinity of a magnetic instability. Electrical resistivity [9] as well as AC-susceptibility $\chi(T)$ (Fig. 3a [2]) and specific heat $C(T)$ (Fig. 3b, [9]) results have indeed revealed a very weak AF phase transition at $T_N = 70$ mK.

T_N increases under the application of external pressure [10]. Extrapolating $T_N(p) \to 0$ one obtains a critical pressure $p_c = -0.3$ (1) GPa, reflecting the fact that a small expansion of the unit-cell volume would tune $T_N \to 0$. This can be achieved by the substitution of Si by the isoelectronic, but larger, Ge. As discussed in Ref. [11] in the system $YbRh_2(Si_{1-x}Ge_x)_2$, the QCP should be met for $x_c = 0.05(1)$. Our attempts to grow a single crystal of $YbRh_2(Si_{0.95}Ge_{0.05})_2$ revealed a very good quality of this sample (cf. its residual resistivity $\rho_0 < 5.5$ μΩ cm, Fig. 2), but an effective Ge concentration x_{eff} of less than 0.02 [11]. Despite its lower effective Ge concentration, we will call this very crystal the $x = 0.05$ sample in the following. $\rho(T)$ measurements on this sample to temperatures as low as 10 mK (Fig. 2) as well

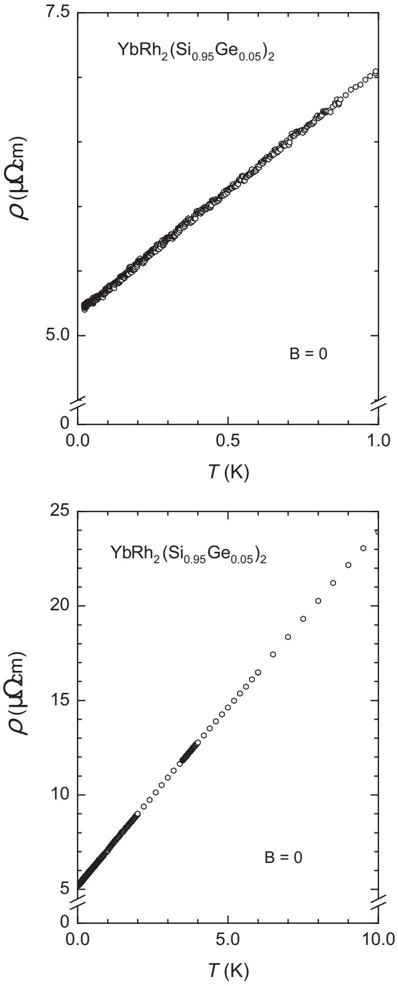

Fig. 2. Resistivity ρ vs. T for $YbRh_2(Si_{0.95}Ge_{0.05})_2$ in the range 10 mK $\leq T \leq$ 10 K.

$\chi(T)$ and $C(T)$ investigations down to almost 20 mK yield no signs of a magnetic phase transition and strongly indicate that T_N is very close to zero temperature. Apart from the lack of the AF transition the behavior of $YbRh_2(Si_{0.95}Ge_{0.05})_2$ is virtually the same as that of the undoped compound. The electrical resistivity depends strictly linearly on temperature over more than three decades, i.e., from 10 mK to above 10 K (Fig. 2). The Sommerfeld coefficient diverges logarithmically below 10 K, i.e., down to 0.3 K (Fig. 3b), and $\chi(T)$ follows a dependence $\chi^{-1} \sim T^{\alpha}$ with $\alpha \approx 0.75$ in the temperature range $0.2\ K \leqslant T \leqslant 1.5\ K$ (Fig. 3a). These observations are phenomenologically closely related to those made for the quantum critical material $CeCu_{5.9}Au_{0.1}$ [12] and hint at a novel kind of local, low-lying critical fluctuations [13,14], qualitatively different from the commonly considered spin excitations of the Fermi sea. Below $T \approx 0.3$ K strong deviations occur from the afore described behavior at higher temperatures. The Sommerfeld coefficient $\gamma(T)$ shows a pronounced upturn (Fig. 3b), while the uniform susceptibility can be well described by a Curie–Weiss law, as also found for $YbRh_2Si_2$ in the temperature range $T_N < T < 0.5$ K (Fig. 3a). Equally large paramagnetic moments, $\mu_{eff} \approx 1.4\mu_B$, and similar Weiss temperatures, $\Theta \approx -0.3$ K, for the $x = 0$ and 0.05 samples are read off as in the inset of Fig. 3a. The observation that the effective moment has the size of the full, i.e., non-Kondo compensated, moment of the Yb^{3+} CF ground-state doublet is, of course, most surprising: For example, measurements of the thermoelectric power reveal a gigantic negative peak near 30 K, which is commonly taken as one of the signatures of the single-ion Kondo scale.

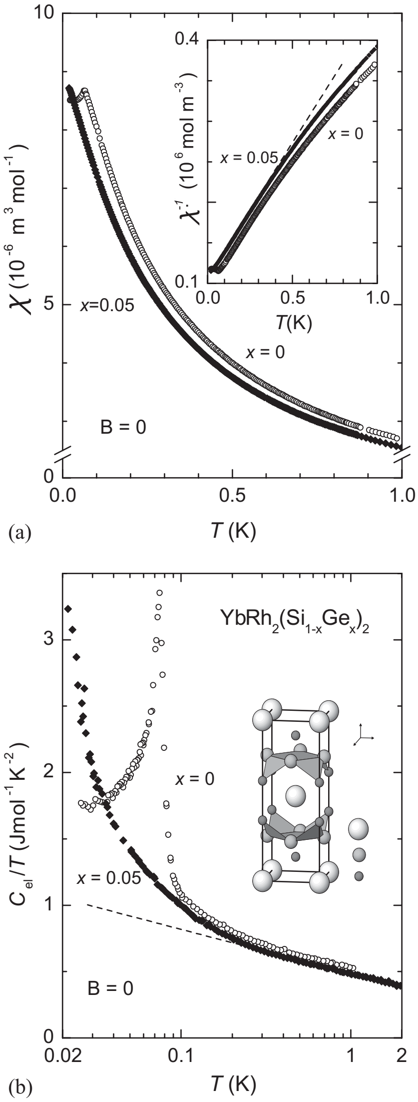

Fig. 3. Low-temperature AC-susceptibility, as χ vs. T (a), and electronic specific heat, as C_{el}/T vs. T (b), for $YbRh_2(Si_{1-x}Ge_x)_2$ with $x = 0$ and $x = 0.05$ (nominal, see text). Inset in (a) shows χ^{-1} vs. T.

The occurrence of uncompensated local magnetic moments in the uniform susceptibility at $T < 10^{-2} T_K$ goes along with a strikingly disparate behavior of $\Delta\rho(T)$ and $\gamma(T)$ below $T \approx 0.3$ K. As mentioned before, at $T > 0.3$ K both quantities show virtually the same T-dependences as found in $CeCu_{5.9}Au_{0.1}$ and described by the "locally critical" scenario [13,14]. For $T < 0.3$ K, $\gamma(T)$ strongly deviates from the $-\log T$ law, while $\Delta\rho(T)$ obeys the linear temperature dependence down to 10 mK. As $\Delta\rho(T)$ is probing the itinerant ("light") component of the "composite quasiparticles", whereas $\gamma(T)$ is probing their dominant local 4f ("heavy") part, these low-T properties seem to indicate a real break up of the heavy-fermion quasiparticles upon the approach to the QCP. Additional information on the nature of these complex quasiparticles can be obtained by using a magnetic field to fine tuning $YbRh_2(Si_{0.95}Ge_{0.05})_2$ away from the QCP [15].

4. Outlook

The two HF metals discussed in this paper are model systems in which the importance of local f degrees of freedom can be convincingly demonstrated.

UPd_2Al_3 is the first superconductor for which tunneling and INS experiments reveal a non-phononic, i.e., magnetic, pairing mechanism. But, in contrast to common belief that the effective pairing attraction in HF superconductors is provided by (strongly over-damped) fluctuations of the spins of the *itinerant* quasiparticles, it was found that here the "exchange boson" has the form of a magnetic exciton. The latter may be regarded as the CF excitation of *localized* 5f states, propagating through the crystal due to substantial U–U interactions. Future experiments should clarify whether this novel pairing mechanism is operating in other U-based HF superconductors as well.

Local f degrees of freedom also play a dominant role in the low-temperature paramagnetic phase of $\mathrm{YbRh_2(Si_{1-x}Ge_x)_2}$, $x_{\mathrm{eff}} \leqslant 0.02$. When approaching the magnetic instability (where $T_{\mathrm{N}} \to 0$), the uniform susceptibility follows a simple Curie–Weiss law, highlighting uncompensated large 4f moments. The latter are weakly coupled antiferromagnetically to each other and/or to the Fermi sea as inferred from a small negative Weiss temperature $\Theta \approx -0.3\,\mathrm{K}$. In the same low-temperature regime, the Sommerfeld coefficient $\gamma(T)$ develops an as yet unexplained additional upturn which, when compared to the unchanged $\Delta\rho \sim T$ dependence, may indicate that the dominating local-f part of the "composite quasiparticles" is more sensitive to the nearby magnetic order than their itinerant conduction-electron component is. This disparate behavior of thermodynamic and transport properties of a HF metal on the approach of a QCP requires further experimental and theoretical investigations.

Acknowledgements

We thank K. Miyake, P. Thalmeier, P. Coleman, C. Pépin, Q. Si and S. Wirth for enlightening discussions.

References

[1] C. Geibel, et al., Z. Phys. B 84 (1991) 1.

[2] O. Trovarelli, et al., Phys. Rev. Lett. 85 (2000) 626.

[3] N.K. Sato, et al., Nature 410 (2001) 340 and references therein.

[4] M. Jourdan, et al., Nature 398 (1999) 47.

[5] W.L. McMillan, J.M. Rowell, Phys. Rev. Lett. 14 (1965) 108.

[6] A.J. Millis, et al., Phys. Rev. B 37 (1988) 4975.

[7] M. Kyougaku, J. Phys. Soc. Jpn. 62 (1993) 4016.

[8] O. Stockert, private communication, 2002.

[9] P. Gegenwart, et al., Phys. Rev. Lett. 89 (2002) 056402.

[10] S. Mederle, et al., J. Magn. Magn. Matter. 226–230 (2001) 254.

[11] C. Geibel, et al., LT 23 proceedings, in press.

[12] A. Schröder, et al., Nature 407 (2000) 351 and references therein.

[13] Q. Si, et al., Nature 413 (2001) 804.

[14] P. Coleman, C. Pépin, cond-mat/0110063, 2 October 2001.

[15] J. Custers, et al., submitted for publication.