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Scaling near a "Quantum" Phase Transition: An Analysis of the Susceptibility and of the Specific Heat of $Ce(Ru_{1-x}Rh_x)_2Si_2$

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The usual scaling equations at a phase transition, employed out of their usual validity range, with T_c a negative constant, fit the susceptibility and the specific heat of these systems of the Non-Fermi Liquid (N.F.L.) window ($0.4 \le x \le 0.6$) where no long range order is observed in $Ce(Ru_{1-x}Rh_x)_2Si_2$. On either side of this window, the same equations also fit the susceptibility of these systems which order, provided the temperature is larger than the Néel temperature T_N. The exponents γ depend on x but seem to approach universal values for these concentrations of the N.F.L. window where $T_N(x)$ cancels.

KEYWORDS: Non-Fermi Liquid, Scaling analysis, Antiferromagnetic phase transition

§1. Introduction

For concentrations $x > 0.6$ the $Ce(Ru_{1-x}Rh_x)_2Si_2$ system is antiferromagnetic at low temperatures. For $0.05 < x < 0.4$ it features spin density waves. The Néel temperature decays and cancels on approaching either side of the concentration window $0.4 \le x \le 0.6$. The alloys in this window do not order and are accepted examples of Non-Fermi Liquid (N.F.L.) behaviour. In a previous paper,[1] we have analysed the susceptibility $\chi(T)$ and the specific heat $C_p(T)$ of the $x = 0.4$ and $x = 0.5$ alloys of the N.F.L. window with the same scaling expressions which we would have used near a standard (ferromagnetic) transition: assuming in this case a correlation length ξ which diverges like[2]

$$\xi/\xi_0 = (1 - T_c/T)^{-\nu}, \tag{1.1}$$

we deduce

$$\chi T/C = (1 - T_c/T)^{-\gamma}, \tag{1.2}$$

$$C_pT^2/A = (1 - T_c/T)^{-\alpha}, \tag{1.3}$$

which reflect the singularity of ξ at T_c.

Differentiating the equation (1.2) or (1.3) we find alternatively

$$\frac{\partial \ln T}{\partial \ln(\chi T)} = -\frac{T - T_c}{\gamma T_c}, \tag{1.4}$$

$$\frac{\partial \ln T}{\partial \ln(C_pT^2)} = -\frac{T - T_c}{\alpha T_c}. \tag{1.5}$$

The equations (1.1) to (1.3) are valid when $\partial \ln T/\partial \ln(\chi T)$ or $\partial \ln T/\partial \ln(C_pT^2)$ is a linear function of T and the corresponding parameters T_c and γ^{-1} (or T_c and α^{-1}) are the intersections of the straight line with the axes.[2)]

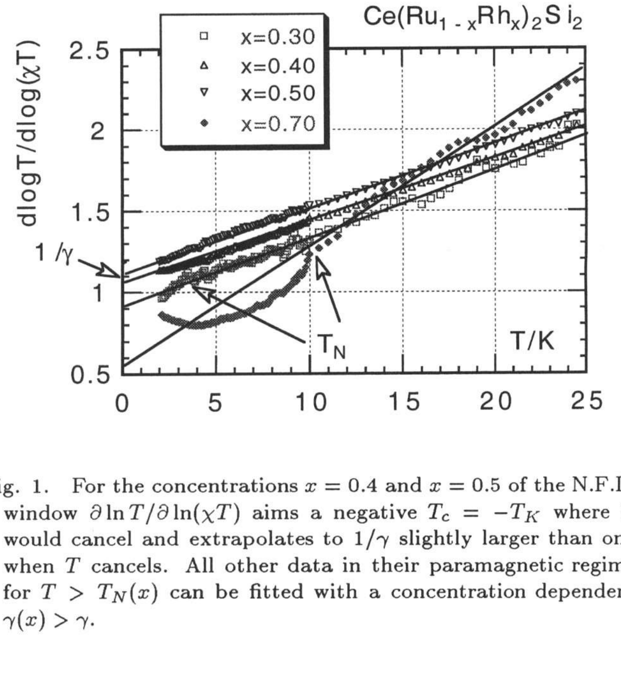

Fig. 1. For the concentrations $x = 0.4$ and $x = 0.5$ of the N.F.L. window $\partial \ln T/\partial \ln(\chi T)$ aims a negative $T_c = -T_K$ where it would cancel and extrapolates to $1/\gamma$ slightly larger than one when T cancels. All other data in their paramagnetic regime for $T > T_N(x)$ can be fitted with a concentration dependent $\gamma(x) > \gamma$.

§2. Results

In the N.F.L. systems $x = 0.4$ and $x = 0.5$ we found[1)] that $\partial \ln T/\partial \ln((\chi - \chi_D)T)$ is a linear function of T from below 2 K to over 200 K, almost 1 decade over the range to which we have, for clarity, restricted our attention in figures 1 and 2. We notice that $T_c = -T_K$ is a negative constant. It follows that the susceptibility χ is well fitted by the equation

$$(\chi - \chi_D)T = C(1 + T_K/T)^{-\gamma}, \tag{2.1}$$

where T_K, γ, C and χ_D are given in Table I. C is the high temperature Curie constant and χ_D a small diamagnetic contribution of the lattice which is easily determined at high temperatures where the variation of

Table I. On the upper four rows we give, for different concentrations x in Rh, the Néel temperature T_N and the parameters χ_D, C, T_K and γ which we deduced from our fit of the c axis susceptibility of $Ce(Ru_{1-x}Rh_x)_2Si_2$ monocrystals with equation (2.1). The additional parameters A and α were deduced from our fit of the specific heat with equation (2.2) and the same value of T_K imposed. On the lower row we give T_K, A and α which we deduced from our fit to the specific heat data of Löhneysen *et al.* in $CeCu_{5.9}Au_{0.1}$. We have neglected the crystal field contribution $\Delta C_p(T)$ in equation (2.2) in all cases.

x	T_N K	χ_D e.m.u./mole	C e.m.u./mole	T_K K	γ	A J.K/mole	α
0.3	2.5	-0.0011	1.28	21.4	1.1		
0.4	0.0	-0.00085	1.24	28.4	0.96	9906	2.80
0.5	0.0	-0.00065	1.19	29.5	0.89	8310	2.75
0.7	10.0	-0.0004	0.98	8.2	1.75		
$CeCu_{5.9}Au_{0.1}$	0.0			7.66		431	2.75

$\chi_D T$ becomes dominant when χT reaches its constant limit C (see Fig. 2).

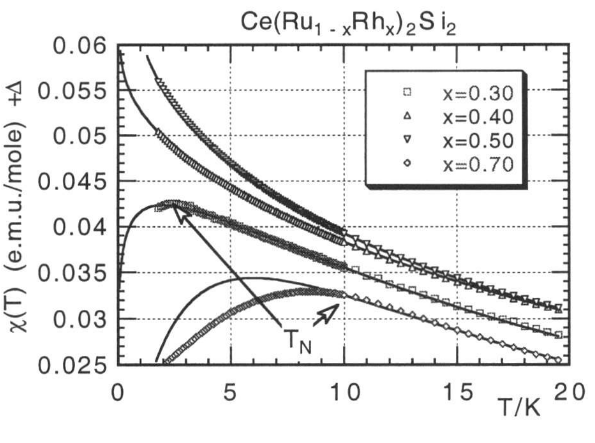

Fig. 2. The equation (1.2) fits the susceptibility at all temperatures for the alloys $x = 0.4$ and $x = 0.5$ of the N.F.L. window with $T_c = -T_K$ and with exponents γ close to one but smaller than one (see Table I) which account for the observed mild divergence of $\chi(T)$ when T cancels. On either side of the N.F.L. window the same equation still describes the data at all $T > T_N$ with a larger exponent which depends on x. For $\gamma(x) > 1$ our model predicts a susceptibility whose continuation below T_N would reach a maximum and then decay to zero. For clarity the data are shifted by a constant $\Delta = 0.005$ for the concentrations $x = 0.4$ and $x = 0.5$ of the N.F.L. window and $\Delta = 0$ otherwise.

The specific heat similarly can be fitted with

$$(C_p(T) - C_{\rm latt})T^2 = A\left(1 + \frac{T_K}{T}\right)^{-\alpha} + \Delta C_p(T)T^2, \quad (2.2)$$

where A and α are also given in Table I for T_K deduced from the susceptibility imposed. We took $C_{\rm latt}$ which fits the measured heat capacity of the non-magnetic isoelectronic system $LaRu_2Si_2$.[1] The excess term $\Delta C_p(T)$ has the shape and the magnitude expected for the incipient contribution due to the splitting, by the crystalline field of the magnetic levels of Ce. It is small in our range and will be neglected in the present discussion.

It turns out that in both systems γ is slightly smaller than one and α is slightly smaller than three. Because γ is close to one $\chi(T)$ nearly follows a Curie Weiss law $\chi = C/(T+T_K)$ but instead of reaching a constant C/T_K limit it features a mild power law divergence $T^{\gamma-1}$ when T cancels. Similarly C_p/T diverges like $T^{\alpha-3}$. From Eq. 2.2 furthermore we derive

$$C_p(T)/T = \frac{A}{T_K^3}\left(1 + \frac{T_K}{T}\right)^{-\alpha}\left(\frac{T_K}{T}\right)^3$$
$$= \frac{A}{T_K^3}\left(1 + \frac{T}{T_K}\right)^{-\alpha}\exp\left((3-\alpha)\ln\frac{T_K}{T}\right). \quad (2.3)$$

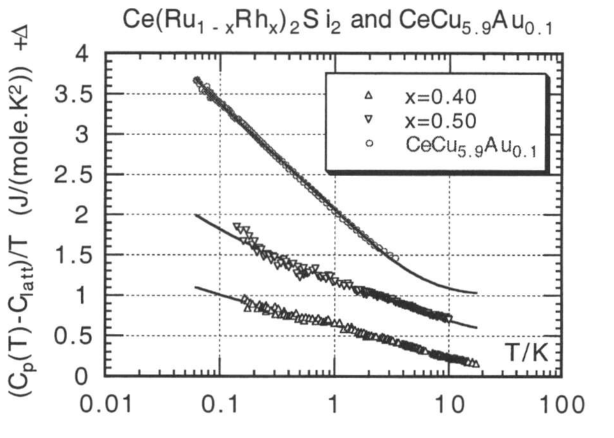

Fig. 3. We show $C_p(T)/T$ vs. $\ln T$ for the concentrations $x = 0.4$ and $x = 0.5$ of the N.F.L. window and for the $CeCu_{5.9}Au_{0.1}$ archetype of N.F.L. behaviour.[3] The data feature a widespread pseudo-logarithmic regime which is well fitted by our equation (1.3) with $T_c = -T_K$ and α just slightly smaller than 3 (see Table I). For the clarity of the figure the different curves have been shifted by a constant $\Delta = 0$ for $x = 0.4$, $\Delta = 0.5$ for $x = 0.5$ and $\Delta = 1$ for $CeCu_{5.9}Au_{0.1}$.

Because $3 - \alpha$ is so small, the exponential in the second member can be expanded as $1+(3-\alpha)\ln T_K - (3-\alpha)\ln T$ over a wide range of temperatures which explains the pseudo-logarithmic regime observed when $C_p(T)/T$ is represented vs. $\ln T$ as in Fig. 3 and is currently an accepted signature of N.F.L. behaviour. For comparison, we have also included the specific heat data of the $CeCu_{5.9}Au_{0.1}$ archetype.[3] In all cases our model permits a better account of the experimental evidence which avoids the difficulty that the extrapolation of the logarithmic trend would imply on the high temperature side. In all cases the exponents although different from each other pertain to the same narrow window close to but smaller than 3. In all cases the entropy which in our model is $S = AT_K^{-2}/[(1-\alpha)(2-\alpha)]$ is very close to $R\ln 2$.[1,2]

We have recently extended our analysis to these alloys, on both sides of the N.F.L. window, which order antiferromagnetically or feature spin density waves. We found that our model also describes the susceptibility of these systems at all temperatures larger than the Néel temperature T_N (see Figs. 1 and 2). In all these systems the exponent γ which we measured resulted larger than in the N.F.L. and actually larger than one: this implies that the continuation of the paramagnetic susceptibility would go through a maximum at T_{max} and then cancel like $T^{\gamma-1}$ when T cancels in striking contrast with the situation which we described in the N.F.L. systems (see Fig. 2). In fact this solution becomes unstable at T_N (which turns out to be very close to T_{max}) and below T_N the susceptibility is described by a different law. The discontinuity of the slope at T_N produces a distinct step on the differential plot of Fig. 1.

Unlike in the case of a ferromagnet for example, T_N is not announced by a "critical regime" where the susceptibility would scale like a power of $T - T_N$: till the last moment $T\chi(T)$ remains a power of $(1 + T_K/T)$ where T_K is not obviously related to T_N and T_N itself appears as a surprise when it occurs. In our model besides, with a negative T_c, the coherence length $\xi(T_N)$ is finite if T_N is finite. Is this the reason why $\gamma(x)$ varies along the $T_N(x)$ line in contrast with what we would expect for a ferromagnet for example ? On the contrary $\xi(T_N)$ diverges when T_N cancels and it seems that some universality is correspondingly recovered: this could explain why the exponents are close to each other for $x = 0.4$ and $x = 0.5$ and close to the values measured in other systems like $CeCu_{5.9}Au_{0.1}$ (for the time being we have no obvious good explanation for the residual scatter which is measured on these values).

§3. Conclusion

We fit the correlations at all temperatures for $0.4 \leq x \leq 0.6$ in the N.F.L. window of $Ce(Ru_{1-x}Rh_x)_2Si_2$ and at all $T > T_N$ on either side of this window. The model[2,5] is an extension of the usual scaling approach of critical phenomena where T_c and the different exponents are permitted to take unconventional values. For T_c negative it produces the power law divergences which we need to describe what is observed when T cancels. However unlike many recent models which also present this feature,[4] it restitutes a regular behaviour (Curie law) when T diverges. This is because, with our scaling variable $J/T_c - J/T$ (eq. 1.1), the thermodynamical quantities remain analytic at high temperature when J/T cancels while the usual (linearized) scaling variable $T - T_c$ does not permit to restitute even the Curie law. For the same reason, χT and C_pT^2 rather than χ and C_p are the pertinent thermodynamical quantities to consider.[2] Our exponents therefore, which are associated with these quantities, differ by 2 and 1 respectively from the corresponding "Griffith's" exponents.[4] For $x = 0.5$ for example with the values given in Table I we have, in any case, $\chi \propto T^{-0.11}$ and $C_p \propto T^{0.75}$ (or $\frac{C_p}{T} \propto T^{-0.25}$). The exponents measured depend on x when $T_N(x)$ depends on x but seem to approach universal values in the N.F.L. window where T_N cancels.

We believe that the scaling equations (1.1-1.5) follow in the framework of a hierarchical argument which is more general than the classical "scaling approach to phase transitions". The latter represents only the singular side of the model.[5]In the $T_c < 0$ case, the singularity sits on the continuation of the expression on the unphysical side of negative temperatures: this type of solution is not prohibited by any thermodynamical rule and it is obviously well adapted to the description of the present situation where we have correlations but no long range order

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