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Effect of conduction band filling on the competition Kondo-magnetism in the Kondo lattice

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Abstract

The variation of the Kondo effect and its competition with magnetism are discussed here as a function of the number of conduction electrons, within a Kondo lattice model which takes into account both the intra-site Kondo exchange and an inter-site antiferromagnetic exchange interaction. By using a mean-field approximation we show that the local Kondo effect is decreased or even suppressed away from half-filling, as well as by antiferromagnetic correlations between neighbours, as seen in our calculation of the magnetic susceptibility. © 2000 Elsevier Science B.V. All rights reserved.

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The single-impurity properties of cerium Kondo systems are well understood. But in a lattice of cerium atoms there exists a strong competition between the Kondo effect on each atom, which tends to suppress the magnetic moment with decreasing temperature, and the RKKY interaction, which, on the contrary, tends to give a magnetic ordering between different rare-earth atoms. The well-known "Doniach diagram" [1] explains the maximum of the Néel temperature observed in several cerium compounds as a function of the intra-site exchange parameter J_K of the exchange Hamiltonian $H = -J_K \mathbf{s}_c \cdot \mathbf{S}$, or experimentally as a function of applied pressure. On the other hand, we have introduced recently a Kondo-lattice model [2] with both intra-site (J_K) and inter-site (J_H) exchange parameters, and we have shown that the actual Kondo temperature T_K can be much smaller than the single-impurity one, T_{K0}, derived within the Doniach diagram. It also remains rather flat as a function of $|J_K|$ (and therefore, of applied pressure) when nearest-neighbour antiferromagnetic correlations are considered [2]. This previous treatment has been performed in the non-magnetic symmetric half-filled case. Such a behaviour has been observed in $CeRh_2Si_2$ [3] and $CeRu_2Ge_2$ [4] under pressure, and in the ternary system $Ce(Ru_{1-x}Rh_x)_2Si_2$, with the variation of x [5]. Moreover, short-range magnetic correlations have been observed in cerium compounds which do not present any long-range magnetic order, such as $CeCu_6$ [6], at a temperature T_{cor} larger than T_K, and this behaviour has also been well accounted for by the model of Ref. [2]. However, the half-filled case introduces a gap at the Fermi energy, and it is not easy to recover a metallic situation with heavy-fermion behaviour for this case [7]. Besides, the actual situation in cerium Kondo compounds corresponds to a number of 4f electrons $n_f = 1$ and a number of conduction electrons $n_c < 1$. Thus, the purpose of the present paper is to study the case $n_c < 1$ in the framework of the Hamiltonian of Ref. [2], given by

$$H = \sum_{k\sigma} \varepsilon_k n^c_{k\sigma} + E_0 \sum_{i\sigma} n^f_{i\sigma} - J_K \sum_i \mathbf{S}^c_i \cdot \mathbf{S}^f_i - J_H \sum_{\langle ij \rangle} \mathbf{S}^f_i \cdot \mathbf{S}^f_j. \quad (1)$$

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As previously, we use a simple mean-field approximation by introducing the two following parameters [8] to describe the non-magnetic phase:

$$\hat{\lambda}_{i\sigma} \equiv \tfrac{1}{2}(c^{\dagger}_{i\sigma} f_{i\sigma} + f^{\dagger}_{i\sigma} c_{i\sigma}),$$
$$\hat{\Gamma}_{ij\sigma} \equiv \tfrac{1}{2}(f^{\dagger}_{i\sigma} f_{j\sigma} + f^{\dagger}_{j\sigma} f_{i\sigma}) \quad (i,j \text{ n.n.}). \tag{2}$$

The case $n_c < 1$ has been already treated elsewhere [8], and there the electronic specific heat has been computed, showing a linear behaviour at low temperatures with an enhanced γ coefficient.

For $n_c < 1$ the situation is no longer symmetric, and both the Fermi energy and the energy E_0 of the 4f band have to be calculated. At $T = 0$, we can solve analytically the mean-field equations, obtaining E_0 as

$$E_0 = -\tfrac{1}{2}(1 - n_c)[D(1 - B) + \sqrt{D^2(1 - B)^2 + 4J_K^2\lambda^2/n_c}] \tag{3}$$

with $B \equiv zJ_H\Gamma/D$, where D is the bandwidth and z the coordination number.

We have also computed the total energy at $T = 0$, and minimized it with respect to λ to obtain the expression for λ in the usual limit of small J_K/D values,

$$\lambda^2 \simeq \frac{4n_c D^2(1 - B)^2}{J_K^2} \exp[2D(1 - B)/J_K]. \tag{4}$$

We see immediately that both the increase of antiferromagnetic short-range interaction, $|J_H|$, and the decrease of the number n_c reduce the parameter λ at $T = 0$. This result generalizes the previous results of Refs. [2,9]. Thus, the effect of increasing $|J_H|$ and decreasing n_c is to reduce the Kondo temperature T_K with respect to the single-impurity value T_{K0}. Numerical calculations have also been performed at finite temperatures. We present in Fig. 1 the results for the temperature dependence of the magnetic susceptibility for representative values of $|J_H|$ and n_c. For small values of $|J_H|$, a kink is observed in the susceptibility at the temperature where λ and Γ become non-zero, which we identify as the Kondo temperature for the lattice. Below this kink, a decreasing susceptibility indicates a Kondo behaviour, i.e. (partial) suppression of the local magnetic moment, which does not vary very much with n_c. As the temperature is further lowered, one notices that the susceptibility rises again. This can be interpreted as a manifestation of the "exhaustion" problem proposed by Nozières [10]: as λ increases, the strength of the local Kondo effect traps the conduction electrons which, being in smaller number, can no longer screen all the local moments. For large values of $|J_H|$, the Kondo effect is considerably reduced, and decreases rapidly with n_c. For $n_c = 0.85$, a small Kondo effect exists below T_K, while there is no Kondo solution ($\lambda = 0$) at all temperatures for $n_c = 0.75$. This is a regime dominated by short-range antiferromagnetic correlations ($\Gamma \neq 0$),

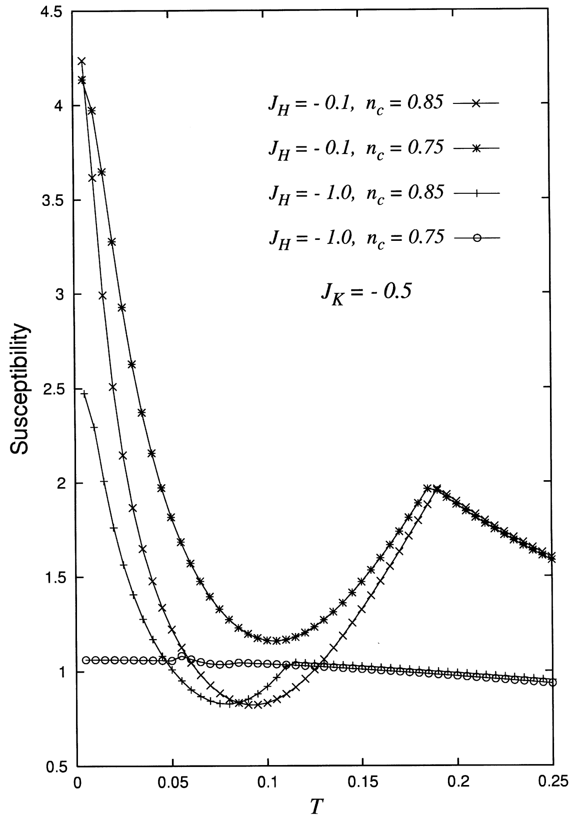

Fig. 1. Magnetic susceptibility as a function of temperature for representative values of $n_c < 1$ in two regimes: small and large $|J_H|$. The exchange parameters are in units of the half-bandwidth.

which also tend to reduce the response of the localized moments to an applied magnetic field, preventing the susceptibility from rising.

The results obtained for $n_c < 1$ confirm, therefore, the decrease of the Kondo temperature obtained previously [2] for $n_c = 1$ in the non-magnetic case within the mean-field approximation and, in addition, provides curves for the specific heat [8] and the magnetic susceptibility (Fig. 1) that can be compared with experimental results. Our present calculation asks again the difficult question about the nature of the ground state and the screening in the Kondo lattice problem. We have shown here that as the number of conduction electrons is reduced the *exhaustion* may be compensated by the formation of intersite singlets of localized spins. Exact calculations for small clusters would be interesting in that a comparison between results with a number of conduction electrons equal or much smaller than the number of 4f electrons localized on the different sites of the clusters could shed new light on this difficult problem. Work in this direction is in progress. Finally, it is interesting to note that taking into account lattice effects is essential for describing the properties of cerium or other anomalous rare-earth compounds at low temperatures, as shown, for example, in photoemission experiments [11]. This certainly stresses the need for a new approach, different from the classical one-impurity one.

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