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Physica B 259–261 (1999) 181–182

PHYSICA B

Mean-field solution of the Kondo lattice away from half-filling

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Abstract

We consider the usual Kondo-lattice, including a Heisenberg-like antiferromagnetic exchange between nearest-neighbor localized spins. Using a fermion representation for the spin operators, we decouple both Kondo and Heisenberg interactions introducing two mean-field parameters: one associated with the local Kondo effect, and the other related to the magnetic correlations between localized spins. We have concentrated on the non-magnetic case. For weak Heisenberg coupling, both mean-field parameters are continuously reduced as the number of conduction electrons departs from one. When the Heisenberg interaction is strong, magnetic-correlations are almost insensitive to band-filling, while the Kondo effect is strongly depleted away from the half-filled band.

Keywords: Kondo lattice; Cerium compounds; Doniach diagram

The denomination Kondo lattice [1] applies to many Cerium compounds, such as $CeAl_3$, $CeCu_6$, $CeCu_2Si_2$, etc. [2], as well as some Uranium and other rare-earth compounds [1], which are characterized by a lattice of localized magnetic moments coexisting with a conduction band. At high temperatures, the localized moments behave as independent impurities, similarly to what happens in dilute alloys. Below a characteristic Kondo temperature T_K a coherent heavy-fermion behavior is observed [1], where the system resembles a Fermi-liquid with enhanced values of parameters such as the specific-heat constant γ and the magnetic susceptibility χ. Deviations from this behavior are observed as some systems can show a magnetically ordered ground state, or strong short-range magnetic correlations even when the Fermi-liquid ground state is stable, if the system is close to the conditions for a magnetic instability. This competition between magnetic correlations and Kondo effect is one of the main issues in the physics of this kind of compounds. The role played by the conduction-band filling is of great relevance as one can move from an underscreened to an overscreened situation depending on the ratio between the number of conduction electrons per site and the magnitude of the localized moments [3]. Here we study the effect of band filling within a mean-field approach that has been used lately to discuss the competition between Kondo effect and magnetism in heavy-fermion compounds [4], as described by the so called Doniach diagram [5].

We choose spin-$\frac{1}{2}$ localized moments, assigning them to "f electrons". The Kondo-lattice Hamiltonian then reads

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

where we have added a Heisenberg-like interaction between nearest-neighbor localized spins. The second term on the right-hand side of Eq. (1) is just a constant provided that we remain in the subspace of unit occupation number for the f electrons at every site. We will actually impose the much weaker condition that the average number of f electrons per site must be equal to one.

We use a fermionic representation for the spin operators, and decouple the products of fermion operators through the mean-field parameters $\lambda = \langle f^\dagger_{i\sigma} c_{i\sigma} \rangle$, which describes the formation of a local Kondo singlet, and $\Gamma = \langle f^\dagger_{i\sigma} f_{j\sigma} \rangle$ (for i and j nearest neighbors), which accounts for magnetic correlations between neighboring

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0921-4526/99/$ – see front matter
PII: S0921-4526(98)00612-7

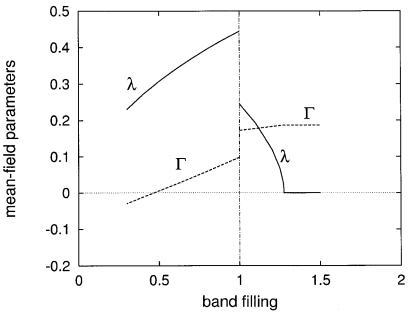

Fig. 1. Mean-field parameters λ and Γ as functions of the band filling n for a fixed temperature ($T \to 0$). The low-$|J_H|$ regime ($J_K = -1.0$, $J_H = -0.2$, in units of the band width) is shown for $n < 1$, while the high-$|J_H|$ regime ($J_K = -1.0$, $J_H = -2.0$) is shown for $n > 1$. (Both regimes are symmetric around $n = 1$.)

localized spins. Here we concentrate on the non-magnetic case, although the local average magnetic moments of both types of electrons could also be taken into account. After diagonalising the mean-field Hamiltonian [4], we solve numerically the self-consistency equations for λ and Γ, together with the conditions that fix the chemical potential μ and the f-electron energy E_0 such that we have a given number n of conduction electrons and a single f electron per site on an average. We check the results by finding the minimum of the free energy in the λ–Γ space.

Our results refer to a semi-elliptical density of states for the conduction band. When $|J_H| \ll |J_K|$, both mean-field parameters present the same critical temperature, while $|J_H|$ comparable to or larger than $|J_K|$ yields a higher critical temperature for Γ, as obtained earlier for the half-filled case [4]. On the left-hand side of Fig. 1 we show a typical example of the variation of the mean-field parameters (near saturation) with the band filling for small $|J_H|$. We see that both parameters are reduced as one moves away from half-filling. The reduction of λ is easily understood as we are increasing the underscreening condition. The fact that Γ is equally sensitive to n suggests that in this regime the inter-site correlations have a strong induced component due to the motion of the conduction electrons and their Kondo coupling to the localized spins. Notice that Γ becomes negative for small n, probably indicating that the correlations have become ferromagnetic, as expected in this limit. The situation is qualitatively changed in the high-$|J_H|$ regime, as shown on the right-hand side of Fig. 1. Now the direct (antiferromagnetic) Heisenberg coupling dominates, keeping Γ almost unchanged, while λ is strongly reduced with n. This puts into evidence the competition between the Kondo effect and magnetism in this system. Due to particle–hole symmetry, the results are symmetric around $n = 1$. In order to address an overscreening situation one has to consider more than one conduction channel.

This work was supported by CNPq (Brazil) and Brazil-France agreement CAPES-COFECUB 196/96. M.A.G. benefitted from the grant FINEP-PRONEX no. 41.96.0907.00 (Brazil). We are indebted to B. Coqblin and C. Lacroix for important remarks and discussions.

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