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A $S = 1$ underscreened Kondo lattice model

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Abstract

The underscreened Kondo lattice model presented here includes both an intra-site Kondo exchange interaction J_K between the conduction band and localized 5f electrons described by $S = 1$ spins, and an inter-site exchange f–f interaction J_H. We write both localized and itinerant spins in a Fermionic representation, and then use a mean-field approximation. We obtain a coexistence of Kondo effect and magnetism which can account for the behavior of some Uranium compounds.

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It is well established that there is a strong competition between the Kondo effect and the magnetic order at low temperature in cerium and ytterbium compounds [1]. On the other hand, the situation seems to be different in uranium systems. Some uranium compounds, such as UBe_{13} [2], URu_2Si_2 [3], UNi_2Al_3 and UPd_2Al_3 [4,5] present a heavy fermion behavior characterized by large values of the electronic specific heat constant and non-Fermi-liquid behavior in C/T, i.e., $C/T \sim \log T$, while they order antiferromagnetically as temperature decreases. Other uranium systems exhibit an unusual behavior among Kondo systems found to date. For example, $U_xTh_{1-x}Cu_2Si_2$ [7], shows a non-Fermi-liquid behavior near a ferromagnetic instability. On the other hand, UTe is a dense Kondo system that undergoes a ferromagnetic ordering at the large Curie temperature of $T_c = 102\,K$ [6], thus presenting a coexistence between the heavy-Fermion behavior and the magnetic order.

Cerium and ytterbium Kondo compounds are well described by the regular Kondo effect corresponding to the $4f^1$ and $4f^{13}$ configurations, while uranium ions in the above-mentioned compounds have a configuration $5f^n$, with $n = 2$ or 3. Our aim is to find a simple theoretical model appropriate to capture the physics of these uranium compounds. We start by considering a lattice of uranium ions in the $5f^2$ configuration with $S = 1$, coupled, through a Kondo-like interaction, to conduction electrons with $\sigma = 1/2$. As $S > \sigma$, this situation corresponds to an underscreened Kondo lattice. The underscreened Kondo effect has been solved exactly for the single-impurity case [8] while, in spite of a large theoretical effort, the underscreened Kondo lattice is still a subject of intensive investigations.

Here we examine the underscreened Kondo lattice model and we demonstrate that there exists a mean field solution correctly describing the coexistence of Kondo behavior and ferromagnetic order. The Kondo lattice Hamiltonian can be written as

$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) n^c_{k\sigma} + \sum_{i\sigma} E_0 (n^{f1}_{i\sigma} + n^{f2}_{i\sigma}) + J_K \sum_i \mathbf{S}_i \boldsymbol{\sigma}_i + \frac{1}{2} J_H \sum_{ij} \mathbf{S}_i \mathbf{S}_j, \quad (1)$$

where the first term describes the conduction band, the second term stands for the two-fold degenerate localized f-levels, the third term describes the intra-site Kondo interaction (with $J_K > 0$) and the fourth term is the

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inter-site interaction between f-magnetic moments (ferromagnetic interaction corresponds to $J_H < 0$).

This underscreened Kondo model is studied in a mean-field approximation (MFA) by employing equations of motion for the matrix Green function (GF) for localized and itinerant spins. All propagators will be written in the Fermionic representation. Within this representation the spin operators of itinerant electrons can be written as: $\sigma_i^+ = c_{i\uparrow}^+ c_{i\downarrow}$, $\sigma_i^- = c_{i\downarrow}^+ c_{i\uparrow}$, $\sigma_i^z = \frac{1}{2}(n_{i\uparrow}^c - n_{i\downarrow}^c)$. The localized f-spins are represented by the zero-width two-fold degenerate f-band coupled to $S = 1$ due to the strong on-site Hund's coupling, which favors the triplet states with respect to the singlet state. Hence, in the following, we consider only triplet states $S = 1$. The analysis is based on a fermionic representation for the spin 1 [9], valid in this constrained triplet Hilbert space.

In MFA we can expand the preceding Hamiltonian according to the four following mean values: magnetization of f-electrons $M = \langle S_i^z \rangle$, magnetization of itinerant electrons $m = \langle \sigma_i^z \rangle$ and a spin-dependent parameter describing the intra-site Kondo correlation $\lambda_\sigma = \sum_\alpha \langle f_{i\sigma}^{\alpha+} c_{i\sigma} \rangle$. Within this approximation the Kondo term is transformed in an effective self-consistent hybridization term [1]. The resulting band scheme consists of two hybridized c–f bands with a localized f-level inside the hybridization gap. The width of the gap for the band with spin σ is proportional to $2J_K^2 \lambda_{\bar{\sigma}}^2$ and it is twice larger than in the $S = 1/2$ f-spin case [1]. The two hybridized bands are given by

$$E_\pm^\sigma(\mathbf{k}) = \frac{1}{2}\left[E_{0\sigma} + \varepsilon_{\mathbf{k}\sigma} \pm \sqrt{(E_{0\sigma} - \varepsilon_{\mathbf{k}\sigma})^2 + 2J_K^2 \lambda_{\bar{\sigma}}^2}\right], \quad (2)$$

where

$$\varepsilon_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} - \mu + J_K \sigma M, \quad (3)$$

$$E_{0\sigma} = E_0 + J_K \sigma m - \frac{1}{2} J_K \lambda_\sigma \lambda_{\bar{\sigma}} + J_H z \sigma M, \quad (4)$$

and $\sigma = \pm 1/2$ corresponds to the $\uparrow$ and $\downarrow$ spins, z being the number of nearest neighbors of a site. It is clear that the bands for $\uparrow$ and $\downarrow$ spins are shifted because of the magnetic polarization, and due to the antiferromagnetic on-site Kondo exchange interaction the f-magnetization M and the conduction band magnetization m have opposite signs. E_0 is the energy of unhybridized f-levels and it is a parameter which tunes the position of the chemical potential for hybridized bands in order to have two f-electrons per site. Then, the equations giving M, m, $\lambda_\uparrow$ and $\lambda_\downarrow$ are obtained by taking a *per site* fixed average number of f-electrons $N_f = \sum_{\sigma,\alpha} \langle n_\sigma^{f\alpha} \rangle = 2$ and of conduction electrons $n_c = \sum_\sigma \langle n_\sigma^c \rangle$. The MFA solutions for the above-mentioned parameters are obtained at $T = 0$ by solving a set of self-consistent equations.

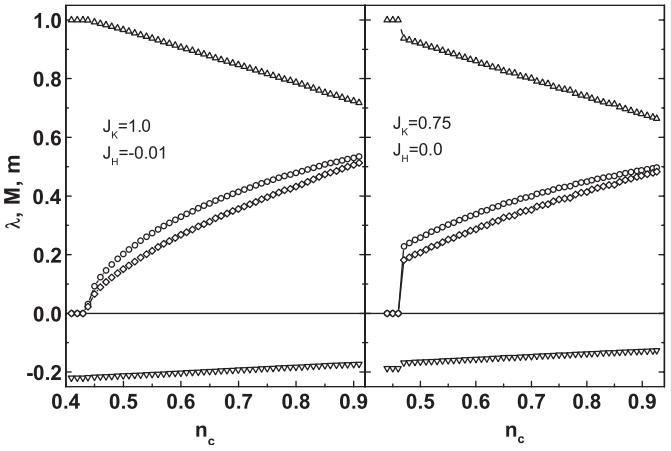

Fig. 1. The Kondo correlations $\lambda_\uparrow$ (○), $\lambda_\downarrow$ (◇), the f-magnetization, M (△) and the c-magnetization m (▽), as a function of the number of conduction electrons, n_c. J_K and J_H are in units of the half-bandwidth, D.

Fig. 1 shows the Kondo correlations $\lambda_\uparrow$, $\lambda_\downarrow$, and the f- and c-magnetization, M and m, as a function of the number of conduction electrons, n_c. We present two cases: one with $J_H/D = 0$ and $J_K/D = 0.75$, and another with $J_H/D = -0.01$ and $J_K/D = 1.0$, D being the half-bandwidth of the bare conduction band. A coexistence between Kondo regime ($\lambda \neq 0.$) and magnetism is observed in both cases. One observes that a Kondo regime with $\lambda_\uparrow \neq \lambda_\downarrow$ is coexisting with partial magnetization of both f- and c-bands for $n_c \geqslant 0.8$, while Kondo correlations vanish for low values of n_c when the f- and c-bands are fully polarized. More results and a detailed discussion will be presented elsewhere.

In conclusion, we have obtained solutions with both finite magnetization ($M \neq 0$, $m \neq 0$) and a Kondo character ($\lambda_\uparrow \neq \lambda_\downarrow \neq 0$). This result can provide a possible explanation for the coexistence between magnetic order and heavy fermion character observed in uranium compounds such as UTe.

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