

Underscreened Kondo lattice model at finite temperature

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Abstract

We have developed an underscreened Kondo lattice model with an intra-site Kondo exchange interaction J_K between the conduction band and localized 5f electrons—described by $S = 1$ spins in the f^2 configuration—and an inter-site ferromagnetic exchange f–f interaction J_H . Using a fermionic representation for the spin operators and a mean-field approximation we obtain, from $T = 0$ up to a critical temperature, a Kondo-ferromagnetic coexistence. This is in agreement with the experimental situation of some Uranium compounds, such as UTe or $UCu_{0.9}Sb_2$, which order ferromagnetically with a Curie temperature of order 100 K and present also a Kondo behavior. The Curie and Kondo temperatures are also determined.

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The normal Kondo-lattice model has been extensively studied to account for the properties of many cerium compounds where the localized electron spin S on each site can be completely screened by the conduction electron spin in the regular Kondo process, or can magnetically order through a RKKY interaction, so resulting in a competition between the magnetic order and the Kondo effect [1]. On the other hand, Uranium compounds present many different behaviors from the mixed valence one to a magnetic one without or with a Kondo effect. As an example, Neptunium and Plutonium metals, as well as some Uranium compounds are close to be magnetic and have been well described by the spin fluctuation model [2]. But, here we are interested only in some Uranium compounds which order ferromagnetically with a large Curie temperature and present also a Kondo behavior. The compound UTe is a dense Kondo system which undergoes a ferromagnetic ordering at the large Curie temperature of $T_c = 102$ K and presents a logarithmic decrease of the magnetic resistivity above it [3]. The compounds $UCu_{0.9}Sb_2$ [4] and $UCO_{0.5}Sb_2$ [5] are also ferromagnetic

Kondo ones: they order ferromagnetically at $T_c = 113$ and 64.5 K, respectively, and they show a Kondo decrease of the resistivity above the Curie temperatures. It is interesting to note that the magnetic moments deduced from magnetic susceptibility experiments are close to the theoretical free ion values of Uranium ions and that the Curie temperatures are much larger here than those of Cerium compounds.

Motivated by these experimental findings, we focus on the coexistence of the Kondo behavior and ferromagnetic ordering at finite temperatures. To account for this Kondo-ferromagnetic coexistence, we study an underscreened Kondo lattice model, assuming that the periodic lattice of magnetic atoms can be modeled by two degenerate f-orbitals interacting with itinerant spins:

$$H = \sum_{k,\sigma} (\epsilon_k - \mu) n_{k\sigma}^c + \sum_{i\sigma\alpha} E_0 n_{i\sigma}^{f\alpha} + J_K \sum_i \mathbf{S}_i \sigma_i + \frac{1}{2} J_H \sum_{ij} \mathbf{S}_i \mathbf{S}_j \quad (1)$$

where the first term represents the conduction band, which we describe by a constant density of states $1/(2D)$, in the interval $[-D, D]$ (and zero otherwise), and where D is the

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half bandwidth, so the bare band energy is $\varepsilon_k \propto |k|$. The second term describes the two-fold degenerate ($\alpha = 1, 2$) f-bands without width, the third term is the intra-site Kondo interaction (with $J_K > 0$) between localized $S = 1$ and itinerant $\sigma = \frac{1}{2}$ spins, and the last term is the ferromagnetic inter-site interaction between localized f-magnetic moments, resulting from two contributions: the effective RKKY interaction, and the direct exchange. As it was shown in Refs. [6,7] the spins $S = 1$ can be replaced by f-Fermi-operators, and we consider only triplet states $S = 1$ [7]. Finally, μ is the bare electron chemical potential and E_0 is a fictitious chemical potential (Lagrange multiplier) for f-fermions, which is fixed by a local constraint for the number of f-electrons per site $n_f = \sum_{\sigma} (n_{\sigma}^1 + n_{\sigma}^2) = 2$.

We use the mean-field (MF) approximation and expand the Hamiltonian (1) according to the following MF values: $M = \langle S_i^z \rangle$, $m = \langle \sigma_i^z \rangle$, $\lambda_{\sigma} = \sum_{\alpha} \langle \sigma_{\sigma}^{\alpha} c_{\sigma} \rangle$. The magnetic moment M arises from f-electrons and m from conduction electrons. The non-zero values of M and m correspond to the formation of the magnetic phase with non-zero total magnetization. The parameter λ_{σ} , which originates from the mean-field (MF) decoupling of the Kondo interaction, describes an effective hybridization between conduction and f-electrons, and it is known as giving a correct phenomenological description of the low-temperature heavy Fermi-liquid properties of the Kondo Lattice Model [1].

We diagonalized the MF Hamiltonian and obtained two non-hybridized f-levels at energy $E_0 + \sigma J_K m / 2 + \sigma J_H M z / 4$ and two hybridized bands with energy:

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

where $\varepsilon_{k\sigma} = \varepsilon_k + J_K \sigma M$ and $E_{0\sigma} = E_0 + J_K \sigma m - \frac{1}{2} J_K \lambda_{\sigma} \lambda_{\bar{\sigma}} + J_H z \sigma M$ with $\sigma = \pm \frac{1}{2}$ for the two spins \uparrow and \downarrow , z being the number of neighboring atoms. The existence of non-zero averages λ_{σ} opens a gap in the energy spectrum, while the bands for \uparrow and \downarrow spins are shifted from each other when one has a non-zero magnetization.

The MF equations giving M , m , λ_{\uparrow} and λ_{\downarrow} are obtained by taking fixed numbers of f-electrons $\langle n_f \rangle = 2$ and of conduction electrons $\langle n_c \rangle = \sum_{\sigma} \langle n_{c\sigma} \rangle$. The solutions at finite temperatures are obtained by solving these equations self-consistently and minimizing the free energy for the Hamiltonian. Finally, we have performed numerical calculations at different values of couplings J_K , J_H and band-filling n_c .

Fig. 1 shows the behavior of the total magnetization $M_{\text{tot}} = M + m$ and $\lambda = \lambda_{\uparrow}$ as a function of the temperature for some parameter sets. At low temperature $T < T_C$ both M and m are non-zero, and due to the breakdown of the spin symmetry $\lambda_{\downarrow} \neq \lambda_{\uparrow}$. In order to keep the figure more transparent we just included in it the temperature dependence of λ_{\uparrow} . In fact, λ_{\downarrow} and λ_{\uparrow} are slightly different only at low temperatures and completely coincide for $T > T_C$ when both magnetizations, M and m , vanish, i.e., when the spin symmetry is restored, and the hybridization of up- and down-spin bands become exactly the same. It is

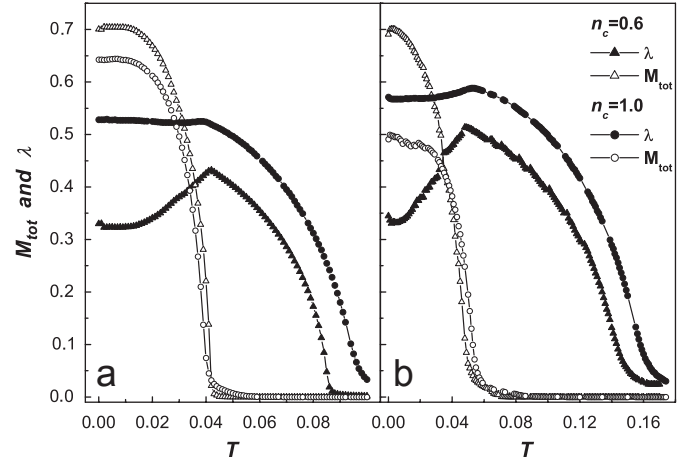


Fig. 1. Temperature dependence of $M_{\text{tot}} = M + m$ and $\lambda = \lambda_{\uparrow}$ for the band fillings $n_c = 0.6$ and $n_c = 1.0$ for values of $J_K = 0.8$ (a) and $J_K = 1.0$ (b). In both panels $J_H = -0.01$. All parameters and the temperature are given in units of the half-bandwidth D .

worth to note that in the magnetic phase the Fermi level lies inside the hybridization gap for the up-spin-band, but inside the conduction band, $E_{\downarrow}^{\downarrow}(k)$, for the down-spin-band. Also, we found a continuous transition from $\lambda \neq 0$ to $\lambda = 0$ regime. This is clear in Fig. 1 for $J_K = 0.8$ and $n_c = 0.6$ while for the other cases we have just $\lambda \approx 0$ because of numerical convergency problems (the Fermi level coincides with the localized f-level when $\lambda = 0$). The resulting characteristic Kondo temperature T_K , that corresponds to the inflexion points of the curves, increases when the Kondo coupling value J_K also increases. One remarkable result is that the Kondo temperature T_K is larger than the magnetic ordering temperature T_C . This is in agreement with experiment for Uranium compounds where a Kondo behavior is observed also above the Curie temperature, like the examples we have quoted before.

To summarize, we present here some results of the MF analysis of the Underscreened Kondo Lattice model at finite temperatures. We have shown that the model delivers good qualitative description of the unconventional properties of the uranium-based ferromagnetic compounds and can also account for the observed coexistence of the ferromagnetism and the heavy-fermion – or Kondo – behavior. Further detailed analysis of the model and results can be found in a forthcoming publication.

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