Competition between magnetic order and Kondo effect in cerium compounds

B. Coqblin,a M.A. Gusmão,b,*, J.R. Iglesiasb, A.R. Ruppenthalb, C. Lacroixc

aUniversité Paris Sud, Laboratoire de Physique des Solides, Bâtiment 510, Orsay 91405, France
bInstituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, RS, Brazil
cCNRS – Laboratoire Louis Néel, B.P. 166, Grenoble 38042, France

Abstract

We present a mean-field analysis of the competition between magnetic order and Kondo effect in a Kondo-lattice model usually employed to discuss properties of certain cerium compounds. A phase diagram is obtained showing an antiferromagnetic phase and a Kondo-compensated regime, in agreement with the Doniach diagram. A general discussion of the mean-field approach is also presented. © 2001 Elsevier Science B.V. All rights reserved.

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It is well-known that there exists a strong competition between Kondo effect and magnetic order in cerium Kondo compounds. It is believed that the ‘Doniach diagram’ [1] can describe this competition, yielding, therefore, a magnetically ordered state (generally an antiferromagnetic one) for small absolute values of the Kondo coupling $J_K$, and a non-magnetic Kondo state for large values of $J_K$. Up to now, we have studied the non-magnetic case within a model which takes into account, besides the Kondo (intra-site) interaction, an inter-site Heisenberg-like exchange term. We found that the Kondo temperature in the lattice is reduced with respect to the single-impurity one by both increasing the inter-site interaction $J_H$ [2] and decreasing the number $n_e$ of conduction electrons [3,4]. This result can account for the relatively flat variation of the Kondo temperature with pressure, observed in cerium compounds such as CeRh$_2$Si$_2$ or CeRu$_2$Ge$_2$ in the non-magnetic regime above the quantum critical point [5–7]. However, many cerium compounds which show a clear heavy-fermion behavior order antiferromagnetically at low temperatures, and some of them become non-magnetic at high pressures.

The purpose of the present paper is to describe the competition between antiferromagnetic order and Kondo effect, within the classical model for the Kondo lattice, including a Heisenberg-like antiferromagnetic exchange between nearest-neighboring localized spins. We consider the Kondo-lattice model, with the usual notations of the Wannier representation,

$$ H = -t \sum_{\langle ij \rangle} c^\dagger_{i\alpha} c_{j\alpha} - J_K \sum_i S_i \cdot S_i - J_H \sum_{\langle ij \rangle} S_i \cdot S_j \quad (1) $$

In two preceding papers [2,3], we decoupled both Kondo and Heisenberg interactions by introducing two mean-field parameters associated with the local Kondo effect and with short-range magnetic correlations. In the present paper, since we are interested in a magnetically ordered state, we use here a different mean-field decoupling, keeping the previously used Kondo mean-field parameter $\lambda$, but introducing as a mean-field parameter the staggered magnetization $M$ instead of the previously used parameter $I$ associated with short-range magnetic correlations.

We assign the localized spins to f electrons, subject to the restriction $\langle n_f^\uparrow \rangle = 1$. In the antiferromagnetic (AF)
case, dividing the system in two sublattices, A and B, the mean-field Hamiltonian takes on the form
\[ H^{MF} = H_A + H_B + H_{AB}, \]
where
\[ H_A = \sum_{\alpha} (E_0 + \sigma M_z J_H) n_{\alpha} - \mu \sum_{\alpha} n_{\alpha}^2 \]
\[ + 2J_K \sum_{\alpha} (c_{\alpha}^d f_{\alpha} + f_{\alpha}^d c_{\alpha}), \tag{2} \]
\[ H_B = H_A(M \rightarrow -M), \]
\[ H_{AB} = -t \sum_{\langle ij \rangle \sigma} (c_{j \sigma}^d c_{i \sigma} + \text{H.c.}). \tag{3} \]
The mean-field parameters satisfy the self-consistency conditions
\[ \lambda = \langle c_{\alpha}^d f_{\alpha} + f_{\alpha}^d c_{\alpha} \rangle / 2 \]
and
\[ M = \langle n_{\alpha}^2 - n_{\alpha} \rangle / 2. \]
The reference energy \( E_0 \) and the chemical potential \( \mu \) have been introduced as Lagrange multipliers for the constraints \( \langle n_{\alpha} \rangle = 1 \) and \( \langle n_{\alpha}^2 \rangle = n_c \), where \( n_c \) is the desired filling of the conduction band.

The above Hamiltonian is numerically diagonalized and we obtain self-consistent solutions for \( \lambda \) and \( M \), with different values of the physical parameters. As usual in the mean-field approximation, the Kondo phase is characterized by a non-zero value of the parameter \( \lambda \), and the antiferromagnetic (AF) order is related to a non-zero magnetization. The Kondo temperature \( T_K \) and the Néel temperature \( T_N \) are defined here as the temperatures at which the corresponding order parameters (\( \lambda \) or \( M \)) go to zero. Our results, shown in Fig. 1, are presented as a phase diagram similar to the Doniach one [1], where we plot the transition temperatures vs. \( |J_K| \) for a fixed (and large) \( J_H = -0.5W \), \( W \) being half the conduction-band width. We choose the electron density \( n_c = 0.9 \) to remain near half-filling but avoiding the Kondo-insulator situation of \( n_c = 1 \). For small values of \( |J_K| \), we obtain antiferromagnetic order at low temperatures, and the Néel temperature is constant since it depends on \( J_H \). On the contrary, for large values of \( |J_K| \), we obtain a Kondo regime, with \( T_K \) rapidly increasing.

The nature of the transition between the AF and Kondo phases is a relevant issue. In fact, we never have a stable 'mixed' phase where both \( \lambda \) and \( M \) have non-zero values. An analysis of the free energy as a function of \( \lambda \) and \( M \) reveals a first-order transition, with regions of metastability of the other solution around the transition line, as shown in Fig. 1. The occurrence of a first-order transition here is an artifact of the mean-field approximation, and one expects that this deficiency can probably be avoided by taking fluctuation corrections into account.

Thus, we have obtained an interesting result giving an AF-Kondo transition for varying \( |J_K| \) with a constant value of \( |J_H| \). We can also use the relation \( J_H = -z J_K^2 \), which was introduced in the non-magnetic case to describe the influence of the RKKY interaction [2]. In this case, however, we tend to have only the AF phase for large \( z \) and only the Kondo phase for small \( z \), because the preceding relation between \( J_H \) and \( J_K \) is too crude a way to describe the RKKY interaction. In fact, the description of both the Kondo effect and the RKKY interaction with the same exchange Hamiltonian is a very long-standing and not really solved problem. Many calculations, including real-space renormalization group [8], have shown that the Kondo-singlet phase is always stable when one considers only the intra-site exchange Hamiltonian, irrespective of the value of the coupling constant. Indeed, it is for this reason that we have explicitly introduced an inter-site exchange term, and the relation with \( z \), but clearly the RKKY interaction has to be more carefully reexamined in the case of a lattice.

In summary, we have obtained here a phase diagram showing a transition with increasing \( |J_K| \) from antiferromagnetic ordering to a Kondo state, as in the Doniach diagram. This result is in agreement with the experimental situation of many cerium compounds which change from magnetic order to heavy-fermion behavior under pressure. Our previous results [2,3] concerning the reduction of the actual Kondo temperature in the non-magnetic case by both increasing the inter-site exchange coupling or decreasing the number of conduction electrons still hold in the present analysis. Improvements of this approach to include fluctuations around the mean-field solution might lead to a better description of the nature of the AF–Kondo transition.

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