ELSEVIER
Journal of Magnetism and Magnetic Materials 226–230 (2001) 115–117
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Competition between magnetic order and Kondo effect in cerium compounds

B. Coqblin[a], M.A. Gusmão[b,*], J.R. Iglesias[b], A.R. Ruppenthal[b], C. Lacroix[c]

[a] *Université Paris Sud, Laboratoire de Physique des Solides, Bâtiment 510, Orsay 91405, France*
[b] *Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, RS, Brazil*
[c] *CNRS – 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.

Keywords: Kondo lattice; Kondo effect; Magnetic ordering

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_c 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 $CeRh_2Si_2$ or $CeRu_2Ge_2$ 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,

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - J_K \sum_i \boldsymbol{S}_i \cdot \boldsymbol{s}_i - J_H \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \,. \tag{1}$$

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 λ, but introducing as a mean-field parameter the staggered magnetization M instead of the previously used parameter Γ associated with short-range magnetic correlations.

We assign the localized spins to f electrons, subject to the restriction $\langle n_i^f \rangle = 1$. In the antiferromagnetic (AF)

* Corresponding author. Tel.: + 55-51-316-6481; fax: + 55-51-319-1762.
E-mail address: magusmao@if.ufrgs.br (M.A. Gusmão).

PII: S0304-8853(00)00762-9

case, dividing the system in two sublattices, A and B, the mean-field Hamiltonian takes on the form $H^{\mathrm{MF}} = H_{\mathrm{A}} + H_{\mathrm{B}} + H_{\mathrm{AB}}$, where

$$H_{\mathrm{A}} = \sum_{i\sigma} (E_0 + \sigma M z J_{\mathrm{H}}) n^{\mathrm{f}}_{i\sigma} - \mu \sum_{i\sigma} n^{\mathrm{c}}_{i\sigma} + 2 J_{\mathrm{K}} \lambda \sum_{i\sigma} (c^{\dagger}_{i\sigma} f_{i\sigma} + f^{\dagger}_{i\sigma} c_{i\sigma}), \quad (2)$$

$H_{\mathrm{B}} = H_{\mathrm{A}}(M \to -M)$, and

$$H_{\mathrm{AB}} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) \,. \quad (3)$$

The mean-field parameters satisfy the self-consistency conditions $\lambda = \langle c^{\dagger}_{i\sigma} f_{i\sigma} + f^{\dagger}_{i\sigma} c_{i\sigma} \rangle / 2$ and $M = \langle n^{\mathrm{f}}_{i\uparrow} - n^{\mathrm{f}}_{i\downarrow} \rangle / 2$. The reference energy E_0 and the chemical potential μ have been introduced as Lagrange multipliers for the constraints $\langle n^{\mathrm{f}}_i \rangle = 1$ and $\langle n^{\mathrm{c}}_i \rangle = n_{\mathrm{c}}$, where n_{c} is the desired filling of the conduction band.

The above Hamiltonian is numerically diagonalized and we obtain self-consistent solutions for λ 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 λ, 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 (λ 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. $|J_{\mathrm{K}}|$ for a fixed (and large) $J_{\mathrm{H}} = -0.5W$, W being half the conduction-band width. We choose the electron density $n_{\mathrm{c}} = 0.9$ to remain near half-filling but avoiding the Kondo-insulator situation of $n_{\mathrm{c}} = 1$. For small values of $|J_{\mathrm{K}}|$, 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 $|J_{\mathrm{K}}|$, 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 λ and M have non-zero values. An analysis of the free energy as a function of λ 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 $|J_{\mathrm{K}}|$ with a constant value of $|J_{\mathrm{H}}|$. We can also use the relation $J_{\mathrm{H}} = -\alpha J_{\mathrm{K}}^2$, 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

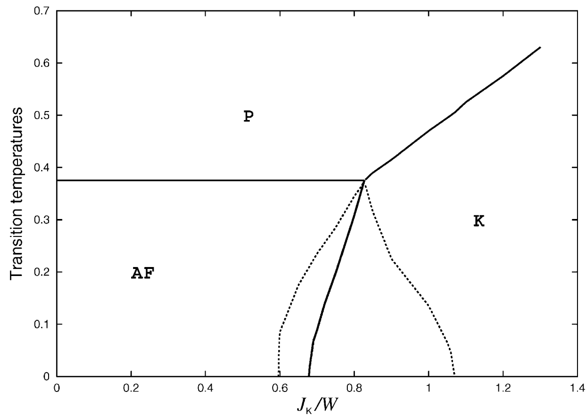

Fig. 1. Phase diagram for fixed $J_{\mathrm{H}} = -0.5\ W$ and $n_{\mathrm{c}} = 0.9$, showing the antiferromagnetic (AF), Kondo (K) and normal paramagnetic (P) regions. The first-order transition line between the AF and Kondo phases lies within the 'coexistence' region, which is delimited by the two dashed lines corresponding to the limits of metastability of the Kondo (left) and magnetic (right) solutions.

large α and only the Kondo phase for small α, 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 α, 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 $|J_{\mathrm{K}}|$ 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.

We acknowledge support from the French–Brazilian agreement CAPES-COFECUB 196/96. M.A.G. benefited from the grant FINEP-PRONEX No. 41.96.0907.00 (Brazil).

References

[1] S. Doniach, Physica B 91 (1977) 231.
[2] J.R. Iglesias, C. Lacroix, B. Coqblin, Phys. Rev. B 56 (1997) 11820.
[3] A.R. Ruppenthal, J.R. Iglesias, M.A. Gusmão, Phys. Rev. B 60 (1999) 7321.
[4] B. Coqblin, J.R. Iglesias, M.A. Gusmão, C. Lacroix, A.R. Ruppenthal, A.S.R. Simões, Physica B 281–282 (50) 2000.
[5] T. Graf, J.D. Thompson, M.F. Hundley, R. Movshovich, Z. Fisk, D. Mandrus, R.A. Fisher, N.F. Phillips, Phys. Rev. Lett. 78 (1997) 3769.
[6] H. Wilhelm, K. Alami-Yadri, B. Revaz, D. Jaccard, Phys. Rev. B 59 (1999) 3651.
[7] S. Sullow, M.C. Aronson, B.D. Rainford, P. Haen, Phys. Rev. Lett. 82 (1999) 2963.
[8] R. Jullien, P. Pfeuty, A.K. Bhattacharjee, B. Coqblin, J. Appl. Phys. 50 (1979) 7555.