Coexistence of Kondo effect and ferromagnetism in the Underscreened Kondo Lattice model

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Abstract. In this work we use a Schrieffer-Wolff transformation in a two-fold degenerate periodic Anderson lattice to describe the coexistence of Kondo effect and ferromagnetism in some uranium and neptunium compounds. We show that the inclusion of a bandwidth for the f electrons can account for a weak delocalization of $5f$ electrons. Using a mean field approximation, we show that a maximum of T_C versus J_K can be found when the bandwidth is proportional to J_K.

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INTRODUCTION

The Kondo effect presents different aspects for $4f$ and $5f$ electrons. In the rare-earth compounds, the $4f$ electrons are well localized and can be described by the Doniach's diagram [1]. In the case of actinide compounds with $5f$ electrons, it is known that some of them exhibit a coexistence of Kondo effect and ferromagnetism. Some uranium and neptunium compounds such as UTe [2, 3, 4], $UCu_{0.9}Sb_2$ [5], $UCo_{0.5}Sb_2$ [6], $NpNiSi_2$ [7] and Np_2PdGa_3 [8] present this behavior, with Curie temperatures of order $T_C \sim 50 - 100$K, which are higher than the magnetic transition temperatures observed in the rare-earth compounds. Another interesting behavior is the variation of T_C as a function of applied pressure in UTe [9, 10], where T_C increases firstly with pressure, goes then through a maximum and finally decreases at very high pressures.

Perkins *et al* [11] proposed an underscreened Kondo Lattice model (UKL) to describe the coexistence of Kondo effect and ferromagnetism in the actinide compounds. The UKL model uses a complete localized description for the $5f$ electrons. However, it is difficult to establish the degree of localization of $5f$ electrons; for example, magnetic measurements in the uranium monochalcogenides show that US lies closest to the itinerant side for the $5f$ electrons, USe is in the middle, and UTe presents more localized $5f$ electrons [4].

Thus, we present here a review of our recent work [12], where we have shown that a delocalization of $5f$ electrons can account for the variation of T_C as a function of pressure. Starting from a two-fold degenerate periodic Anderson lattice, we use a Schrieffer-Wolff (SW) transformation [13] to obtain an effective bandwidth for the f electrons. The dependence of the effective bandwidth appears to be very important for

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the variation of T_C with the Kondo parameter J_K.

EFFECTIVE MODEL

To describe the coexistence between Kondo effect and ferromagnetism, we start from a periodic Anderson lattice model with two orbitals per site and 2 f electrons on these orbitals, which allows to treat the case of $S = 1$ spins. The Hamiltonian can be written as:

$$H = H_s + H_f + H_{\text{hyb}}\,, \tag{1}$$

where H_s is the kinetic energy of conduction electrons, H_f represents the energy of $5f$ electrons and H_{hyb} is the hybridization between the conduction and $5f$ electrons. Then,

$$H_s = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma}\,, \tag{2}$$

$$\begin{aligned} H_f = \sum_{i\alpha\sigma} \varepsilon_f n^f_{i\alpha\sigma} + \sum_i \Big[& U(n^f_{i1\uparrow} n^f_{i1\downarrow} + n^f_{i2\uparrow} n^f_{i2\downarrow}) + U'(n^f_{i1\uparrow} n^f_{i2\downarrow} + n^f_{i1\downarrow} n^f_{i2\uparrow}) \\ & + (U' - J)(n^f_{i1\uparrow} n^f_{i2\uparrow} + n^f_{i1\downarrow} n^f_{i2\downarrow}) - J(f^{\dagger}_{i1\uparrow} f_{i1\downarrow} f^{\dagger}_{i2\downarrow} f_{i2\uparrow} + h.c.) \Big]\,, \end{aligned} \tag{3}$$

$$H_{\text{hyb}} = \sum_{i\vec{k}\alpha\sigma} (V_{\vec{k}\alpha} e^{i\vec{k}\cdot\vec{R}_i} c^{\dagger}_{\vec{k}\sigma} f_{i\alpha\sigma} + V^*_{\vec{k}\alpha} e^{-i\vec{k}\cdot\vec{R}_i} f^{\dagger}_{i\alpha\sigma} c_{\vec{k}\sigma})\,, \tag{4}$$

and we define

$$H_0 = H_s + H_f\,, \tag{5}$$

where $\varepsilon_{\vec{k}}$ is the energy of conduction electrons, ε_f is the energy of the two-fold degenerate f electrons, U and U' are the Coulomb repulsion integrals between the f electrons in the same and in different orbitals α ($\alpha = 1, 2$) and J is the Hund's coupling constant. $c^{\dagger}_{\vec{k}\sigma}$ ($c_{\vec{k}\sigma}$) creates (destroys) a quasiparticle with momentum $\vec{k}$ and spin σ, $f^{\dagger}_{i\alpha\sigma}$ ($f_{i\alpha\sigma}$) is the creation (destruction) operator for f electrons in the site i, orbital α and spin σ, and $n^f_{i\alpha\sigma}$ is the operator for the number of f electrons.

To perform the SW transformation, we have to define the eigenstates of Hamiltonian H_0. We assume that the triplet states have lower energy comparing with the singlet states and they will be the groundstates. It means that we consider that the energy $U' - J$ is much smaller than $U' + J$ and U. We study the SW transformation in this limit, considering that just the triplet states, $S = 1$, are initial and final states of the scattering process that give rise to the transformed Hamiltonian $H_{\text{trans}} = H_0 + \tilde{H}$. The equation (6) describes the scattering process which plays the main role in the SW transformation [13]:

$$\tilde{H} = \frac{1}{2} \sum_c \langle b|H_{\text{hyb}}|c\rangle \langle c|H_{\text{hyb}}|a\rangle \left(\frac{1}{E_a - E_c} + \frac{1}{E_b - E_c} \right) |b\rangle\langle a|\,, \tag{6}$$

where $|a\rangle$, $|b\rangle$ and $|c\rangle$ are the eigenstates of H_0 and E_a, E_b and E_c are the eigenenergies, respectively.

Among the different terms that come from the SW transformation, we obtain a Kondo-like term that represents the interaction between the spins $S = 1$ of localized $5f$ electrons and the spins $s = 1/2$ of conduction electrons and also a term that represents an effective bandwidth for the f electrons.

From the SW transformation we obtain the $s - f$ interaction as:

$$H_{sf} = \frac{1}{2} \sum_{i\vec{k}\vec{k}'} J_K \left[c^{\dagger}_{\vec{k}'\uparrow} c_{\vec{k}\downarrow} S_i^{f-} + c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}\uparrow} S_i^{f+} + (c^{\dagger}_{\vec{k}'\uparrow} c_{\vec{k}\uparrow} - c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}\downarrow}) S_{zi}^{f} \right], \tag{7}$$

where the operators $S_i^{f+} = n^f_{i1} f^{\dagger}_{i2\uparrow} f_{i2\downarrow} + n^f_{i2} f^{\dagger}_{i1\uparrow} f_{i1\downarrow}$, $S_i^{f-} = n^f_{i1} f^{\dagger}_{i2\downarrow} f_{i2\uparrow} + n^f_{i2\sigma} f^{\dagger}_{i1\downarrow} f_{i1\uparrow}$, $S_i^{fz} = n^f_{i1\uparrow} n^f_{i2\uparrow} - n^f_{i1\downarrow} n^f_{i2\downarrow}$ and $n^f_{i\alpha} = n^f_{i\alpha\uparrow} + n^f_{i\alpha\downarrow}$, satisfying the usual commutation rules for the spin operators. J_K is the Kondo parameter and it is given by $J_K = \frac{2|V_{kf}|^2}{\mu - E_0^f}$, where $E_0^f = U' - J + \varepsilon_f$ is the energy difference between one and two f electrons with $S = 1$ in the periodic Anderson model given by the equation (1). μ is the chemical potential and V_{kf} is the Anderson hybridization.

The introduction of the f bandwidth improves the decription of the f electrons in the uranium and neptunium compounds. The effective f bandwidth can be written in the mean field approximation as:

$$A_{\vec{k}\sigma} = -P \frac{J_K}{2} \left(\langle n^f_{\sigma} \rangle^2 + \frac{1}{2} \langle n^f_{\sigma} \rangle \langle n^f_{\bar{\sigma}} \rangle + \frac{1}{4} \langle n^f_{\bar{\sigma}} \rangle^2 \right) \varepsilon_{\vec{k}}, \tag{8}$$

where P is a parameter, $\langle n^f_{\sigma} \rangle$ is the mean value of the number of f electrons per site and per orbital. In the original SW transformation for a localized spin $S = 1/2$ lattice, an effective bandwidth term is also found. However, as the behavior of $4f$ electrons are almost localized, this term is usually not considered. The effective Hamiltonian to be analyzed is:

$$H_{\text{eff}} = H_0 + H_{sf} + \sum_{\vec{k}\alpha\sigma} A_{\vec{k}\sigma} f^{\dagger}_{\vec{k}\alpha\sigma} f_{\vec{k}\alpha\sigma} + \frac{1}{2} J_H \sum_{\langle ij \rangle} \vec{S}_i^f \cdot \vec{S}_j^f. \tag{9}$$

The last term represents the RKKY interaction between the f spins in different sites. As we want to study the coexistence of Kondo effect and ferromagnetism, this term is added to take into account the ferromagnetic interactions between the f spins, where J_H is a ferromagnetic interaction parameter. Thus in our model, both J_H and the second order term in J_K contribute to the determination of the Curie temperature.

RESULTS AND CONCLUSION

We have calculated the Kondo (T_K) and Curie (T_C) temperatures as a function of the Kondo parameter J_K. This allows us to obtain a comparison with the experimental results for the variation of T_K and T_C with applied pressure and our results present a

good agreement with the experimental results for the compound UTe [9, 10]. T_K and T_C are defined within the mean field approximation by the temperatures at which the magnetization and the mean value $\langle \lambda_\sigma \rangle = \langle c^\dagger_{\vec{k}\sigma} f_{i\alpha\sigma} \rangle$ are respectively tending to zero. We consider that the density of states for the conduction electrons is constant and equal to $2D$. All energies are defined in units of D. We analyzed the effect of the f bandwidth on the magnetic properties of the system, considering three different forms for the f bandwidth, defined as W:

- (a) W is constant.
- (b) W is proportional to the Kondo parameter, $W = QJ_K$.
- (c) W is defined in agreement with our present result obtained by the SW transformation, $W = 2A_{\vec{k}\sigma}/\varepsilon_{\vec{k}}$.

In figure 1, we show the variation of T_C and T_K as a function of the Kondo parameter J_K for the three cases, where we used $W = 0.05$ for case (a), $Q = 0.12$ for case (b), and $P = 0.12$ for the case (c). For all figures we fixed the number of f and c electrons as $n^f_{\rm tot} = 2$ and $n^c_{\rm tot} = 0.8$, respectively.

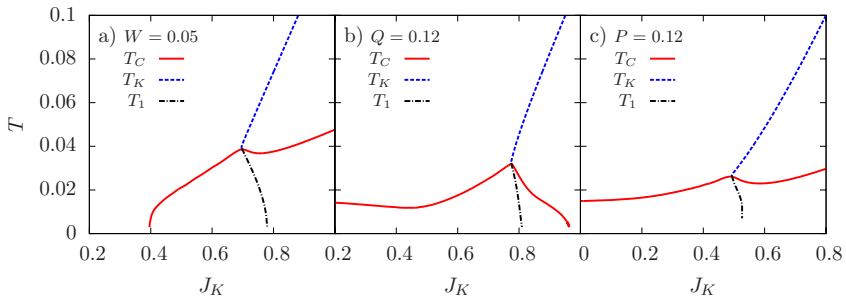

FIGURE 1. T_C and T_K *versus* J_K for the three cases described in the text: (a) $W = 0.05$, (b) $Q = 0.12$, and (c) $P = 0.12$, for $J_H = -0.01$ [12].

Cases (b) and (c), where the f bandwidth is proportional to the Kondo parameter, show a maximum for T_C for a given value of J_K and a decrease of T_c for larger J_K; the increase of J_K can be connected with an increase of pressure, because, when the pressure increases, the energy E^f_0 comes closer to the Fermi level μ, which results, as usual, in an increase of the value of J_K. We can conclude that the decrease of T_C is related with the decrease of localization of f electrons. This result is in agreement with the experimental results obtained for UTe [9, 10] and is in favor of the UKL model [11, 12] that we have proposed to describe the coexistence between Kondo effect and ferromagnetism in some uranium and neptunium compounds.

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