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The S=1 Underscreened Anderson Lattice model for Uranium compounds

C. Thomas[1,2], A. S. R. Simões[1], J. R. Iglesias[1], C. Lacroix[2], N. B. Perkins[3] and B. Coqblin[4]

[1] Inst. de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, Brazil
[2] Institut Néel, CNRS-UJF, BP 166, 38042 Grenoble Cedex 9, France
[3] Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA
[4] L. P. S., Université Paris-Sud, UMR-8502 CNRS, 91405 Orsay, France

Abstract. Magnetic properties of uranium and neptunium compounds showing coexistence of the Kondo effect and ferromagnetic order are investigated within the degenerate Anderson Lattice Hamiltonian, describing a $5f^2$ electronic configuration with $S = 1$ spins. Through the Schrieffer-Wolff transformation, both an exchange Kondo interaction for the $S = 1$ f-spins and an effective f-band term are obtained, allowing to describe the coexistence of Kondo effect and ferromagnetic ordering and a weak delocalization of the $5f$-electrons. We calculate the Kondo and Curie temperatures and we can account for the pressure dependence of the Curie temperature of UTe.

1. INTRODUCTION

The interplay between Kondo effect and magnetism is very important in cerium, ytterbium, uranium or other anomalous rare-earth and actinide systems [1, 2]. In contrast to $4f$-electrons, the $5f$-electrons in actinide compounds can be either localized or itinerant or in-between, depending on the studied system [3, 4, 5, 6, 7].

The difference between the $4f$- and $5f$-electrons leads to different magnetic properties. In the case of cerium Kondo compounds, the competition between the Kondo effect on each Ce atom and the magnetic ordering is described by the "Doniach diagram" [8], which gives rather low ordering temperatures, typically of order 5 to 10 K. On the other hand, some uranium compounds, like UTe [9], $UCu_{0.9}Sb_2$ [10] or $UCo_{0.5}Sb_2$ [11] present a ferromagnetic order with large Curie temperatures (equal respectively to 102 K, 113 K and 64.5 K) and also exhibit a logarithmic Kondo-type decrease of the resistivity above T_C. Recently, a similar behavior has been observed in two neptunium compounds $NpNiSi_2$ [12] and Np_2PdGa_3 [13], with T_C equal to respectively 51.5 K and 62.5 K.

Thus, it is clear that Kondo effect and ferromagnetic order coexist in some uranium and neptunium compounds. However, the localization of the $5f$-electrons is a difficult question and in fact the values of the magnetic moments observed for example in UTe are substantially smaller than the free-ion values for either the $5f^2$ or the $5f^3$ configurations [9]. On the same side, in the series of uranium monochalcogenides, US lies closest to the itinerant side for the $5f$-electrons, USe is in the middle and the $5f$-electrons are more localized in UTe, as evidenced by magnetization measurements [9]. Moreover, the Curie temperature of UTe is passing through a maximum and is then decreasing with applied pressure, which is interpreted

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as a weak delocalization of the $5f$-electrons under pressure [4, 9]. The dual nature of the $5f$-electrons, assuming two localized $5f$-electrons and one delocalized one, has been also introduced to account for the properties of some uranium compounds [5] .

The coexistence between the Kondo effect and the ferromagnetism in some uranium compounds was described by the Underscreened Kondo Lattice (UKL) model which considers localized f-spins $S = 1$ without any f-band width [14]. Here we will present a recent work in which a finite $5f$-bandwidth is introduced within the Underscreened Anderson Lattice (UAL) model, in order to describe a weak delocalization of the $5f$-electrons and to account for the pressure dependence of the Curie temperature of UTe [15, 16]. In contrast with $S = 1/2$ case, Kondo screening in Kondo $S = 1$ is not complete [17] and this allows coexistence of Kondo effect and magnetism.

2. THE EFFECTIVE $S = 1$ HAMILTONIAN.

We start here from the UAL Hamiltonian with two f-electrons per site (in different orbitals α=1,2) forming a $S = 1$ spin. The UAL model, which is explicitely given in Ref. [15], is composed of a conduction band of energy $\epsilon_{\mathbf{k}}$, a two-fold degenerate f-level at the energy E^f, a $c - f$ hybridization term, and Coulomb interactions between f-electrons: U and U' among electrons in respectively the same and different orbitals and Hund's coupling J. Then, we use the Schrieffer-Wolff (SW) transformation [18] and we obtain an effective Hamiltonian: $H = H_c + H_{cf} + H_W$. The first term describes the conduction electrons, the second one is the usual Kondo exchange Hamiltonian, but here with f-spins $S = 1$, and it is given by:

$$H_{cf} = \frac{1}{2}\sum_{i\mathbf{k}\mathbf{k}'} J_K \left[c^\dagger_{\mathbf{k}'\uparrow} c_{\mathbf{k}\downarrow} S^-_i + c^\dagger_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} S^+_i + (c^\dagger_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow}) S^z_i \right] \tag{1}$$

with the different components of the spin $S = 1$ given by: $S^z_i = n^f_{i1\uparrow} n^f_{i2\uparrow} - n^f_{i1\downarrow} n^f_{i2\downarrow}$, $S^+_i = n^f_{i1} f^\dagger_{i2\uparrow} f_{i2\downarrow} + f^\dagger_{i1\uparrow} f_{i1\downarrow} n^f_{i2}$ and a similar expression for S^-_i. J_K is the usual Kondo interaction integral. The third term H_W of the new derived Hamiltonian yields an effective f-band term, with a bandwidth proportional to J_K. Detailed calculations can be found in Refs [15] and [16].

Besides these two terms H_{cf} and H_W, we add an exchange interaction J_H between the localized spins to account for the effective intersite ferromagnetic exchange. In fact, the exchange interaction J_K can in principle yield both the Kondo effect and magnetic order, but the addition of the exchange interaction J_H is necessary to really describe the magnetic order, as already well established theoretically [2, 14, 19]. Here J_H is considered as a ferromagnetic interaction between nearest neighbor f-spins.

Thus, the total mean field Hamiltonian is :

$$H_{tot} = \sum_{\mathbf{k}\sigma} \epsilon^c_{\mathbf{k}\sigma} n^c_{\mathbf{k}\sigma} + \sum_{i\sigma\alpha} E^f_{0\sigma} n^f_{i\alpha\sigma} + \sum_{\mathbf{k}\sigma\alpha} \Lambda_\sigma (c^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\alpha\sigma} + h.c.) + \sum_{\mathbf{k}\sigma\alpha} A_{\mathbf{k}\sigma} f^\dagger_{\mathbf{k}\alpha\sigma} f_{\mathbf{k}\alpha\sigma} + C \tag{2}$$

The effective f-hopping term $A_{\mathbf{k}\sigma}$ is given by :

$$A_{\mathbf{k}\sigma} = -\epsilon_{\mathbf{k}} \frac{J_K}{2} \left[(n^f_\sigma)^2 + \frac{1}{2} n^f_\sigma n^f_{\bar{\sigma}} + \frac{1}{4} (n^f_{\bar{\sigma}})^2 \right] , \tag{3}$$

while the effective $c - f$ hybridization is equal to $\Lambda_\sigma = -\frac{J_K}{4}(\lambda_\sigma + \lambda_{\bar{\sigma}})$, with $\epsilon^c_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + \Delta_\sigma$ and $\Delta_\sigma = J_K \sigma M^f$.

$E^f_{0\sigma}$ is the effective position of the f-level given by :

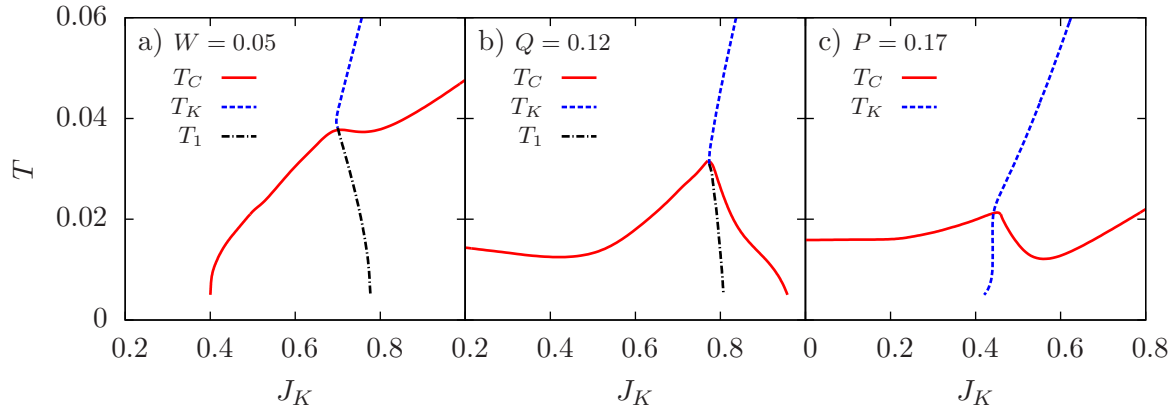

Figure 1. Plots of T_C, T_K and T_1 versus J_K for the three cases (a), (b) and (c), with $J_H = -0.01$, $n^c = 0.8$ and $n^f_{\rm tot} = 2$ and the values of the different parameters given in the figures (all the temperatures and the energies are expressed in units of D).

$$\begin{aligned} E^f_{0\sigma} &= E^f + U' n^f_{\bar{\sigma}} + (U' - J) n^f_{\sigma} + J_K \sigma m^c \\ &\quad - \tfrac{J_K}{8}(\lambda_\uparrow + \lambda_\downarrow)^2 + J_H z \sigma M^f \ , \end{aligned} \tag{4}$$

and C is equal to :

$$\begin{aligned} C &= -2U' N n^f_\uparrow n^f_\downarrow - (U' - J) N [(n^f_\uparrow)^2 + (n^f_\downarrow)^2] \\ &\quad + \tfrac{J_K}{2} N (\lambda_\uparrow + \lambda_\downarrow)^2 - \tfrac{J_H}{2} z N (M^f)^2 \\ &\quad - J_K N m^c M^f \end{aligned} \ , \tag{5}$$

with $\sigma = \pm\frac{1}{2}$, $M^f = n^f_\uparrow - n^f_\downarrow$ and $m^c = \frac{1}{2}(n^c_\uparrow - n^c_\downarrow)$.

$n^f_{i\alpha\sigma}$ is the number of f-electrons per site, spin and orbital α, $n^f_\sigma = < n^f_{i\alpha\sigma} >$ and n^c the total number of conduction electrons. The f and c magnetizations $M^f = n^f_\uparrow - n^f_\downarrow$, $m^c = \frac{1}{2}(n^c_\uparrow - n^c_\downarrow)$ and Kondo parameter $\lambda_\sigma = \langle c^\dagger_{\mathbf{k}\sigma} f_{i\alpha\sigma} \rangle$ should be calculated selfconsistently [14, 16].

The diagonalization of the Hamiltonian gives one pure f-band with dispersion given by: $E^{f-band}_{\mathbf{k}\sigma} = E^f_{0\sigma} + A_{\mathbf{k}\sigma}$

and two hybridized $f - c$ bands $E^\pm_{\mathbf{k}\sigma}$ given by :

$E^\pm_{\mathbf{k}\sigma} = \frac{1}{2}[\epsilon_{\mathbf{k}} + A_{\mathbf{k}\sigma} + E^f_{0\sigma} + \Delta_\sigma \pm S_{\mathbf{k}\sigma}]$,

with:

$S_{\mathbf{k}\sigma} = \sqrt{[\epsilon_{\mathbf{k}} - A_{\mathbf{k}\sigma} - E^f_{0\sigma} + \Delta_\sigma]^2 + 8(\Lambda_\sigma)^2}$.

3. RESULTS and CONCLUSIONS.

We present here the main results obtained by the present calculations. The Kondo (T_K) or Curie (T_C) temperatures are defined in the mean field approach as the temperatures at which respectively the λ_σ parameters or the magnetizations vanish. T_K depends essentially on J_K,

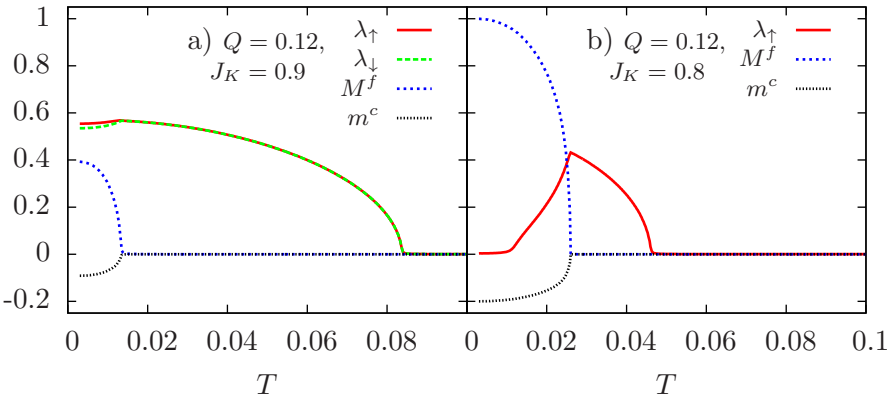

Figure 2. M^f, m^c and λ_σ versus temperature (expressed in units of D) for the case (b), with $Q = 0.12$, $J_H = -0.01$, $n^c = 0.8$, $n^f_{\rm tot} = 2$, and respectively two values of $J_K = 0.9$ (Figure 2.a) and $J_K = 0.8$ (Figure 2.b).

while T_C depends obviously on both J_K and J_H. We consider a constant density of states for the conduction electron band with a band width $2D$, and in the following all energies and temperatures are expressed in units of D.

Our basic interest is here to study the effect of the finite f-band width W on the magnetic properties. Thus, we have considered the three following cases:
- case (a) : W is taken constant,
- case (b) : W is taken proportional to the exchange Kondo integral, i.e. $W = QJ_K$,
- case (c) : W is given by our present derivation of the SW transformation, i.e. $W = 2PA_{\mathbf{k}\sigma}/\epsilon_{\mathbf{k}}$.

Figure 1 gives both T_K and T_C, as a function of the Kondo exchange integral J_K, for the three cases (a), (b) and (c) defined above, with respectively the following parameters: $W = 0.05$, $Q = 0.12$ and $P = 0.17$. For small J_K values, there is no Kondo effect and T_C increases continuously with J_K, while for large J_K values, T_K increases rapidly with J_K. Two effects have to be pointed out: (1) in some cases T_C decreases for large J_K; (2) there is a "peculiar behavior" of T_K for the two cases (a) and (b): in a certain J_K range, λ is non-zero only between two temperatures T_K and T_1 and vanishes below T_1.

Then, we present on Figure 2 two plots of M^f, m^c and λ_σ versus temperature for $n^c = 0.8$, $J_H = -0.01$ and for the case (b) with $Q = 0.12$, but for two different values of J_K equal to 0.9 (Figure 2a) and 0.8 (Figure 2b). Figure 2a shows clearly that both the Kondo effect and ferromagnetism exist together for $J_K = 0.9$ down to the lowest temperatures, with T_K larger than T_C. Figure 2b corresponding to the "peculiar behavior" shows that for $J_K = 0.8$, with decreasing temperature, Kondo effect occurs at T_K, then there is a coexistence of Kondo and ferromagnetism, and finally the Kondo effect disappears at T_1 to yield only a strong ferromagnetism at very low temperatures. This behavior can be interpreted in the following way: Kondo effect for a spin $S = 1$ cannot be complete when there is only one screening channel [17]. Thus if exchange is large enough, the ordering of the remaining f-moments occurs in the Kondo phase. However, at lower temperature, when these ordered magnetic moments are large, they act as an internal magnetic field and Kondo effect is destroyed by this effective magnetic field. One should notice that there is at present no experimental evidence in favor or in contrast of such an effect in actinide compounds at very low temperatures.

Finally, the decrease of the Curie temperature observed in the cases (b) and (c) of Figure 1 for large J_K values above the intersection point with T_K can probably be considered as resulting from a possible effect of "delocalization" of the $5f$-electrons. Let us also remark that J_K increases with increasing pressure and that the two figures corresponding to the cases (b) and

(c) can give a good description of the experimentally observed variation of T_C with pressure in UTe compound, which is passing through a maximum and then decreasing with applied pressure [4, 9].

We can conclude that the present calculation improves the previous $S = 1$ UKL model of Ref. [14]. The model described in Ref. [14] started from a localized description of the $5f$-electrons in the $5f^2$ configuration, while here we started from an Anderson Hamiltonian and derived by the Schrieffer-Wolff transformation a new Hamiltonian with a non zero f-band width, in addition to the usual Kondo exchange term. This new Hamiltonian can describe the onset of the "delocalization" of the $5f$-electrons and the new curves giving a maximum of T_C as a function of J_K can account for the pressure dependence of T_C in UTe. Thus, the present work yields an improvement with respect to the UKL model of Ref. [14] for the description of the $5f$-electrons in some uranium compounds.

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