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The Schrieffer-Wolff transformation for the S=1 Underscreened Kondo Lattice model : Application to Uranium compounds

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It is well known that the interplay between the Kondo effect and magnetism plays a very important role in Cerium, Ytterbium, Uranium or other anomalous rare-earth and actinide systems. Both effects depend strongly on the hybridization between the f and conduction electrons, which in turn significantly depends on the level of localization of the f electrons. In the case of Cerium compounds, 4f-electrons are usually well localized, while in the case of Uranium and other actinide compounds, 5f-electrons can be either localized or itinerant or in between, depending on the studied system. The difference between 4f- and 5f-electrons can lead to very different magnetic properties of rare-earth and actinide compounds.
It is now established that some actinide compounds exhibit a co-existence between magnetic order and Kondo effect. This phenomenon was observed in several Uranium compounds, like UTe, UCu0.9Sb2, UCo0.5Sb2 or UNiSi2, in which a ferromagnetic order with large Curie temperatures (equal respectively to Tc = 102K, 113K, 64.5K and 95K) and a logarithmic Kondo-type decrease of the resistivity above Tc have been experimentally observed [1] [2]. Moreover, the Curie temperature of UTe is passing through a maximum and is then decreasing with applied pressure, which is interpreted as a weak delocalization of the 5f electrons under pressure [3] [4]. A similar observation has been done in the Neptunium compound NpNiSi2 with a Curie temperature equal to 51.5K [5]. This behaviour is very different from that of Cerium compounds, in which there is a competition between the Kondo effect and the magnetic ordering of the Ce moments, leading to rather low ordering temperatures, typically of order 5 to 10 K.
The first attempt to describe the coexistence of ferromagnetism and Kondo effect in Uranium compounds has been performed within an underscreened Kondo lattice (UKL) model which considers localized f-spins Sf = 1 to describe a 5f2 configuration of Uranium ions with 2 f-electrons [6]. This model describes the interaction between the localized spins and s=1/2 spins of conduction electrons through the local Kondo interaction, JK, and the inter-site exchange interaction between the f-spins, JH. The UKL model gives a new diagram for the Curie Tc and the Kondo TK temperatures versus JK: at a critical value of JK, there is a steep increase of TK, while Tc increases smoothly above this critical value of JK. This diagram, which is different from the Doniach diagram used for Cerium compounds, can account for the coexistence of ferromagnetism and Kondo effect and for the increase of Tc with pressure at low pressures in UTe. However, this model is based on the assumption of localized 5f-electrons, which does not reflect the situation of several Uranium compounds. Thus, it is necessary to include in the UKL model the possibility of describing the 5f electron delocalization and this will be done here by considering a finite f-band width.
Here we start with an underscreened Anderson Lattice (UAL) Hamiltonian and transform it to an effective Kondo-type spin Hamiltonian by use of a generalized Schrieffer-Wolff (SW) transformation [7]. Namely, the SW transformation yields the usual exchange Kondo-type term for Sf =1 spins with an exchange interaction

proportional to the square of the hybridization parameter Vkf between conduction and f-electrons, and a new scheme for the bands, giving two hybridized bands and one f-band which has a spin-dependent width given by W = -JKA⊠/2, with A⊠ = [(nf⊠)2 −(1/2)nf⊠nf-⊠ −(1/4)(nf-⊠)2], where nf⊠⊠ is the average number of f-electrons per site i in one of the orbitals 1 or 2 and spin ⊠.
We discuss now the results obtained by this improved UKL model. In the joint Figure 1, we plot Tc and TK temperatures versus the Kondo interaction parameter JK , obtained for the two following cases: in case (a), the f-band width is proportional to JK, W = QJK with Q=0.12 and in case (b), the relation between W and JK is that previously derived by the SW transformation and is spin-dependent, W= PJKA⊠, with here P= -2.

Figure 1. Plots of the Curie temperature, Tc, and the Kondo temperature, TK, versus JK, in the two cases explained in the text. The parameters are: JH= -0.01, a total number of 5f electrons equal to 2, a number of conduction electrons <nc> = 0.8, U'= J = 0 and U infinite.

In the case (a), we obtain a maximum at the crossing point between Tc and TK and finally Tc is tending to zero. Since JK increases with pressure, this dependence can provide a possible explanation for the pressure dependence of Tc in UTe compound. In the case (b) the behaviour Tc with JK is qualitatively similar. Thus, for low values of JK, there are no Kondo effect and only a ferromagnetic order, as resulting from the exchange interaction JH. On the other hand, at a sufficiently large JK, there is a very steep increase of the Kondo temperature, indicating that the Kondo screening takes place and, at large JK, a ferromagnetic-Kondo regime is realized. However, as expected, the Kondo effect tends to suppress the ferromagnetic order and as a result, the Curie temperature Tc is passing through a maximum and decreasing with JK.
In conclusion, taking into account a f-band width, derived correctly from the SW transformation for Sf =1 spins, improves considerably the description of the Kondo-ferromagnetism coexistence and presents a first approach for describing the decrease of the localization of the 5f electrons when the Kondo effect arises or when pressure increases.

References
[1] J. Schoenes, O. Vogt, J. Lohle, F. Hulliger and K. Mattenberger, Phys. Rev. B 53, 14987 (1996).
[2] V. H. Tran, R. Troc, Z. Bukowski, D. Badurski and C. Silkowski, Phys. Rev. B71, 094428 (2005).
[3] P. Link, U. Benedict, J. Wittig and H. Wuhl, J. Phys. Condens. Matter 4, 5585 (1992)
[4] Q. G. Sheng and B. R. Cooper, J. Mag. Mag. Mater. 164, 335 (1996)
[5] E. Colineau, F. Wastin, J. P. Sanchez and J. Rebizant, J. Phys. Condens. Matter 20, 075207 (2008)
[6] N. B. Perkins, M. D. Nunez-Regueiro, B. Coqblin and J. R. Iglesias, Phys. Rev. B 76, 125101 (2007).
[7] J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149, 491 (1966).

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