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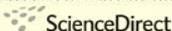


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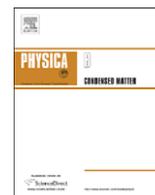
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The Schrieffer–Wolff transformation for the underscreened Anderson lattice

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ABSTRACT

We present a derivation of the Schrieffer–Wolff transformation for the Anderson Lattice Hamiltonian with a two-fold degenerate f-level in each site. The degeneracy of the f-electrons has been taken into account in order to describe uranium and other actinide magnetic compounds with a spin larger than $\frac{1}{2}$, for example a total $S = 1$ spin for the f-electrons. The transformed Hamiltonian has several terms as in the $s = \frac{1}{2}$ classical case, but we have obtained here both an exchange (Kondo) interaction between the $S = 1$ f-spins and the spins of the conduction electrons, and also an effective f-band term. This f-band term describes better the underscreened Kondo lattice model which has been recently developed to explain the Kondo-ferromagnetism coexistence observed in uranium compounds such as UTe [N.B. Perkins, M.D. Nunez-Regueiro, J. R. Iglesias, B. Coqblin, Phys. Rev. B 76 (2007) 125101].

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The properties of cerium, ytterbium and other anomalous rare-earth systems have been extensively studied and many compounds present a Kondo effect [2–4]. More recently, cerium or ytterbium Kondo compounds have been analyzed within the Kondo lattice model with localized f-electron spins $S = \frac{1}{2}$ [5,6]. A competition between Kondo effect on each Ce atom and magnetic ordering of the Ce moments has been obtained, which can account for the separation of anomalous compounds in two groups: the non-magnetic heavy fermion ones and those which magnetically order but at a rather low Néel or Curie temperature, typically of order 5–10 K [3,7,8].

The situation in actinides compounds is more complex because the 5f electrons are generally less localized than the 4f electrons of rare-earths. However, it has been shown that some uranium compounds, like UTe [9,10], $\text{UCu}_{0.9}\text{Sb}_2$ [11] or $\text{UCo}_{0.5}\text{Sb}_2$ [12] present a ferromagnetic ordering with large Curie temperatures (equal, respectively, to $T_c = 102, 113$ and 64.5 K) and also exhibit a logarithmic Kondo-type decrease of the resistivity above T_c . Very recently, a similar behavior has been observed in the neptunium compound NpNiSi_2 [13].

As previously noticed, the 5f electrons in uranium compounds are in a crossover region between a localized and an itinerant behavior. It is also difficult to decide, on the basis of the experimental data, between a Kondo behavior corresponding to a $5f^n$ configuration and an intermediate valence situation. For example, in uranium monochalcogenides, US lies closest to the

itinerant side for the 5f electrons, UTe is the closest to the localized side and USe is in between [10,16]. Photoemission experiments on UTe have been interpreted as favoring itinerant magnetism [17], while previous results of ultraviolet photoemission spectroscopy (UPS) [18] and X-ray photoemission spectroscopy (XPS) [19] were interpreted in terms of localized electrons in UTe. Finally, the results of the magnetic moments deduced from magnetic susceptibility experiments in this compound are close to the free ion values of uranium, which implies that the 5f electrons are relatively well localized in UTe within a $5f^2$ configuration [10,14].

An underscreened Kondo lattice (UKL) model that considers localized f-spins $S^f = 1$ (corresponding to the $5f^2$ configuration of uranium ions) has been recently studied [1]. This model starts with localized S^f -spins interacting through an exchange (Kondo) interaction, J_K , with the electrons of a non-degenerate conduction band. The local spins $S = 1$ are fermionized using a method developed in Ref. [15] and the resulting fermion Hamiltonian is treated within a generalized mean field approach. A phase diagram is obtained providing the Kondo and the Curie temperature as a function of the Kondo exchange interaction constant, J_K , which differs from the Doniach diagram of cerium compounds. The main difference is that when increasing the exchange, J_K , the system goes from a ferromagnetic phase to a phase where the magnetic order coexists with the Kondo state. This model is the first one to present a theoretical explanation of the coexistence of ferromagnetic order and Kondo effect in uranium compounds. However, it presents some shortcomings: on one hand the f-electrons of uranium are described as completely localized, while on the other hand the mean field approach

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considers a non-zero term that may be interpreted as a charge transfer among the f-levels and the conduction band. Finally the model cannot be applied to describe compounds with intermediate valence behavior.

In this paper we start from an Anderson lattice Hamiltonian where a term of charge transfer from and to the conduction band is present from the beginning. We transform this Hamiltonian using a generalized Schrieffer–Wolff transformation and we will see that the resulting Hamiltonian can well describe both the limit of completely localized f-electrons as well as the intermediate valence case when n_f is close to an integer value of two electrons *per site*.

We first write the Anderson lattice model with 2 degenerate orbitals on each site, and we consider that there are two f-electrons *per site*, $f_{1\sigma}$ and $f_{2\sigma}$ (indices 1 and 2 refer to the 2 degenerate orbitals). The resulting Hamiltonian describes a conduction band with dispersion energy ε_k defined with respect to the Fermi energy, a two-fold degenerate f-band with an energy ε_f (that does depend neither on the site nor on the level label), then an hybridization term between conduction and f-electrons, with the same hybridization matrix element for the two f-electrons. Finally, the last term describes all Coulomb and exchange interactions between two f-electrons on the same site. Thus, the Anderson lattice Hamiltonian can be written as

$$\mathbb{H} = H_{band} + H_{hyb} + H_{corr}, \quad (1)$$

with

$$H_{band} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i\alpha\sigma} \varepsilon_f n_{i\alpha\sigma}^f, \quad (2)$$

$$H_{hyb} = \sum_{ik\alpha\sigma} (V_{k\alpha} c_{k\sigma}^\dagger f_{i\alpha\sigma} + V_{k\alpha}^* f_{i\alpha\sigma}^\dagger c_{k\sigma}), \quad (3)$$

$$H_{corr} = \sum_i [U(n_{i1\uparrow}^f n_{i1\downarrow}^f + n_{i2\uparrow}^f n_{i2\downarrow}^f) \quad (4)$$

$$+ U'(n_{i1\uparrow}^f n_{i2\downarrow}^f + n_{i1\downarrow}^f n_{i2\uparrow}^f) + (U' - J)(n_{i1\uparrow}^f n_{i2\uparrow}^f + n_{i1\downarrow}^f n_{i2\downarrow}^f) + J(f_{i1\uparrow}^\dagger f_{i1\downarrow}^\dagger f_{i2\downarrow}^\dagger f_{i2\uparrow}^\dagger + c. c.)]. \quad (5)$$

Then we perform a Schrieffer–Wolff type transformation [20] on the preceding Hamiltonian. The aim of the calculation is to describe a situation where the ground state of the last term H_{corr} is the spin triplet $S = 1$ with atomic wave functions

$$\begin{aligned} c_{k\sigma}^\dagger f_{i1\uparrow}^\dagger f_{i2\uparrow}^\dagger |0\rangle, \quad S_{zi}^f = 1, \\ \frac{c_{k\sigma}^\dagger}{\sqrt{2}} (f_{i1\uparrow}^\dagger f_{i2\downarrow}^\dagger + f_{i1\downarrow}^\dagger f_{i2\uparrow}^\dagger) |0\rangle, \quad S_{zi}^f = 0, \\ c_{k\sigma}^\dagger f_{i1\downarrow}^\dagger f_{i2\downarrow}^\dagger |0\rangle, \quad S_{zi}^f = -1. \end{aligned}$$

It is interesting to note that the last term of H_{corr} guarantees that these three states are degenerate and correspond to the ground state, with an energy eigenvalue: $U' - J$. Thus, we can assume the intra-orbital Coulomb term U infinite, keeping only U' and J finite.

So, we obtain a transformed Hamiltonian \mathcal{H} , as follows :

$$\mathcal{H} = H_1 + H_2 + H_3 + H_4, \quad (6)$$

with

$$H_1 = \sum_{ik\mathbf{k}'} J_{k\mathbf{k}'} [c_{k\uparrow}^\dagger c_{k\downarrow} S_i^- + c_{k\downarrow}^\dagger c_{k\uparrow} S_i^+ + (c_{k\uparrow}^\dagger c_{k\uparrow} - c_{k\downarrow}^\dagger c_{k\downarrow}) S_{zi}^f], \quad (7)$$

where we define

$$\begin{aligned} S_i^{f+} &= n_{i1\uparrow}^f f_{i2\downarrow}^\dagger f_{i2\downarrow} + f_{i1\uparrow}^\dagger f_{i1\downarrow} n_{i2}^f, \\ S_i^{f-} &= n_{i1\downarrow}^f f_{i2\downarrow}^\dagger f_{i2\uparrow} + f_{i1\downarrow}^\dagger f_{i1\uparrow} n_{i2}^f, \end{aligned}$$

$$S_{zi}^f = n_{i1\uparrow}^f n_{i2\uparrow}^f - n_{i1\downarrow}^f n_{i2\downarrow}^f, \quad (8)$$

$$\begin{aligned} H_2 &= -2 \sum_{ijk\mathbf{k}'\sigma\sigma'\alpha\beta} W_{k\mathbf{k}'} c_{k'\sigma'}^\dagger c_{k\sigma}^\dagger c_{k\sigma'} c_{k'\sigma'} f_{j\beta\sigma'}^\dagger f_{i\alpha\sigma''} \\ &+ \sum_{ijk\mathbf{k}'\sigma\sigma'\alpha\beta} W_{k'\mathbf{k}'} c_{k\sigma}^\dagger c_{k'\sigma'}^\dagger c_{k'\sigma'} c_{k\sigma} f_{j\beta\sigma''}^\dagger f_{i\alpha\sigma''}, \end{aligned} \quad (9)$$

$$\begin{aligned} H_3 &= \sum_{ik\mathbf{k}\sigma\sigma'} J_{k\mathbf{k}'} \left[(1 - 2\delta_{k\mathbf{k}'}) n_{i1\sigma}^f n_{i2\sigma}^f + \frac{1}{2} (1 - \delta_{k\mathbf{k}'}) \right. \\ &\left. (n_{i1\sigma}^f n_{i2\sigma'}^f + f_{i1\sigma}^\dagger f_{i1\sigma'}^\dagger f_{i2\sigma}^\dagger f_{i2\sigma'}^\dagger) \right] c_{k\sigma'}^\dagger c_{k\sigma}, \end{aligned} \quad (10)$$

and

$$\begin{aligned} H_4 &= 2 \sum_{ik\mathbf{k}'\sigma\sigma'\alpha} J_{k\mathbf{k}'} [c_{k'\sigma'}^\dagger c_{k\sigma}^\dagger c_{k\sigma'} c_{k'\sigma'} (f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} + f_{i\alpha\sigma'}^\dagger f_{i\alpha\sigma'}) \\ &+ \sum_{\sigma''} (\delta_{\sigma'\sigma} + 1) c_{k'\sigma''}^\dagger c_{k\sigma'}^\dagger c_{k\sigma'} c_{k'\sigma''} (f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} + f_{i\alpha\sigma'}^\dagger f_{i\alpha\sigma'})], \end{aligned} \quad (11)$$

where

$$J_{k\mathbf{k}'} = -\frac{1}{2} V_k^* V_{k'} \left(\frac{1}{U' - J + \varepsilon_f - \varepsilon_k} + \frac{1}{U' - J + \varepsilon_f - \varepsilon_{k'}} \right), \quad (12)$$

and

$$W_{k\mathbf{k}'} = V_k^* V_{k'} \left(\frac{1}{\varepsilon_f - \varepsilon_k} + \frac{1}{\varepsilon_f - \varepsilon_{k'}} \right). \quad (13)$$

This is the more general form of the transformed Hamiltonian. However, we have drop some terms: (a) we do not allow f-electrons to jump from one orbital to the other inside the same site and (b) we do not allow, in average, more than two f-electrons per site neither less than two.

So, the resulting Hamiltonian, Eq. (6) contains a first term, H_1 , that gives the s–f exchange interaction for the spins $S = 1$, as in the original Schrieffer–Wolff transformation for $s = \frac{1}{2}$. If the dependence of $J_{k\mathbf{k}'}$ with \mathbf{k} and \mathbf{k}' is neglected, we get the usual local Kondo coupling between the localized spin $S = 1$ and the conduction electron spin on the same site, in the same way as in Ref. [1]. But it is interesting to remark that the exchange integral $J_{k\mathbf{k}'}$ contains in the denominators a term $U' - J + \varepsilon_f - \varepsilon_k$ which is different from the classical exchange term obtained for a spin $s = \frac{1}{2}$. In fact the denominator is the energy difference between the ground state of two f-electrons: $U' - J + 2\varepsilon_f$ and the energy of the intermediate state with one f-electron: $\varepsilon_f + \varepsilon_k$.

The following terms have a different physical meaning. Some of them could be found for the $s = \frac{1}{2}$ spin in the original paper of Schrieffer and Wolff [20] and are generally neglected when one is studying the Kondo effect. All these terms here are composed of six fermion field operators and some kind of decoupling will be needed to treat them.

The second term, H_2 , is important and new, since it connects operators $f_{i\alpha\sigma}$ on two different sites i and j , and, therefore, can be considered as an effective band term for the 5f electrons. The other terms are less important for the study of the underscreened Kondo model. The term H_3 will introduce a renormalization of the energy of the conduction band depending on the number of f-electrons in each orbital and spin state and H_4 describes spin flip processes of the f-electrons in the same or in different orbitals and we are going to neglect them in the future.

Concluding, the transformation presented here describes an effective exchange Hamiltonian that can be useful for the study of uranium and actinide compounds with more than one f-electron. If we neglect the effective f-band term (H_2) we recover the main ingredients of the spin one Kondo Hamiltonian studied in Ref. [1]. But if we keep this term we can include charge transfer effects

that could be important for the case of less localized f-states. In this sense, the present derivation yields a clear progress for the study of the Underscreened Kondo lattice model.

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