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NON LOCAL INTERACTION IN THE KONDO LATTICE

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Abstract. — A Kondo lattice has been obtained applying the Schrieffer-Wolff transformation [1] on an Anderson lattice, keeping the term corresponding to non-local Kondo interaction. Using the Integral Functional method, proposed by Lacroix and Cyrot [2], we study the influence of that interaction on the phase diagram of the Kondo lattice, restricted to the nearest neighbour case.

Introduction

Many attempts have been made to discuss the ground state of the so-called Kondo lattice [2-5]. In such a system a mechanism of competition between the RKKY interaction, tending to stabilize a magnetic phase, and the Kondo effect, tending to compensate the magnetic moments, is argued to account for the inexistence of an ordered magnetic phase in CeAl₃ or the existence of an ordered one in some rare-earth compounds like for example in CeAl₂ or CeB₂. On the other hand, it is well known that the Schrieffer-Wolff transformation [1] gives an equivalence between the Anderson lattice Hamiltonian and the Kondo lattice one. In the present paper we first obtain the S-W transformation starting from the Anderson lattice Hamiltonian, retain the terms arising from the non local Kondo interaction with spin-flip, restricted to the nearest neighbours and then we study the influence of this term on the ground state of the Kondo lattice for \( T = 0 \) K.

The model and approximations

A detailed calculation will be given elsewhere [6]. Here we present the final transformed Hamiltonian for the case of one electron per atom in the local state.

\[
H = H_0 + H_1 + H_2 + H_3 + H_4 \tag{1}
\]

\[
H_0 = \sum_{k,\sigma} c_k c_{k\sigma} + E_0 \sum_{i,\sigma} f_{i\sigma} f_{i\sigma} \tag{2}
\]

\[
H_1 = \frac{J_0}{2} \sum_{i,\sigma} c_{i\sigma} c_{i-\sigma} f_{i-\sigma} f_{i\sigma} \tag{2a}
\]

\[
H_2 = \frac{J_0}{2} \sum_{i,\sigma} f_{i-\sigma} f_{i-\sigma} c_{i\sigma} c_{i\sigma} \tag{2b}
\]

\[
H_3 = -J_1 \sum_{i,j,\sigma} \left( f_{i-\sigma} f_{i\sigma} c_{j\sigma} c_{i-\sigma} + c_{j-\sigma} c_{j\sigma} f_{i\sigma} f_{i-\sigma} \right) \tag{2c}
\]

\[
H_4 = J_1 \sum_{i,j,\sigma} \left( f_{i\sigma}^+ f_{j-\sigma} c_{j\sigma}^+ c_{i\sigma} + c_{j\sigma}^+ c_{j\sigma} f_{i\sigma}^+ f_{j-\sigma} \right) \tag{2d}
\]

where \( J_0 < 0 \) and \( J_1 \), coming from the S-W transformation of the Anderson lattice, are the usual exchange interaction constants between local f-states and conduction electrons. \( J_0 \) corresponds to the interaction on the same site and \( J_1 \) is the non local exchange interaction constant within the nearest neighbour approximation. The sign of \( J_1 \) will be discussed later.

In order to approximate \( H_1 \) and \( H_3 \), we use the Functional Integration Approach [7] in a similar way as in the reference [2]. \( H_2 \) and \( H_4 \), responsible for the polarization of the conduction electrons will be treated in the Hartree-Fock approximation.

The partition function is obtained from the well known Stratanovitch-Hubbard identity [7]. The result is very similar to that of reference [2] with the addition of new term corresponding to the non-local Kondo interaction. Such a term is equivalent to a fictitious time dependent s-f mixing \( \alpha_{ij} (\tau) \). Using the static approximation, which gives results qualitatively correct for the case a single impurity [8] and a Kondo lattice without non local interaction [2]. Further, assuming the hermiticity of the Hamiltonian and using the translation symmetry, the final Hamiltonian is now:

\[
H = H_0 + \frac{J_0}{2} \sum_{i,\sigma} x_i \left( f_{i\sigma}^+ c_{i\sigma} + c_{i\sigma}^+ f_{i\sigma} \right) + \frac{J_1}{2} \sum_{i,\sigma} \left( f_{i\sigma}^+ f_{i-\sigma} c_{i\sigma} + c_{i\sigma}^+ c_{i\sigma} f_{i\sigma} f_{i-\sigma} \right) \tag{3}
\]
tion on the integral functional by the maximum value of the integrand, the partition function can be solved and the free energy obtained. However, in the present case we will discuss a particular situation considering the Kondo state as the state without net magnetic moment, called pure Kondo phase (PKS) [2]. Supposing that the system is homogeneous \( x_i = x \) and in a preliminary simplified approach, we assume that there is no \( k \)-dependence in \( \alpha_{ij} \) making \( \alpha_{ij} = \alpha \). Work is in progress to improve this calculation [6], where the self-consistent determination of the difference \( \Delta F(x, \alpha) \) between the pure Kondo phase and the state without \( s-f \) mixing.

\[ \Delta F(x, \alpha) \] is calculated from conduction electrons and local states propagators. In the PKS \( \langle f_{i\sigma}^+ f_{i\sigma} \rangle = 1/2 \) and \( \langle c_{i\sigma}^+ c_{i\sigma} \rangle = n/2 \), being \( n \) the number of conduction electrons per atom. In the presence of interaction the density of states (DOS) for both the conduction electrons and the local states can be obtained in terms of the non interacting conduction band DOS. It is supposed to be:

\[ \rho_0(\epsilon) = \frac{1}{2}D, \quad -D < \epsilon < D \quad \text{and} \quad \rho_0(\epsilon) = 0, \quad \text{otherwise}. \]

The feature of the total DOS has the same form as that found in reference [2] but its gap and the width of its peaks after and before the gap is now of the order of \( (J_0 x + 2J_1 \alpha)^2 / D \) for \( n \approx 1 \).

The energy corresponding to the PKS can be calculated. Analogously from the density of states without \( s-f \) mixing, we can calculate the energy corresponding to this phase. Both energies can be calculated self-consistently, including the determination of the difference correlation functions \( \langle c_{i\sigma}^+ c_{j\gamma} \rangle \) for the Kondo phase and an identical expression of \( \eta^s \), for the phase without \( s-f \) mixing, for which some analytical expressions are known [10]. However, to simplify we suppose that the difference correlation functions would not change appreciably from one phase to another making \( \eta^s = \eta^k \). Although it appears a very rough assumption it does not change qualitatively the behaviour of the function \( \Delta F(x, \alpha) \) as we will see. In such approximation, except for a self consistent determination of the occupation number \( n \), the contribution of \( \eta^s \) and \( \eta^k \) is proportional to their difference and disappears at the end of the calculation of \( \Delta F(x, \alpha) \). Then we get:

\[ \Delta F(x, \alpha) = -\frac{1}{4} P^{1/2} - \frac{1}{2} J_0 x^2 - 2xJ_1 \alpha^2 + 2K \ln \frac{P^{1/2} - nD}{P^{1/2} + nD} + \frac{nD}{4} \]

where

\[ K = \left( \frac{J_0 x + 2J_1 \alpha}{8D} \right)^2 \]

and

\[ P = n^2 D^2 + n(J_0 x + 2J_1 \alpha)^2. \]

and \( z \) is the coordination number.

In order to determine the Kondo phase we have to find the minimum of this function. For \( J_1 = 0 \), it is possible to have a Kondo phase only if \( J_0 < 0 \) [2]. For \( J_1 < 0 \) and \( J_0 < 0 \) the Kondo effect is reinforced and no important effect is obtained. On the other hand, if \( J_1 > 0 \) there is an important consequence because the magnetic phase seems to emerge strongly. In this case the function \( \Delta F(x, \alpha) \) does not have a global minimum at all, except for \( \alpha = 0 \). In this case the result of Lacroix and Cyrot is recovered and it is possible to construct a phase diagram depending on \( J_0 \) and \( n \).

**Conclusion**

We have seen that in the absence of the non local interaction there is a minimum of the function \( \Delta F(x, \alpha) \). However, within the approach used here, as soon as \( \alpha \neq 0 \) this function has no more a minimum value and it seems that the magnetic phase would be stable. This is in qualitative agreement with a previous study of one dimensional Kondo lattice by renormalization group technique [5], that shows that the behaviour of the singlet-triplet gap favours the magnetic order as soon as \( J_1 (> 0) \) exists. We have to be careful about the inexistence of the Kondo phase within the static approximation of the Integral Functional Method, particularly because we overestimated the nearest neighbour interaction by eliminating the \( k \)-dependence on \( \alpha \). It would be interesting to perform the complete self-consistent solution and work is in progress in this sense.

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