Phase diagram of the Kondo necklace: a mean-field renormalization group approach

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In this paper we investigate the magnetic properties of heavy fermions in the antiferromagnetic and dense Kondo phases in the framework of the Kondo necklace model. We use a mean field renormalization group approach to obtain a temperature versus Kondo coupling \((T - J)\) phase diagram for this model in qualitative agreement with Doniach’s diagram, proposed on physical grounds. We further analyze the magnetically disordered phase using a two-sites approach. We calculate the correlation functions and the magnetic susceptibility that allow to identify the crossover between the spin-liquid and the local moment regimes, which occurs at a coherence temperature.

I. INTRODUCTION

It is well known that the nature of the ground state of dense Kondo compounds results basically from the competition between the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and the Kondo effect. In a simple picture it is governed by a single parameter, the ratio \(J/W\), where \(J\) is the effective exchange between localized moments and conduction electrons and \(W\) is the bandwidth of the latter. The value of this ratio is usually tunable experimentally by pressure or composition ratio of the compounds. The RKKY interaction is an indirect magnetic interaction between localized moments, mediated by the polarized conduction electrons, with an energy scale of order \(J_{RKKY} \propto \frac{J^2}{W}\), that produces a long-range ordered magnetic ground state. On the other hand, the Kondo effect favors the formation of singlet states between localized moments and conduction electrons generating a non-magnetic ground state and, in the single impurity case, has a characteristic energy scale of order \(k_B T_K = W e^{-W/J}\). As result of the interplay between these two effects, some Kondo compounds are non-magnetic and are characterized by a heavy-fermion behavior (Fermi-liquid) at very low temperatures, while others order magnetically, generally antiferromagnetically. The study of this interplay is easily formulated using the Kondo lattice model, which emphasizes the importance of spin fluctuations neglecting charge fluctuations of the localized electrons, and has been well characterized by the “Doniach phase diagram” [1]. In this simple picture, the ordering temperature \(T_N\) initially increases with increasing \(J\), then passes through a maximum and vanishes at a critical coupling \(J_c\). At this quantum critical point, a second order phase transition between an antiferromagnetic ground state for small values of \(J\) and a dense Kondo state for strong couplings \(J\) occurs. This behavior of \(T_N\) has been experimentally observed in many Cerium compounds by varying the pressure applied on the system [2,3] or the relative concentration in the compounds [4].

In this paper we are interested in studying the \(T x J\) phase diagram of Kondo compounds. For that purpose, we use an analog of the symmetric Kondo lattice with complete absence of charge fluctuations, the Kondo necklace model (KNM). This model was proposed by Doniach [5], and its ground state has been investigated by a variety of methods [6–10]. In order to assess the critical behavior of the Kondo necklace, we apply the mean field renormalization group (MFRG), first proposed by Indekeu et al. [11], on the KNM. This method combines mean field results for small clusters of spins and renormalization group ideas. While mean field theory identifies the order parameter of the cluster with the order parameter of the entire system, the MFRG assumes that the cluster order parameter rescales with cluster size [12]. Using this method we obtain the phase diagram of the Kondo necklace as a function of temperature and Kondo coupling, which is qualitatively identical to the Doniach diagram. Within a two-site approach [13], we calculate the finite temperature magnetic susceptibility and investigate the behavior of short-range magnetic correlations in the magnetically disordered phase. As a result of this investigation, we increase the phase diagram with a crossover line, which is associated to a coherence temperature that separates Kondo spin-liquid and localized moments regimes.

This paper is organized as follows: In the next section we present the Kondo lattice and Kondo necklace models and discuss their analogies. In section III we apply the mean-field renormalization group approach in the Kondo necklace model and obtain the Doniach phase diagram, which we compare with experimental results. In section IV we apply a two-sites method on the non-magnetic phase, in order to study the role of short-range correlations on the system. We also calculate the magnetic susceptibility and then obtain a coherence temperature. In section V we summarize and discuss our results.
II. THE MODEL

The Kondo lattice model (KLM) is a theoretical model for heavy fermions that can be derived from the more fundamental Anderson Lattice Model, in the case of well-developed local spin moments [10]. It consists of two different types of electrons, the localized spins whose charge degrees of freedom are suppressed, and the conduction electrons that propagate as charge carriers. It is described by

\[ H = -t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + J \sum_i S_i \cdot c_{i,\alpha}^\dagger c_{i,\beta}. \]  

(1)

The first term represents the conduction band \((c_{i,\sigma}^\dagger c_{j,\sigma} \text{ is the creation operator, } t \text{ is the hopping between nearest neighbors})\) and the second term is the interaction between conduction electrons and localized moments \(S_i \) via the intra-site exchange \(J\), where \(\sigma\) are the Pauli matrices.

In order to study the interplay between Kondo screening and the RKKY interaction, Doniach proposed a simplified model related to the one-dimensional Kondo lattice, called the Kondo necklace model (KNM). In this model, the conduction electrons are replaced by a spin chain with \(XY\) coupling which eliminates charge fluctuations [1].

\[ H_{KN} = W \sum_{\langle i,j \rangle} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y) + J \sum_i S_i \cdot \tau_i. \]  

(2)

where \(\tau_i\) and \(S_i\) are independent sets of spin 1/2 Pauli operators. The first term mimics electron propagation, and in one dimension can be mapped by the Jordan-Wigner transformation onto a band of spinless fermions. The second term is the magnetic interaction between conduction electrons and localized spins \(S_i\) via the coupling \(J\), as in Eq. (1).

Although the KLM is mapped onto the KNM only in one dimension, it is clear that, even in higher dimensions, \(H_{KN}\) has the same magnetic tendencies of the Kondo lattice. Since the essential features of the original model are kept, we expect that the main physical properties of the Kondo lattice will be maintained in the model described by Eq. (3).

III. MEAN-FIELD RENORMALIZATION GROUP

The mean-field renormalization group was first proposed by Indekeu et al. [13] for computing critical properties of lattice spin systems. This method has been applied to many statistical physics problems, both classical and quantum systems, with [17] and without disorder [13], and the resulting critical exponents deviate from those obtained from standard mean field theories (including Bethe lattice calculations) [14].

The main idea of the MFRG is the comparison of two clusters with \(N\) and \(N'\) sites respectively, subjected to symmetry-breaking boundary conditions. The interactions within the clusters are treated exactly, and the effect of surrounding sites is replaced by a mean field which is supposed to scale in the same way as the order parameter.

For a generic spin system, one considers each boundary spin fixed and equal to \(b\) and \(b'\) for the \(N\) and \(N'\) spin clusters, respectively. After computing the order parameter \(O_N\) and \(O_N'\) for both clusters one imposes a scaling relation between them

\[ O_N'(K', b') = \xi O_N(K, b), \]  

(3)

with \(K\) and \(K'\) being the coupling constants of the two rescaled systems. Assuming a similar relation between the mean-fields \((b' = \xi b)\) and knowing that these fields have to be very small near the second order phase transition, one can expand equation (3) for small values of \(b\) and \(b'\) to obtain

\[ \frac{\partial O'_N(K', b')}{\partial b'} \bigg|_{b'=0} = \frac{\partial O_N(K, b)}{\partial b} \bigg|_{b=0}, \]  

(4)

which is independent of the scaling factor \(\xi\). Equation (4) can be interpreted as a recursion relation for the coupling constant \(K\), from which the critical point \(K_c\) is extracted.

We can apply this method to the Kondo necklace in its simplest version, that is, we consider two cells containing one and two sites each, as sketched in figure 1 for a 2D hiper cubic lattice.

\[ H'' = \sum_i S_i \cdot \tau_i. \]  

(5)

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(6)

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(7)

FIG. 1. Clusters considered in the calculations of the 2D case. Each site contains two spins, one spin \(S\) (open circle) connected by a solid line to one spin \(\tau\) (filled circle). The interaction between sites is mediated by the spins \(\tau\), where the dashed bonds represent interactions with the boundary symmetry breaking fields \(b'\) and \(b\).
As we are dealing with an incipient antiferromagnetic ordering and the antiferromagnetism in the Kondo necklace occurs in the XY plane, we consider a D-dimensional hypercubic lattice and divide the system in two sub-lattices $A$ and $B$. The order parameter is then the staggered magnetization of the spins $\tau$, taken along the $x$ direction (see Eq. (3) and (4) below). The $x$ component of the boundary spins in the smallest cluster is fixed to be $-b'$ since all the first neighbors of $\tau_1$ are in the same sub-lattice. In the two-sites cluster, $\tau_1$ and $\tau_2$ are in different sub-lattices, so the $x$ component of their neighboring boundary spins have different signs and are fixed at $-b$ and $b$ respectively.

Let us first consider the Hamiltonian for a one-site cluster taken on a sub-lattice $A$:

$$H_1 = J' S_1 \cdot \tau_1 - z b' W' \tau_1^x,$$

where $J'$ is the scaled coupling interaction, and the spin $\tau_1$ interacts with its $z$ nearest neighbors through the term $z b' W' \tau_1^x$.

Similarly, the Hamiltonian for the two-sites system (one in each sub-lattice) is given by:

$$H_{12} = J \sum_{i=1}^{2} S_i \cdot \tau_i + W(\tau_1^x \tau_2^x) - (z-1) b W(\tau_1^x - \tau_2^x) .$$

(6)

In this case the spin $\tau_1$ interacts directly with $\tau_2$ through a term $W(\tau_1^x \tau_2^x)$ and both $\tau_1$ and $\tau_2$ interact with their $(z-1)$ nearest neighbors through $-(z-1) b W \tau_1^x$ and $(z-1) b W \tau_2^x$, respectively.

This method can be used to study quantum systems ($T = 0$), for which there are few available renormalization group techniques. For that purpose, we compute the ground state $|0\rangle_1$ and $|0\rangle_{12}$ of the two systems and their corresponding staggered magnetizations along the $x$ direction. In the vicinity of the phase transition, $b$ and $b'$ can be assumed small and

$$M_1^x = \langle 0 | \tau_1^x | 0 \rangle = - \frac{z}{2j'} b',$$

$$M_{12}^x = \frac{\langle 0 | (\tau_1^x - \tau_2^x) | 0 \rangle}{2} = - \frac{2(z-1)(\sqrt{16 j^2 + 1} + 1)^2}{(1 + 16 j^2 + \sqrt{16 j^2 + 1})(-1 + \sqrt{16 j^2 + 1})} b,$$

where $j = \frac{J}{W}$ and $j' = \frac{J'}{W'}$.

The main assumption of the MFRG is the imposition of the same scaling relations between $M_1^x$ and $M_{12}^x$, $b$ and $b'$. By doing this we arrive at the renormalization group recursion relation for $j$ and $j'$. The associated fixed point equation is

$$z = \frac{4(z-1)(\sqrt{16 j^2 + 1} + 1)^2}{(1 + 16 j^2 + \sqrt{16 j^2 + 1})(-1 + \sqrt{16 j^2 + 1})} .$$

(7)

By solving Eq. (7) we obtain the antiferromagnetic quantum critical point (QCP) in any space dimension $D$. For $z = 2$, which corresponds to a one dimensional system, we obtained $j_c = 0.64$. The critical ratios $j_c$ for other coordination numbers are: $z = 4 \rightarrow j_c = 1.66$, $z = 6 \rightarrow j_c = 2.67$. This values can be compared with recent results [26,12] and the relative errors are $12.67\%$ for 2D and 1.5% for 3D showing that the results are most reliable for higher dimensions.

It is worth mentioning that the diagonalization of $H_{12}$ is not a simple task. However, as we are interested in small values of the mean field, a perturbative expansion can be worked out in order to obtain the eigenvalues and eigenvectors in powers of $b$ [18]. We follow the same prescription in order to calculate the staggered magnetizations for $T \neq 0$.

As we have more then one variable, we cannot determine a complete renormalization flow in the $[j, T]$ plane. However, for a fixed $j$ we can calculate $T_N$ or vice-versa. In order to obtain the critical values, we consider the solutions of the fixed point equation associated with eq. (4), that is,

$$\frac{\partial M_1^x(T_N,j)}{\partial b'} \bigg|_{b'=0} = \frac{\partial M_{12}^x(T_N,j)}{\partial b} \bigg|_{b=0} ,$$

(8)

where for each $j < j_c$ we obtain a $T_N(j)$ and the set of all critical points yields the temperature dependent phase diagram of the Kondo necklace. The critical line for a 3D system ($z = 6$), is depicted in figure 3. Close to the zero temperature fixed point it behaves as:

$$|\delta| = |j - j_c| \propto e^{-\alpha(z,j_c)\beta N}, \quad \beta N = \frac{1}{k_B T_N}$$

(9)

This dependence is characteristic of this approach and appears for any dimension.
In figure [11], Endstra et al. calculated the $J$ coupling of many Cerium and Uranium compounds based fundamentally on the atomic radii and interatomic distances of these systems [23]. More recently, Cornelius and Schilling, based on the variation of the lattice parameters generated by pressure and substitution of Si by Ge (negative pressure) in $CeM_2Si_2-Ge_x$ compounds (where $M=Rh,Ru,Pd$) [22], found a relation between the Néel temperature $T_N$ and the coupling $J$ for $CeRu_2Si_2$, $CeRh_2Si_2$ and $CePd_2Si_2$ [23]. Their results fall in Doniach-like curves, that when normalized by the maximum of $T_N$ ($T_{max}$) and its equivalent $J_{t_{max}}$ collapse onto a single universal curve.

We observe that in the experimental results, the Néel temperature goes to zero in the weak coupling regime at a value of $J$ greater than zero, differently from the theoretical predictions for the Kondo Lattice. By shifting the experimental results along the $J$ axis in order to obtain $T_N = 0$ at $J = 0$, and using the same normalization used in Ref. [22], we obtain the results of figure 1 ($z = 6$ (3D)), where one can see that the behavior of the theoretical curve is in good agreement with the experimental values. We can conclude that these Kondo systems behave qualitatively as proposed by Doniach although in practice the long range magnetic order vanishes before the theoretical $J = 0$ value is attained.

As we are dealing with a mean-field like approach using small clusters we do not obtain a precise value for the QCP for one dimension case ($J = 0$) such as in previous works [1] [23]. Nevertheless, this method has the advantage of being very simple to implement at finite temperature and produce reliable values of the QCP for higher dimensions, as discussed before.

The main feature of our MFRG method in its simplest approach (1 and 2 site cells) is that it yields the $[T,j]$ phase diagram for heavy fermions as proposed by Doniach on physical grounds [1] which, as far as we know, has never been obtained before. This is so because this method captures the essential physics of the Kondo lattice problem, namely, the competition between the RKKY and Kondo interactions. However, it is important to note that the present method can be applied to larger clusters, which provides better information concerning the lattice topology of the system [14], in order to obtain more accurate values for the quantum critical point for lower dimensions.

IV. SHORT-RANGE CORRELATIONS

In the magnetically disordered phase, where the mean fields $b$ and $b'$ are identically zero, we can still calculate some properties of the system by means of a two-site approximation. This method consists on solving exactly a Hamiltonian of two sites, i.e., Eq. (6) with $b = 0$. As the system does not present long-range (magnetic) order, we expect that this approach will unravel some aspects of this phase. We can investigate the behavior of short-range magnetic correlations as well as the intra-site correlations between localized moments and conduction electrons, which are related to the Kondo effect. The results of the calculations are shown in figures 3(a) and 3(b).

The localized-delocalized spin correlation function $< S \cdot \tau >$ characterizes the condensation of singlet states. At $T = 0$, this function decreases for increasing values of $j$, saturating at the value $\frac{1}{2}$, which is consistent with the strong coupling limit [11], where the system condenses into independent singlets in each site. As the temperature increases, this correlation rapidly falls to zero and we observe that, since coherence in the KNM is a collective phenomena, even low temperature excitations can destroy the Kondo spin-liquid regime. The inter-site correlation function $< \tau_i \tau_j^*$ > represents the short-range magnetic correlations. This function has a minimum at a low temperature and then gradually vanishes as $T$ increases. Differently from $< S \cdot \tau >$, it has a smooth behavior for large $T$ and its asymptotic behavior is independent of $|\delta| = |j - j_c|$.

The competition between these two kind of correlations produces a change in the behavior of the system, as illustrated in figure 3. For low temperatures, the correlation $< S \cdot \tau >$ is stronger and the system is in a condensate of singlets, typical of the Kondo spin-liquid regime [12]. Near the minimum of the magnetic correlation function $< \tau_i \tau_j^* >$ there is a crossover: $< \tau_i \tau_j^* >$ begins to dom-

![FIG. 3. Correlation functions $< S \cdot \tau >$ (a) and $< \tau_i \tau_j^* >$ (b) for different values of $|\delta| = |j - j_c|$ as a function of temperature.](image)
inate and destroys these singlet states giving rise to a paramagnetic regime with localized moments. The inflection point in the magnetic correlation function, where it crosses \(< S \cdot \tau >\), defines the crossover or coherence temperature which separates two different regimes in the non-magnetic region of the phase diagram.

![Figure 4](image)

**FIG. 4.** Competition between two kind of correlations: the intra-site \(< S \cdot \tau >\) (dashed line) and the inter-site \(< \tau^x_1 \tau^x_2 >\) (solid line) for \(|\delta| = 0.5\).

The magnetic susceptibility (figure 4), calculated according to eq. (10), illustrates the difference between these two regimes.

$$\chi_0 = Z^{-1} N^{-1} \beta \sum_m e^{-\beta E_m} (M_{\text{total}}^x)^2,$$

(10)

$$Z = \sum_m e^{-\beta E_m}, \quad \beta = \frac{1}{k_B T}.$$ At low temperatures, as we are dealing with the symmetric case of the Kondo lattice, the system is an insulator and there is a singlet-triplet gap. At a higher temperature there is a maximum in the susceptibility where the gap closes and finally, at high \(T\), we can see an asymptotic Curie-Weiss regime, typical of localized moments. For \(|\delta| = 0\) the system has only the Curie-Weiss regime and the susceptibility can be fitted as, \(\chi_0 \propto T^{-1}\).

The coherence temperature can be calculated by finding the zero of \(\frac{\partial^2 < \tau^x_1 \tau^x_2 >}{\partial T^2}\) and at low temperatures it is quadratic in \(|\delta|:\)

$$T_{\text{coh}} \propto |\delta|^2.$$ (11)

The gap at \(T = 0\) in the critical regime, for \(|\delta| \to 0\), also has a power law behavior with the same exponent of the coherence temperature.

The Doniach diagram discussed in the previous section can be generalized in order to include two other regimes in the magnetically disordered region of the phase diagram, separated by the coherence line. Figure 5 illustrates the extended diagram obtained using these two methods.

![Figure 5](image)

**FIG. 5.** Complete phase diagram of the Kondo necklace model (for \(z = 6\)). The curve \(T_N(J)\) is shown here as a full line, whereas the dashed line represents \(T_{\text{coh}}(J)\).

V. CONCLUSIONS

We have successfully applied the MFRG on the Kondo necklace model. Using the simplest choice of clusters, we obtained the quantum critical point for the 2D and 3D cases that are in good agreement with previous calculations. We obtained for the first time a theoretical calculation of the Doniach diagram and compared it with experimental results for some Cerium compounds obtaining qualitatively good agreement. In the magnetic disordered phase we calculate, using a two-sites method, the short-range magnetic correlation function, the localized-delocalized spin correlation function as well as the magnetic susceptibility as a function of temperature and characterized two well-defined regimes: at low temperatures, a condensate of singlets with a singlet-triplet gap and at high temperatures, a Curie-Weiss regime. The crossover line close to the QCP has been analytically calculated and presents a power-law behavior.

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