A Kondo cluster-glass model for spin glass Cerium alloys

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Abstract.

There are clear indications that the presence of disorder in Ce alloys, such as Ce(Ni,Cu) or Ce(Pd,Rh), is responsible for the existence of a cluster spin glass state which changes continuously into inhomogeneous ferromagnetism at low temperatures. We present a study of the competition between magnetism and Kondo effect in a cluster-glass model composed by a random inter-cluster interaction term and an intra-cluster one, which contains an intra-site Kondo interaction $J_k$ and an inter-site ferromagnetic one $J_0$. The random interaction is given by the van Hemmen type of randomness which allows to solve the problem without the use of the replica method. The inter-cluster term is solved within the cluster mean-field theory and the remaining intra-cluster interactions can be treated by exact diagonalization. Results show the behavior of the cluster glass order parameter and the Kondo correlation function for several sizes of the clusters, $J_k$, $J_0$ and values of the ferromagnetic inter-cluster average interaction $I_0$. Particularly, for small $J_k$, the magnetic solution is strongly dependent on $I_0$ and $J_0$ and a Kondo cluster-glass or a mixed phase can be obtained, while, for large $J_k$, the Kondo effect is still dominant, both in good agreement with experiment in Ce(Ni,Cu) or Ce(Pd,Rh) alloys.

Recent experimental results for CePd$_{1-x}$Rh$_x$ [1] and CeNi$_{1-x}$Cu$_x$ [2] alloys show a complex scenario coming from the competition between the RKKY and Kondo interaction in the presence of disorder displaying, for instance, a cluster glass state (CSG). In the particular case of CeNi$_{1-x}$Cu$_x$, the small doping region ($x < 0.2$) is dominated by the Kondo effect. However, for the intermediate doping regime (0.3 < $x < 0.6$), short range ferromagnetic correlations induce the formation of clusters that become frozen in a CSG order when the temperature decreases, the CSG is replaced by a ferromagnetic phase at very low temperatures.

From a theoretical point of view, several models have been analyzed in order to account the experimental results described above. The models consider the Kondo-Ising Lattice (KIL) model with an additional Ising intersite interaction between disordered localized spins [3, 4]. Despite of the relative success to reproduce the experimental phase diagram of the CeNi$_{1-x}$Cu$_x$ in Ref. [4], this approach has a shortcoming that the phase diagram can be dependent of the particular replica solution scheme [5]. Quite recently, a van Hemmen (vH) like interaction [6] for the Ising term has recently been studied in the KIL, which allows to treat the disorder without the use of replica method [7]. Furthermore, this model gives results in which a Kondo phase is found for large $J_k$ (the strength of Kondo coupling). For smaller $J_k$ values, a spin glass phase, a mixed spin glass-ferromagnetic one and finally a ferromagnetic (FE) phase are found by decreasing temperature. Theses results are in agreement with the experimental ones of the CeNi$_{1-x}$Cu$_x$, but nevertheless it considers canonical spins.
In the present work, the competition between Kondo effect and cluster glass is studied in the following Kondo Lattice Cluster Glass (KLCG) model (see Ref. [8] and references therein) given by:

\[
\hat{H} = \sum_{a, i, j} t_{0a}^{ij} d_{\sigma a}^{j} d_{\bar{\sigma} a}^{i} + J_k \sum_{a, i, j=1}^{n_s} \left( \hat{S}_{ia}^{+} \hat{S}_{ja}^{-} + \hat{S}_{ia}^{-} \hat{S}_{ja}^{+} \right) - J_0 \sum_{a, i, j=1}^{n_s} \hat{S}_{ia}^{z} \hat{S}_{ja}^{z} - \sum_{a<b} J_{ab} \hat{S}_{a}^{z} \hat{S}_{b}^{z}
\]

(1)

where \(N_{cl}\) is the number of clusters and \(n_s\) is the number of sites in each cluster. The indices \((a, b)\) and \((i, j)\) indicate clusters and sites inside a cluster, respectively. The three first terms represent intra-cluster interactions and the last one is an inter-cluster disordered coupling, in which \(J_{ab}\) is a random variable given as in the vH model: \(J_{ab} = \frac{1}{N_{cl}} (\xi_a \eta_b + \eta_a \xi_b) + \frac{1}{n_s} \). In this interaction, \(q_1\) is the ferromagnetic average inter-cluster interaction while \(\xi_a\) and \(\eta_a\) are random variables that follow the bimodal distribution: \(P(x) = \frac{1}{2} [\delta(x - 1) + \delta(x + 1)]\).

In Eq. (1), the hopping \(t_{0a}^{ij}\) is only inside the cluster, the second term is the Kondo interaction and the third term is a ferromagnetic intra-cluster interaction. The spin operators are defined as: \(\hat{S}_{ia}^{+} = f_{ia}^{\dagger} f_{ia}^{\dagger}, \hat{S}_{ia}^{-} = (\hat{S}_{ia}^{+})^{\dagger}, \hat{S}_{ia}^{z} = (\hat{S}_{ia}^{+})^{\dagger} \) and \(\hat{S}_{a}^{z} = \sum_{i=1}^{n_s} \hat{S}_{ia}^{z} = \sum_{\alpha} \xi_{ia}^{\dagger} f_{ia}^{\dagger} f_{ia}^{\dagger} \), where \(f^{\dagger} (f)\) is a localized fermion creation (annihilation) operator and \(d^{\dagger} (d)\) is a conduction fermion creation (annihilation) operator.

To write the partition function \(Z\) of equation (1), the inter-cluster disorder can be treated in a mean field approach without the use of replica method. For that, the order parameters \(q_1 = 1/N_{cl} \sum (\xi_{ia} \eta_{ib} / n_s)\), \(q_2 = 1/N_{cl} \sum (\eta_{ia} \xi_{ib} / n_s)\) and \(m = 1/N_{cl} \sum (\xi_{ia} / n_s)\) (magnetization) are introduced in \(Z\). Particularly, the saddle-point approximations are used to obtain \(q_1\), \(q_2\) and \(m\). As a result of this calculation, one can obtain an effective one-cluster problem with the free energy per cluster given by:

\[
\beta F = \frac{\beta I_0 m^2}{2} + \beta J q^2 - \frac{1}{n_s} \langle \ln Tr T e^{-\beta \hat{H}_{eff}} \rangle
\]

(2)

where \(\langle \cdots \rangle\) means the average over \(\xi\) and \(\eta\), \(\beta = 1/T\) (\(T\) is the temperature), \(q = q_1 = q_2\) and:

\[
\hat{H}_{eff} = \sum_{i,j,\sigma} t_{ij}^{\sigma} d_{\sigma i}^{\dagger} d_{\sigma j} + J_k \sum_{i=1}^{n_s} \left\{ \hat{S}_{i}^{+} \hat{s}_{i}^{-} + \hat{S}_{i}^{-} \hat{s}_{i}^{+} \right\} - J_0 \sum_{i<j}^{n_s} \hat{S}_{i}^{z} \hat{s}_{j}^{z} - 2 h(m, q) \sum_{j=1}^{n_s} \hat{s}_{j}^{z}
\]

(3)

with the internal field \(h(m, q) = I_0 m + J q (\xi + \eta)\).

Numerical results are obtained by exact diagonalization of the effective Hamiltonian given by (3), where it is used a basis of states that satisfies the following criteria: each site is exactly occupied by one localized fermion (only two states per site: spin up or down), while four possible conduction fermion occupancies at each site are allowed (sites unoccupied, single occupied and double occupied). The intrachannel hopping term \(t_{ij} = 5 J\) and size of cluster \(n_s\) (=4 or 5) are constants. The intrachannel interaction between localized fermions \(J_0\) is ferromagnetic.

The behavior of order parameters as a function of temperature is exhibited in Fig. (1) for \(J_0 / J = 1\), different values of \(J_k\) and \(I_0\). In particular, Fig. (1-a) shows results for \(I_0 = 0\), where the cluster spin glass order parameter \(q\) becomes greater than zero at the freezing temperature \(T_f\). For increasing \(J_k\), \(T_f\) and \(q\) are decreased and the correlation \(\lambda = \frac{1}{n_s} \sum_{i=1}^{n_s} \hat{S}_{i} \hat{s}_{i}^{z} > 0\) has nonzero values (\(s_{i} = \sum_{\sigma} d_{\sigma i}^{\dagger} d_{\sigma i}\)). Figure (1-b) shows results when \(I_0 / J = 0.1\). In this situation, the magnetization \(m\) also appears at \(T_c\) for temperatures lower than \(T_f\) (\(T_c < T_f\)), which characterizes the mixed phase CSG-FE with both \(q > 0\) and \(m > 0\). For \(J_k / J = 2\) (see dashed lines of Fig. (1)), the critical temperatures decrease while \(\lambda\) increases, which suggests that the suppression of the magnetic order is a result of the enhancement of Kondo effect.
Figure 1. Order parameters versus temperature for $n_s = 4$ and two values of $J_k/J = 0.0$ and $2.0$. Panels (a) and (b) present results for $I_0/J = 0$ and $I_0/J = 0.1$, respectively.

The effects of $J_k$ on the order parameters become more evident in Fig. (2), where the behaviors of $q$, $m$ and $\lambda$ versus $J_k$ are exhibited for $I_0/J = 1$ and two temperatures: $T/J = 0.4$ and $T/J = 0.2$. For instance, the CSG order parameter decreases towards zero when $J_k$ increases. On the contrary, the correlation $\lambda$ enhances with $J_k$ and it assumes higher intensities at low temperatures in the region where $q = 0$. In this figure one can also analyze the role of $I_0$. When $I_0 > 0$ it is possible to find the order parameter $m$ (see Fig. (2-b)) that is also decreased by the increase of $\lambda$. Therefore, the interaction $J_k$ is able to destroy the CSG and the mixed phase at the same time that the correlation $\lambda$ is enhanced. This behavior can be associated with the Kondo interaction that could dominate at higher values of $J_k$.

Figure 2. Order parameters versus $J_k$ for $n_s = 4$ and two values of $T/J = 0.4$ and 0.2. Panels (a) and (b) present results for $I_0/J = 0$ and $I_0/J = 0.1$, respectively.

The short range intra-cluster interaction $J_0$ also has an important role in this problem. For example, Fig. (3) exhibits a comparison between results for order parameters with $J_0/J = 1$ (full lines) and $J_0/J = 1.5$ (dashed lines) with a constant $I_0/J = 0.1$. This shows that the increase of $J_0$ enhances the range of $T$ (Fig. (3-a)) and $J_k$ (Fig. (3-b)) where the magnetic orders occur.

Figure (4) shows results for $n_s = 5$, $J_0/J = 1$ and $I_0/J = 0.1$, where the correlation $\lambda$ is also enhanced with $J_k$ (see Fig. (4-b)). However, the mixed phase region is increased by the cluster size when the results of $n_s = 5$ are compared with those ones for $n_s = 4$. Therefore, the cluster size is relevant to the magnetic properties of the KLCG model.

In conclusion, a Kondo lattice cluster model with an inter-cluster magnetic disordered spin...
Figure 3. Panel (a) presents \( q, m \) and \( \lambda \) as a function of \( T \) for \( J_k/J = 2 \). Panel (b) shows \( q, m \) and \( \lambda \) versus \( J_k \) for \( T/J = 0.2 \). These results are for \( n_s = 4, I_0/J = 0.1 \) and two values of \( J_0/J = 1 \) and 1.5.

Figure 4. Panel (a) presents \( q, m \) and \( \lambda \) as a function of \( T/J \) for \( J_k/J = 0 \) and 2. Panel (b) presents \( q, m \) and \( \lambda \) versus \( J_k/J \) for \( T/J = 0.2 \). These results are for \( n_s = 5 \) and \( I_0/J = 0.1 \).

glass interaction is studied. The results show a competition between the Kondo effect and the magnetic orders, cluster spin glass (CSG) and mixed phase (CSG+FE). These magnetic orders are strongly dependent on the ferromagnetic inter-cluster interaction \( I_0 \) and the Kondo exchange interaction \( J_k \). For example, the CSG phase can be found when \( J_k \) is small, but it can present a transition to the mixed phase at lower temperatures if \( I_0 \) assumes small values. However the Kondo effect becomes dominant for large \( J_k \).

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