The random cluster approach in the Kondo Lattice model

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Abstract. We present here a Kondo Lattice model with an intersite random coupling between localized magnetic moments, which is composed of two terms, a random one given by the van Hemmen model and a ferromagnetic one. This model can be used to study new experimental evidences indicating the existence of a complex magnetic arrangement in CeNi₁₋ₓCuₓ alloys showing, with decreasing temperature, a glassy Kondo behavior and then a disordered ferromagnetism. We treat here the randomness without the replica method and found a phase which describes some features of the spin glass approach within the van Hemmen model. This approach, which takes both Kondo and ferromagnetic interactions, is suitable to describe correctly the phase diagram of CeNi₁₋ₓCuₓ alloys, with in particular the existence of the mixed spin glass-ferromagnetic at very low temperatures.

1. Introduction

The interplay between disorder and strong electronic correlations has been extensively studied in f-electron systems and in particular in Kondo systems [1]. Alloys such as CeNi₁₋ₓCuₓ [2, 3] or CePd₁₋ₓRhₓ [4] present very complex phase diagrams with magnetic orders (antiferromagnetism or ferromagnetism). Kondo phases but also disordered phases showing a spin glass state or even a more complicated state with magnetic clusters. The peculiar behavior of CeNi₁₋ₓCuₓ alloys has been studied since many years from both an experimental and theoretical point of view. CeCu presents an antiferromagnetic order at low temperatures and CeNi has a Kondo behaviour at low temperatures. The situation is more complex for intermediate concentrations x and a phase diagram with the occurrence of a spin glass phase followed at lower temperatures by a ferromagnetic order was initially observed experimentally [5]. The first theoretical explanation was based on the Kondo-Ising Lattice (KIL) model with a Kondo intrasite interaction and an intersite magnetic interaction described by the Sherrington-Kirkpatrick model, which gives firstly a Kondo phase and a spin glass one [6] and then a Kondo-spin glass-magnetic order [7]. But more sophisticated experiments have recently shown the appearance of disordered magnetic clusters; the size of the clusters increases with decreasing temperature, leading to a “cluster glass” phase below a freezing temperature and then, by a percolative process without a real transition, to a ferromagnetic phase with larger magnetic clusters [3]. A similar behaviour giving a Kondo-Cluster-Glass state has been also observed recently in CePd₁₋ₓRhₓ [4]. Our
purpose is to present here new theoretical models able to better describe recent improvements in the experimental data.

2. The theoretical model.
Our starting point is the KIL model given by:

\[ H = \sum_{i,j} t_{ij} n_{i\sigma} + e_0 \sum_{i,\sigma} n_{i\sigma}^f + J_K \sum_{i} [S_{fi}^z s_{ci}^z + S_{fi}^+ s_{ci}^+] - \sum_{(i,j)} J_{ij} S_{fi}^x S_{fj}^x. \] (1)

The spin operators in the KIL model given by the equation (1) are defined as usual [6] by:

\[ S_{fi}^x = \frac{1}{2} [n_{i\uparrow}^f - n_{i\downarrow}^f], \quad S_{fi}^+ = f_{i\uparrow}^f f_{i\downarrow}^\dagger, \quad s_{ci}^z = c_{i\uparrow}^c c_{i\downarrow}^c \] (2)

In the equations (1) and (2), \( S_{fi}^z = (S_{fi}^+)^\dagger, s_{ci}^z = (s_{ci}^+)^\dagger, n_{i\sigma}^f = f_{i\sigma}^f f_{i\sigma}^\dagger, \) \( n_{i\sigma}^c = c_{i\sigma}^c c_{i\sigma}^\dagger \) where \( f_{i\sigma}^\dagger (f_{i\sigma}) \) and \( c_{i\sigma}^\dagger (c_{i\sigma}) \) are fermionic creation (destruction) operators of localized \( f \) and conduction \( c \) electrons, respectively, with \( \sigma = \| \text{ or } \downarrow \) indicating the spin projections.

The first term of equation (1) describes the conduction band, the second term the f-band without width and the third term the classical intrasite Kondo exchange interaction (with a positive Kondo interaction \( J_K \)). But, the real difficulty comes here from the fourth term which describes the intersite randomly distributed exchange term between different localized spins. In previous works [6, 7], we have used the Sherrington-Kirkpatrick model [8] in which the exchange integral \( J_{ij} \) is approximated by a Gaussian distribution with a zero center to describe the spin glass-Kondo phase diagram [6] or a non zero one for the spin glass(SG)-Kondo-Ferromagnetic(FE) case [7]; a phase diagram giving temperature \( T \) versus \( J_K \) has been obtained in which there are a Kondo state and magnetic phases as SG, FE and a mixed phase. This diagram provides a first good explanation of the experimental phase diagram of CeNi\(_{1-x}\)Cu\(_x\) alloys, except for the fact that we have obtained a Curie temperature \( T_c \) always larger than the freezing one \( T_f \), in contradiction with experiment.

Thus, we have built again a new model [9] with a modified description of the disorder and we have taken for \( J_{ij} \) a generalization of the Mattis model [10] used extensively to study complex systems [11] given as:

\[ J_{ij} = \frac{J}{2N} \sum_{\mu=1}^{p} \xi_{i}^\mu \xi_{j}^\mu \] (3)

where \( \xi_{i}^\mu \) is a random variable which follows a bimodal distribution.

We have introduced a parameter to control the level of frustration [9] and we have obtained a phase diagram with a mixed Kondo phase, a SG phase which is replaced with decreasing temperature by Mattis states which have the same thermodynamics as a ferromagnetic phase [11]. Thus, the change from SG to FE with decreasing temperature is in good agreement with experiment, but here we have obtained a first-order transition from SG to the equivalent FE without any mixed phase, which is again not in good agreement with experiment.

Thus, we will try to improve again the agreement with the experimental case of CeNi\(_{1-x}\)Cu\(_x\) alloys and we introduce, in the KIL model, a new kind of disordered coupling \( J_{ij} \) given by van Hemmen (VH) [12] as:

\[ J_{ij} = \frac{J}{N} (\xi_i n_j + \eta_j \xi_j) + \frac{J_0}{N} \] (4)

with \( \xi \) and \( \eta \) being random variables which follow the bimodal distribution:

\[ P(x) = \frac{1}{2} [\delta(x - 1) + \delta(x + 1)] \] (5)
where $\delta(x)$ is the Dirac delta function.

In the equation (4), we take both a random contribution and a ferromagnetic one, which can account for both the SG and the ferromagnetic phases. The detailed calculations will be published elsewhere [13], but the present model is treated here, as usual, in the mean field approximation but without the use of the replica technique, as shown in the classical and quantum van Hemmen model [12, 14], which represents an important advantage with respect to the problems treated with the replica method. In particular, because there is no need of replicas, the cluster problem in Ref [16] would become more tractable using the coupling $J_{ij}$ given in Eq. (4). On the other hand, in Refs. [7, 9] as well as in the present work, canonical spins have been used. This description is obviously not enough to capture the complexity of the cluster glass state which is found for instance in $\text{CeNi}_{1-x}\text{Cu}_{x}$. However, earlier results for a mean field formulation of the cluster glass indicate that there is no essential differences between canonical spins and clusters as concerned the phase boundaries [15]. Therefore, one can expect that most of the previous discussion concerning phase boundaries can be preserved even if the problem is formulated in terms of clusters of spins instead of canonical ones [16].

We have then performed a classical mean field calculation and derived the order parameters, $\lambda$ corresponding to the average $\langle f_{i\sigma}^{\dagger}c_{\sigma} \rangle$ for the Kondo state, the f-magnetization for the ferromagnetic order and $q$ for the spin glass. Finally, the free energy can be found as [13]:

$$\beta f = \beta Jq^2 + \frac{\beta J_0 m^2}{2} + 2\beta J_K\lambda^2 - \left\langle \frac{1}{\beta D} \int_{\beta D}^{\beta D} dx \ln\left[\cosh\frac{x + h}{2} + \cosh\sqrt{\Delta}\right]\right\rangle$$

where $h = \beta J(\xi + \eta)q + \beta J_0 m$, $\Delta = (x - h)^2 / 4 + \beta^2 J_K^2\lambda^2$, $\beta = 1/T$ and $\langle \cdot \cdot \rangle$ denotes the average over the random variables $\xi$ and $\eta$.

We have obtained a phase diagram with the three following phases, SG, FE and a mixed one (FE+SG) and the result depend obviously on the ratio $J_0/J$. We have plotted in figure 1 the phase diagram giving the different phases in a plot temperature $T/J$ versus Kondo coupling $J_K/J$ for a given value of $J_0/J$. We obtain, for large $J_K$, a Kondo phase and, for smaller $J_K$, a

**Figure 1.** Phase diagram $T/J$ versus $J_K/J$ for $J_0/J = 1.3$ and $D = 12$. 

International Conference on Magnetism (ICM 2009) IOP Publishing
Journal of Physics: Conference Series 200 (2010) 012023 doi:10.1088/1742-6596/200/1/012023
sequence with decreasing temperature from the paramagnetic phase to a SG phase and finally to a mixed spin glass-ferromagnetic phase, in agreement with the phase diagram of $\text{CeNi}_{1-x}\text{Cu}_x$ alloys.

3. Conclusions.
In fact, the problem of the mixed spin glass-ferromagnetic phase in $\text{CeNi}_{1-x}\text{Cu}_x$ or other disordered Cerium alloys is a very difficult one, because the magnetic behaviour is going with decreasing temperature from a paramagnetic phase to a spin glass-like one and finally to a disordered ferromagnetic order. In fact, when temperature decreases, a percolative process has been observed from a cluster glass behavior with magnetic clusters to a disordered ferromagnetism with larger and more ferromagnetic clusters, as recently observed [3]. Experiments on $\text{CePd}_{1-x}\text{Rh}_x$ alloys have shown firstly a non-Fermi-liquid behaviour [17], but evidence for the absence of a ferromagnetic quantum critical point has been interpreted in terms of a Kondo-cluster-glass [4].

Our present van Hemmen model improves the description of the experimental data of $\text{CeNi}_{1-x}\text{Cu}_x$, because it gives both a ferromagnetic state below the spin glass phase and a mixed SG-ferromagnetic order at very low temperatures, in progress with respect to previous models of refs. [7, 9]. However, more recent and sophisticated experiments have shown evidence of a cluster glass. In a preceding recent theoretical model [16], we have taken magnetic clusters with only a small number of magnetic atoms within the Kondo Lattice model with an inter-cluster random Gaussian interaction like in the Sherrington-Kirkpatrick model and we have obtained a coexistence at low temperatures between the Kondo effect and a cluster glass phase. Work is presently in progress to compute within the van Hemmen model both the spin-spin correlation function and the spin glass order parameter, in order to better describe the cluster glass behaviour observed in Cerium alloys at low temperatures.

References
[1] B. Coqblin, M.D. Nunez-Regueiro, A. Theumann, J.R. Iglesias, S.G. Magalhaes, Philosophical Magazine 86, 2576 (2006).
[2] N. Marcano, J.C. Gomez Sal, J.I. Espeso, L. Fernandez Barquin and C. Paulsen, Phys. Rev. B 76 224419 (2007).
[3] N. Marcano, S. G. Magalhaes, B. Coqblin, J.C. Gomez Sal, J.I. Espeso, F. M. Zimmer, J.R. Iglesias, presented at ICM2009.
[4] T. Westerkamp, M. Deppe, R. Kuchler, M. Brando, C. Geibel, P. Gegenwart, A. P. Pikul, F. Steglich, Phys. Rev. Lett. 102, 206404 (2009).
[5] J. Garcia Soldevilla, J.C. Gomez Sal, J.A. Blanco, J.I. Espeso and J. Rodriguez Fernandez, Phys. Rev. B 61 6821 (2000).
[6] A. Theumann, B. Coqblin, S. G. Magalhaes, A. A. Schmidt, Phys. Rev. B 63 54409 (2001).
[7] S. G. Magalhaes, A. A. Schmidt, A. Theumann, B. Coqblin, Eur. Phys. J. B 30 419 (2002).
[8] S. Kirkpatrick, D. Sherrington, Phys. Rev. B 17, 4384 (1978).
[9] S. G. Magalhaes, F. M. Zimmer, P. R. Krebs, B. Coqblin, Phys. Rev. B 74 014427 (2006).
[10] D. J. Mattis, Phys. Lett. 56A, 421 (1977).
[11] D. J. Amit, Modelling Brain Function. The world of Attractor Neural Networks (Cambridge University Press, Cambridge, England, 1989).
[12] J. L. van Hemmen, Phys. Rev. Lett. 49, 409 (1982).
[13] S. G. Magalhaes, F. M. Zimmer, B. Coqblin, to be published.
[14] J. R. Viana, Y. Nogueira and J. Ricardo de Souza, Phys. Rev. B 66, 113307 (2002).
[15] C. M. Sokoulis, K. Levin, Phys. Rev. B 18 1439 (1978).
[16] F.M. Zimmer S.G. Magalhaes and B. Coqblin, presented at SCES2008, Buzios, Brazil.
[17] A.P. Pikul, N. Caroca-Canles, M. Deppe, P. Gegenwart, J.G. Sereni, C. Geiel and F. Steglich, J. Phys.: Condens. Matter, 18, L-535 (2006).