

Spin glass and ferromagnetism in Kondo lattice compounds

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Abstract. The Kondo lattice model has been analyzed in the presence of a random inter-site interaction among localized spins with non zero mean J_0 and standard deviation J . Following the same framework previously introduced by us, the problem is formulated in the path integral formalism where the spin operators are expressed as bilinear combinations of Grassmann fields. The static approximation and the replica symmetry ansatz have allowed us to solve the problem at a mean field level. The resulting phase diagram displays several phase transitions among a ferromagnetically ordered region, a spin glass one, a mixed phase and a Kondo state depending on J_0 , J and its relation with the Kondo interaction coupling J_K . These results could be used to address part of the experimental data for the $\text{CeNi}_{1-x}\text{Cu}_x$ compound, when $x \leq 0.8$.

PACS. 64.60.Cn Order-disorder transformations; statistical mechanics of model systems – 75.10.Nr Spin-glass and other random models – 75.30.Mb Valence fluctuation, Kondo lattice, and heavy-fermion phenomena

1 Introduction

The magnetism in strongly correlated f -electron systems has become a source of great interest due to the physics involved [1] like, for instance, quantum phase transitions and Non-Fermi liquid behavior [2]. The anti-ferromagnetic s - f exchange coupling of conduction electrons to localized spins can be responsible for the competition between the Kondo effect, that reduces the localized magnetic moments, and the RKKY interaction among magnetic impurities which, in turn, may give rise to magnetic long range order.

Recently, an experimental magnetic phase diagram of the Kondo $\text{CeNi}_{1-x}\text{Cu}_x$ compound has been proposed [3] showing the existence of a spin glass like state. In the CeCu limit, the negative magnetic interaction is dominant enough to produce an anti-ferromagnetic long range order with no indications of the Kondo effect. When Cu is substituted by Ni, there is a phase transition around $x = 0.8$ from the antiferromagnetic (AF) to a ferromagnetic (FM) ordering, which finally disappears at roughly $x = 0.2$; the Curie temperature is roughly equal to 1 K and is slowly decreasing down to $x = 0.4$ and then disappears at $x = 0.2$. Above the ferromagnetic phase, a spin-glass (SG) phase was identified by magnetic susceptibility measurements and the SG transition temperature

increases from 2 to 6 K for x varying from 0.7 to 0.2. For $x < 0.2$ a Kondo behaviour has been proposed, and finally CeNi is an intermediate valence compound. Thus, at very low temperatures, the phase sequence FM-SG-Kondo has been observed with decreasing x and in the range 0.7 – 0.2 for x , the sequence FM-SG is obtained with increasing temperature. It is quite rare to observe a ferromagnetic phase in cerium Kondo compounds, while antiferromagnetic phases are often observed and for example the sequence of SG-AF-Kondo transitions is obtained with increasing x in $\text{Ce}_2\text{Au}_{1-x}\text{Co}_x\text{Si}_3$ alloys [4].

Quite recently, a model has been introduced [5] to study the interplay between spin glass ordering and a Kondo state. This model is based on the previously introduced Kondo lattice model [6] with an intrasite s - f exchange interaction and an intersite long range random interaction of zero mean that couples the localized spins. The use of the static approximation and the replica symmetry ansatz has made possible to solve the problem at a mean field level. This fermionic problem is formulated by representing the spin operators as a bilinear combination of Grassmann fields and the partition function is found through the functional integral formalism [7–10]. The results are shown in a phase diagram of T/J versus J_K/J where T is the temperature, J_K is the intrasite Kondo exchange interaction and J is the standard deviation of the random inter-site interaction. For high temperatures and small values of J_K , a paramagnetic phase is found.

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In this situation, if the temperature is decreased a second order phase transition to a spin glass phase appears at T_f . The model shows a transition line $J_K^c(T)$ separating the paramagnetic and the spin glass phases from the Kondo phase.

In the present work, the model mentioned in the previous paragraph has been extended in order to include the proper elements that produce also a ferromagnetic ordering by taking the mean random interaction J_0 to be different from zero. Therefore, the magnetization can be introduced in addition to the other order parameters and solved coupled to them.

From this procedure a quite non-trivial phase diagram is obtained which contains ferromagnetism, a mixed phase [12,13] (ferromagnetism and spin glass), a spin glass phase and a Kondo state. For instance, one of the achievements of the present work is the finding of a mixed phase whose existence should not be discarded in the magnetic measurement of $\text{CeNi}_{1-x}\text{Cu}_x$, as mentioned in reference [3]

This paper is organized as follows. In Section 2 we present the model and its development in order to obtain the free energy and the saddle point coupled equations for the order parameters. The phase diagram of the temperature T/J versus J_K/J is shown for several values of J_0 . The Almeida-Thouless line is also calculated. Discussions and concluding remarks are presented in the last section.

2 The model and results

The model considered in this work was introduced before in reference [5] to study spin glass ordering in a Kondo lattice compound so the Hamiltonian is

$$\mathcal{H} - \mu_c N_c - \mu_f N_f = \sum_{k,\sigma} \epsilon_k n_{k\sigma} + \epsilon_0 \sum_{i,\sigma} n_{i\sigma}^f + J_K \sum_i [S_{fi}^+ s_i^- + S_{fi}^- s_i^+] - \sum_{i,j} J_{ij} S_{fi}^z S_{fj}^z \quad (1)$$

where $J_K > 0$ and the sum runs over N lattice sites. In the present case the random intersite interaction J_{ij} in the Hamiltonian is infinite ranged with a Gaussian distribution where $\langle J_{ij} \rangle = 2J_0/N$ and $\langle J_{ij}^2 \rangle = 8J^2/N$. This particular scaling compensates the factors 1/2 that originate in the definition of the operators S^z in equation (2) and also in changing from sum over sites to sum over bonds.

The spin variables $S_{fi}^{(+)}$ (s_{ci}^{+-}), S_{fi}^- are bilinear combinations of the creation and destruction operators [5] for localized (conduction) fermions $f_{i\sigma}^\dagger$, $f_{i\sigma}$ ($d_{i\sigma}^\dagger$, $d_{i\sigma}$) with the spin projection $\sigma = \uparrow$ or \downarrow :

$$\begin{aligned} S_{fi}^+ &= f_{i\uparrow}^\dagger f_{i\downarrow}; & s_{ci}^+ &= d_{i\uparrow}^\dagger d_{i\downarrow} \\ S_{fi}^- &= f_{i\downarrow}^\dagger f_{i\uparrow}; & s_{ci}^- &= d_{i\downarrow}^\dagger d_{i\uparrow} \\ S_{fi}^z &= \frac{1}{2} [f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow}]. \end{aligned} \quad (2)$$

The μ_f (μ_c) are the chemical potential for the localized (conduction) band. The energy ϵ_0 is referred to μ_f while ϵ_k is referred to μ_c .

The partition function is expressed in terms of functional integrals using anticommuting Grassmann variables $\varphi_{i\sigma}(\tau)$ and $\psi_{i\sigma}(\tau)$ associated with the conduction and the localized electrons respectively. Therefore,

$$Z = \int D(\psi^* \psi) D(\varphi^* \varphi) \exp \left\{ \int_0^\beta d\tau [L_0(\psi^*, \psi) + L_0(\varphi^*, \varphi) + L_{SG} + L_K] \right\} \quad (3)$$

where

$$\begin{aligned} L_0(\psi^*, \psi) &= \sum_{ij\sigma} \psi_{i\sigma}^*(\tau) \left[\frac{\partial}{\partial \tau} - \epsilon_0 \right] \delta_{ij} \psi_{j\sigma}(\tau), \\ L_0(\varphi^*, \varphi) &= \sum_{ij\sigma} \varphi_{i\sigma}^*(\tau) \left[\frac{\partial}{\partial \tau} \delta_{ij} - t_{ij} \right] \varphi_{j\sigma}(\tau), \\ L_{SG} &= \sum_{ij} J_{ij} S_{fi}^z(\tau) S_{fj}^z(\tau), \\ L_K &= \frac{J_K}{N} \sum_{i\sigma} [\varphi_{i-\sigma}^*(\tau) \psi_{i-\sigma}(\tau)] \\ &\quad \times \sum_{j\sigma} [\psi_{j\sigma}^*(\tau) \varphi_{j\sigma}(\tau)]. \end{aligned} \quad (4)$$

In the static approximation [7–10], it is possible to solve the problem in a mean field theory where the Kondo state is described by the complex order parameters [5,6]:

$$\begin{aligned} \lambda_\sigma^* &= \frac{1}{N} \sum_{i,\omega} \langle \psi_{i\sigma}^*(\omega) \varphi_{i\sigma}(\omega) \rangle \\ \lambda_\sigma &= \frac{1}{N} \sum_{i,\omega} \langle \varphi_{i\sigma}^*(\omega) \psi_{i\sigma}(\omega) \rangle. \end{aligned} \quad (5)$$

Following the treatment for the Kondo part in the partition function as introduced in reference [5], where it was assumed that $\lambda_\sigma^* \approx \lambda^*$ ($\lambda_\sigma \approx \lambda$), we show in the Appendix that first the conduction electron degrees of freedom may be integrated out to give

$$\frac{Z}{Z_d^0} = e^{[-2N\beta J_K \lambda^* \lambda]} Z_{eff} \quad (6)$$

where

$$Z_{eff} = \int D(\psi^* \psi) \exp \left\{ \sum_{\omega\sigma} \sum_{i,j} g_{ij}^{-1}(\omega) \psi_{i\sigma}^*(\omega) \times \psi_{j\sigma}(\omega) + A_{SG} \right\}, \quad (7)$$

Z_d^0 is the partition function of the free conduction electrons,

$$g_{ij}^{-1}(\omega) = (i\omega - \beta\epsilon_0) \delta_{ij} - \beta^2 J_K^2 \lambda^* \lambda \gamma_{ij}(\omega), \quad (8)$$

while $\gamma_{ij}^{-1} = i\omega\delta_{ij} - \beta t_{ij}$ is the inverse d -electron Green's function and $\beta = 1/T$ is the inverse temperature.

The free energy is given by the replica method

$$\beta F = 2\beta J_K \lambda^* \lambda - \lim_{n \rightarrow 0} \frac{1}{Nn} (\langle \langle Z_{\text{eff}}^n(J_{ij}) \rangle \rangle_{ca} - 1) \quad (9)$$

and the averaged replicated partition function can be linearized by means of the usual Hubbard-Stratonovich transformation. Therefore,

$$\langle \langle Z_{\text{eff}}^n(J_{ij}) \rangle \rangle_{ca} = \int \Pi_{\alpha\beta} dq_{\alpha\beta} \int \Pi_{\alpha} dm_{\alpha} \exp \left\{ -N \times \left[\frac{\beta^2 J^2}{2} \sum_{\alpha\beta} q_{\alpha\beta}^2 + \frac{\beta J_0}{2} \sum_{\alpha} m_{\alpha}^2 \right] \right\} \Lambda(q_{\alpha\beta}, m_{\alpha}) \quad (10)$$

with $\alpha = 0, 1, \dots, n$ being the replica index and

$$\Lambda(q_{\alpha\beta}, m_{\alpha}) = \int D(\psi_{\alpha}^* \psi_{\alpha}) \exp \left\{ \sum_{i,j,\sigma,\omega} g_{ij}^{-1}(\omega) \times \sum_{\alpha} \psi_{i\sigma\alpha}^*(\omega) \psi_{j\sigma\alpha}(\omega) + \beta J_0 \sum_{i\alpha} 2S_i^{\alpha} m_{\alpha} + \beta^2 J^2 \sum_{ij\alpha\beta} 4S_i^{\alpha} S_j^{\beta} q_{\alpha\beta} \right\}. \quad (11)$$

A more detailed derivation of equations (10) and (11) is given in the Appendix.

This problem is analysed within the replica symmetric ansatz where $q_{\alpha\neq\beta} = q$ is the spin glass order parameter, $m_{\alpha} = m$ is the magnetization and $q_{\alpha\alpha} = q + \bar{\chi}$, ($\bar{\chi} = \frac{\chi}{\beta}$) with χ being the static susceptibility. The sum over replica indices also gives quadratic terms which can be linearized again by introducing new auxiliary fields in equation (10):

$$\Lambda(q_{\alpha\beta}, m_{\alpha}) = \int Dz_j \int D(\psi^* \psi) \times \exp \left\{ \sum_{i,j,\sigma,\omega} g_{ij}^{-1} \sum_{\alpha} \psi_{i\sigma\alpha}^*(\omega_n) \psi_{j\sigma\alpha}(\omega_n) + \beta J_0 m \sum_{\alpha} 2S_i^{\alpha} + \beta J \sqrt{2q} \sum_i z_i 2S_i^{\alpha} \right\} \times \int D\xi_j^{\alpha} \exp \left\{ - \sum_{\alpha j} (\xi_j^{\alpha})^2 + \beta J \sqrt{2\bar{\chi}} \xi_j^{\alpha} 2S_j^{\alpha} \right\} \quad (12)$$

where $Dx = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx$ and

$$S_i^{\alpha} = \frac{1}{2} \sum_{\omega_n \alpha\sigma = \pm} \sigma \psi_{\alpha\sigma}^*(\omega_n) \psi_{\alpha\sigma}(\omega_n).$$

The functional integral in equation (12) can be performed and the saddle point solution for the free energy

is given by

$$\beta F = 2\beta J_K \lambda^2 + \frac{1}{2} \beta^2 J^2 (\bar{\chi}^2 + 2q\bar{\chi}) + \frac{\beta J_0}{2} m^2 - \lim_{n \rightarrow 0} \frac{1}{Nn} \left\{ \int \Pi_i D z_i \times \int \Pi_{\alpha,i} D \xi_i^{\alpha} \exp \left[\sum_{\omega\sigma} \ln [\det G_{ij\sigma}^{-1}(\omega)] \right] - 1 \right\} \quad (13)$$

where in the previous equation we introduced the inverse Green's function

$$G_{ij\sigma}^{-1}(\omega) = g_{ij}^{-1}(\omega) - \delta_{ij} \sigma h(z_i, \xi_i^{\alpha}) \quad (14)$$

with an effective field

$$h(z_i, \xi_i^{\alpha}) = \beta J_0 m + \beta J \sqrt{2q} z_i + \beta J \sqrt{2\bar{\chi}} \xi_i^{\alpha}. \quad (15)$$

A problem is presented by the calculation of the Green's function $G_{ij\sigma}(\omega)$ in equation (14) where there is a random Gaussian field $h(z_i, \xi_i^{\alpha}) \equiv h_{i\alpha}$ applied at every site i of n replicated lattices with N sites. The decoupling used at this point is the same as for reference [5], *i.e.*, the original Green's function $G_{ij\sigma}(\omega)$ is replaced by a Green's function $\Gamma_{\mu\nu\sigma}(\omega)$ where there is a uniform field $h_{i\alpha}$ applied in every site μ, ν of a fictitious Kondo lattice. Therefore, going to the reciprocal space and assuming a constant density of states for the conduction electron band $\rho(\epsilon) = \frac{1}{2D}$ for $-D < \epsilon < D$, the sum over Matsubara's frequencies ω can be performed in equation (13) and the resulting free energy is

$$\beta F = 2\beta J_K \lambda^2 + \frac{1}{2} \beta^2 J^2 \{ \bar{\chi}^2 + 2\bar{\chi}q \} + \frac{\beta J_0}{2} m^2 - \int_{-\infty}^{+\infty} Dz \ln \left[\int_{-\infty}^{+\infty} D\xi e^{E(\xi)} \right] \quad (16)$$

where

$$E(\xi) = \frac{1}{\beta D} \int_{-\beta D}^{+\beta D} dx \ln \{ S(\xi, x) \},$$

$$S(\xi, x) = \cosh(h_x^+) + \cosh(\sqrt{\Delta}),$$

$$\Delta = (h_x^-)^2 + (\beta J_K \lambda)^2 \quad \text{and} \quad h_x^{\pm} = \frac{h \pm x}{2}.$$

The saddle point equations for the order parameters q , m , $\bar{\chi}$ and λ can be found from equation (16).

The limit of stability for the order parameters solutions with replica symmetry is achieved if the Almeida-Thouless eigenvalue becomes negative:

$$\lambda_{AT} = 1 - 2\beta^2 J^2 \int_{-\infty}^{+\infty} Dz \left\{ \frac{\int_{-\infty}^{+\infty} D\xi e^{E(\xi)} \Omega(T)}{\int_{-\infty}^{+\infty} D\xi e^{E(\xi)}} - \left[\frac{\int_{-\infty}^{+\infty} D\xi e^{E(\xi)} T_1(\xi)}{\int_{-\infty}^{+\infty} D\xi e^{E(\xi)}} \right]^2 \right\}^2 \quad (17)$$

where

$$\Omega(T) = [T_1(\xi)]^2 - T_2(\xi) + T_3(\xi)$$

$$T_1(\xi) = \frac{1}{2\beta D} \int_{-\beta D}^{\beta D} dx \left[\frac{\sinh(h_x^+) + \frac{\sinh(\sqrt{\Delta})}{\sqrt{\Delta}}(h_x^-)}{S(\xi, x)} \right]$$

$$T_2(\xi) = \frac{1}{4\beta D} \int_{-\beta D}^{\beta D} dx \left[\frac{\sinh(h_x^+) + \frac{\sinh(\sqrt{\Delta})}{\sqrt{\Delta}}(h_x^-)}{S(\xi, x)} \right]^2$$

$$T_3(\xi) = \frac{1}{4\beta D} \int_{-\beta D}^{\beta D} dx \left[\frac{\cosh(h_x^+) + \frac{\sinh(\sqrt{\Delta})}{\sqrt{\Delta}}}{S(\xi, x)} \right. \\ \left. + \frac{\left[\cosh(\sqrt{\Delta}) - \frac{\sinh(\sqrt{\Delta})}{\sqrt{\Delta}} \right] \frac{(h_x^-)^2}{\Delta}}{S(\xi, x)} \right].$$

3 Discussion

We have studied in this work a Kondo lattice model where the localized moments interact through a random inter-site interaction which has an average different from zero. The static approximation and replica symmetry ansatz lead to a mean field solution for the problem. The resulting coupled saddle point equations for the order parameters produce solutions which give a Kondo state and magnetic ordering like ferromagnetism, spin glass and a mixed phase. In principle, we would be able to build up transition surfaces among those phases in a space T/J (temperature) versus J_0/J (the inter-site interaction average) and J_K/J (the Kondo coupling) where J (the inter-site interaction standard deviation) is kept constant. These parameters J_K , J_0 , J and the temperature are the set of energy scales in the present model. The conduction electrons bandwidth D is kept constant.

The result shown in Figure 1 represents a cut in the cited space transversal to the J_K/J axis. For this situation and using $J_K/J=4$, the Kondo state is still not turned on (it means $\lambda=0$). The obtained phase diagram for this fermionic model resembles the classical one [11, 13] (it depends basically on J_0 and its relation to J) except that the numerical values of the transition temperatures are smaller. If $J_0 < 1.46J$, for decreasing temperature, there is a second order transition from a paramagnetic to a spin glass phase ($m=0, q \neq 0$). For that region, the Almeida-Thouless (AT) line coincides with the transition line. However, for $J_0 \geq 1.46J$, for decreasing temperature, the model shows a transition from a paramagnetic to a ferromagnetic phase ($m \neq 0, q \neq 0$). The AT line is located at higher temperature than the calculated replica symmetry line transition $T^*(J_0)$ between the ferromagnetic and the spin glass phases. Therefore, this fermionic model shows a transition from a ferromagnetic to a replica symmetry breaking spin glass phase with a large number

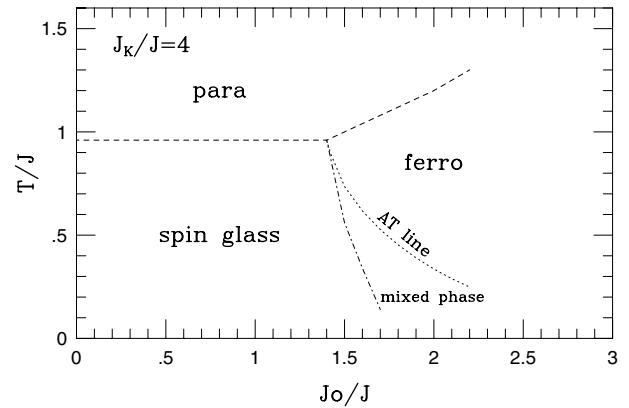


Fig. 1. Cut in the phase transition space transversal to the J_K/J axis for $J_K=2$, $J=0.5$ and $D=10$. The Kondo state is not turned on yet and the transitions among the ferromagnetism and the spin glass phases depend on the value of J_0 . The dashed line shows the transition from the paramagnetic phase to the ferromagnetic and the spin glass phases. The dotted line is the Almeida-Thouless (AT) line which, for lower values of J_0 , coincides with the paramagnetic – spin glass transition line (horizontal dashed line). The dot-dashed and the AT line delimit the mixed phase between the ferromagnetic and spin glass phases.

of degenerate states but still with non-zero spontaneous magnetization which is called a mixed phase [12, 13].

Figure 2 shows the cut in the phase space transversal to the J_0/J axis. For values of J_0/J close to zero (see Fig. 2a), the phase diagram resembles the scenario already found in reference [5], that is a paramagnetic phase at high temperatures, a spin glass phase below the freezing temperature T_f and a line $J_K=J_K^c(T)$ separating both phases from a Kondo state. For that situation, the AT line is at T_f and follows the line $J_K=J_K^c(T)$.

As the value of J_0/J is increased (for small J_K/J) (see Figs. 2b, c and d), the phase diagram starts to show the presence of a ferromagnetic phase which has a transition temperature $T_c(J_0)$ increasing with J_0 , the AT line and the calculated replica symmetric line $T^*(J_0)$ decreasing with J_0 . Nevertheless the AT line is always above $T^*(J_0)$. In that scenario, for decreasing temperature, first a transition from paramagnetic to a ferromagnetic phase appears followed by a transition from the ferromagnetic to a mixed phase. This behavior is reminiscent of that one described for the cut transversal to J_K/J (Fig. 1). For some value of J_0/J , the mixed phase finally disappears and that region of the phase diagram is totally occupied by the ferromagnetic phase. For larger values of J_K/J , the phase diagram goes to a Kondo state where the transition line $J_K^c(T)$ does not depend on J_0 .

A remark should be made about the transition line between the spin glass phase and the Kondo state. At low temperatures, this is a first order transition line and so multiple possible solutions for the order parameters can be found. Nonetheless, the actual stable solutions can be obtained from the minimization of the free energy. In the case of $J_0/J < 1.46$ the hatched region in Figure 2a

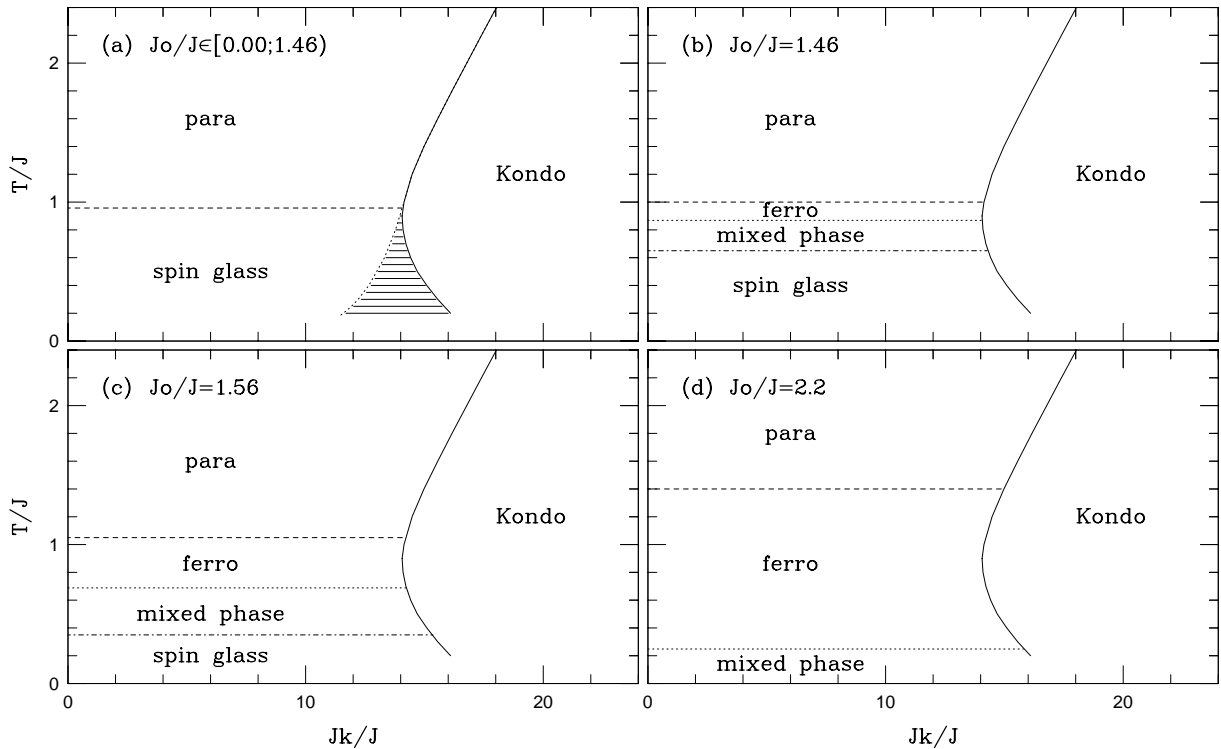


Fig. 2. Cut in the phase transition space transversal to the J_0/J axis for several values of J_0 , $J = 0.5$ and $D = 10$. The solid line shows the thermodynamically stable transition from the Kondo phase to the other ones. For lower temperatures, a hatched region in panel (a) delineates a multiple solution region where the solid line to the right corresponds to the thermodynamically stable solution. The horizontal dashed, dotted and dot-dashed lines have the same meaning as in Figure 1. The AT line follows the horizontal dotted line up to the Kondo transition point. Beyond that, for larger values of J_K , the AT line follows the transition line from the Kondo phase and the mixed and spin glass phases (solid line, lower temperatures). One can notice that, as J_0 increases, a ferromagnetic and a mixed phase start to appear and, for some value of J_0 , the spin glass phase finally disappears.

displays where these multiple solutions occur. By computing the free energy we have found the thermodynamically stable solutions. The solid line to the right of the hatched region in Figure 2a corresponds to these solutions and the hatched region itself corresponds to metastable solutions. Such a careful analysis can be considered an improvement with respect to our previous work [5] where such a discussion had not been done. Nevertheless the previous SG-Kondo state transition line shown there is approximately the same as the one presented here. Thus, the hatched regions corresponding to the one displayed in Figure 2a have not been presented in Figures 2b–d.

4 Conclusions

In this work it has been studied a Kondo lattice model in the presence of a random inter-site interaction which produces paramagnetism, ferromagnetism, a spin glass phase, a mixed phase and a region where the magnetic moments of the localized electrons are suppressed by the screening of the conduction ones (Kondo state). The model has four energy scales: the temperature, J_0 (the average inter-site interaction), J (the inter-site interaction variance) and J_K (the Kondo coupling). As a re-

sult one has a three dimensional phase diagram with axes J_0/J , J_K/J and temperature. Some cuts of this diagram transversal to the J_K/J and J_0/J , planes are shown in the Figures 1 and 2. The position of the transition line separating the Kondo state from the magnetic phases is not affected by J_0 . This energy scale is basically responsible for locating several magnetic orderings along the temperature range.

One can try to address the experimental phase diagram found in reference [3] for the alloys $\text{CeNi}_{1-x}\text{Cu}_x$, but theoretically if we vary only J_K with x , we have found a ferromagnetic phase above the spin glass, in disagreement with the experimental result. However, the equivalence between their experimental phase diagram and ours (see Figs. 1 and 2) is not so straightforward since the Ni content would have to be associated to both J_0 and J_K . This could be an indication that the ergodicity breaking mechanism for the formation of magnetic phases like spin glass and ferromagnetism in $\text{CeNi}_{1-x}\text{Cu}_x$ is far more complicated than the modelling by a random inter-site interaction can address. Although recent investigations on the ferromagnetic transverse Ising spin glass suggest also the existence of a spin glass transition below the Curie temperature [14], it is plausible that this be a characteristic of the Sherrington–Kirkpatrick model with a high degree of frustration. Less

frustrated spin glass models [15] may sustain spin glass order above the Curie temperature and they can be more indicated for the study of the $\text{CeNi}_{1-x}\text{Cu}_x$ compounds.

To conclude, in reference [5] a Kondo lattice model with strong frustration (at mean field level) has been solved showing the existence of a SG and a Kondo state depending on J_K/J (as defined in Sect. 2). These results could address part of the experimental phase diagram of $\text{CeNi}_{1-x}\text{Cu}_x$ [4]. The purpose of the present work has been to examine a wider and more complex region of this experimental phase diagram which includes ferromagnetism. Therefore, we have improved our previous work by choosing a non-zero average of the random coupling J_0 . From this approach we have been able to generate a quite non-trivial phase diagram with a spin glass phase, ferromagnetism, a Kondo state and a mixed phase (spin glass and ferromagnetism). Nevertheless the calculated spin glass freezing temperature is lower than the Curie temperature in contrast with some experimental findings [3]. However, as pointed out in reference [3], a mixed phase can not be discarded as a possible explanation for the magnetic measurements. The calculations with the ferromagnetic phase has also shown an improvement with respect to our previous work [5] regarding the actual location of the SG-Kondo first order transition line. The present approach might also explain the frustration in antiferromagnetic Kondo systems like $\text{Ce}_2\text{Au}_{1-x}\text{Co}_x\text{Si}_3$ alloys. This work is now on progress.

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Appendix

We outline here briefly the method used in reference [5]. In order to obtain equations (10) and (11) of Section 2 we must first use the static approximation in the Fourier transform of L_K in equation (4) and introduce the Kondo order parameter by means of the identity

$$\begin{aligned} \exp \left\{ \int_0^\beta L_K d\tau \right\} &= \int_{-\infty}^{\infty} \Pi_\sigma d\lambda_\sigma^\dagger d\lambda_\sigma \Pi_\sigma \\ &\times \delta \left(\lambda_\sigma^\dagger N - \sum_{j,w} \psi_{j\sigma}^\dagger(w) \varphi_{j\sigma}(w) \right) \\ &\times \delta \left(\lambda_\sigma N - \sum_{j,w} \varphi_{j\sigma}^\dagger(w) \psi_{j\sigma}(w) \right) \\ &\times \exp \left\{ \beta J_k N [\lambda_\uparrow^\dagger \lambda_\downarrow + \lambda_\downarrow^\dagger \lambda_\uparrow] \right\} \quad (18) \end{aligned}$$

and using the integral representation for the δ function we obtain, after some algebra,

$$Z = \int \Pi_\sigma d\lambda_\sigma^\dagger d\lambda_\sigma \exp \left\{ -N\beta J_K \sum_\sigma \lambda_\sigma^\dagger \lambda_\sigma \right\} Z_{stat} \quad (19)$$

where

$$\begin{aligned} Z_{stat} &= \int D(\psi^* \psi) D(\varphi^* \varphi) \\ &\times \exp \left\{ \int_0^\beta d\tau [L_0(\psi^*, \psi) + L_0(\varphi^*, \varphi) + L_{SG}] \right\} \\ &\times \exp \left\{ \beta J_K \sum_\sigma \left[\lambda_{-\sigma}^\dagger \sum_{j,w} \varphi_{j\sigma}^\dagger(w) \psi_{j\sigma}(w) \right. \right. \\ &\quad \left. \left. + \lambda_\sigma \sum_{j,w} \psi_{j\sigma}^\dagger(w) \varphi_{j\sigma}(w) \right] \right\}. \quad (20) \end{aligned}$$

The mean field approximation adopted here is based on two assumptions: first, fluctuations in time are ignored (static approximation); second, fluctuations in space are also ignored in the definition of the order parameters. Both assumptions lead us to a quadratic form in the Grassmann variables φ and φ^* in equation (20) and shifting the representation to Matsubara's frequencies we can perform the functional integrals to obtain equation (6), where now the order parameters λ_σ^\dagger , λ_σ are taken at their saddle point value. We also have

$$\int_0^\beta d\tau L_{SG} = \sum_{ij} J_{ij} S_{fi}^z S_{fj}^z \quad (21)$$

where

$$S_{fi}^z = \frac{1}{2} \sum_\omega [\psi_{i\uparrow}^*(\omega) \psi_{i\uparrow}(\omega) - \psi_{i\downarrow}^*(\omega) \psi_{i\downarrow}(\omega)]. \quad (22)$$

Hence, in order to get the configurational average over the random coupling J_{ij} , we use a Gaussian distribution with average and variance given in Section 2. So

$$\langle Z_{eff}^n(J_{ij}) \rangle_{ca} = \int D(\psi^* \psi) \exp \left\{ A_0^{eff} + A_{SG}^{replc} \right\} \quad (23)$$

where

$$A_0^{eff} = \sum_{ij\sigma\alpha} \sum_{\omega_n} \psi_{i\sigma\alpha}^*(\omega_n) g_{ij}^{-1}(\omega_n) \psi_{j\sigma\alpha}(\omega_n)$$

and

$$\begin{aligned} A_{SG}^{replc} &= \frac{1}{N} \left\{ \frac{\beta^2 J^2}{2} \sum_{\alpha\beta} \left[\sum_i 4S_i^\alpha S_i^\beta \right]^2 \right. \\ &\quad \left. + \frac{\beta J_0}{2} \sum_\alpha \left[\sum_i 2S_i^\alpha \right]^2 \right\}. \end{aligned}$$

In the previous equation, $g_{ij}^{-1}(\omega_n)$ has been defined in Section 2. The static approximation is also used to write the S_i^α in terms of Grassmann fields as in equation (22) and the resulting equation can be linearized by standard procedures [10], introducing the order parameters $q_{\alpha\beta}$ and m_α which gives equations (10) and (11).

References

1. B. Coqblin, B.H. Bernhard, J.R. Iglesias, C. Lacroix, K. Le Hur, *Proc. International Workshop on Electron Correlations and Materials Properties, 1988, Crete, Greece*
2. P. Coleman, *Physica B* **259-261**, 353 (1999)
3. J. Garcia Soldevilla, J.C. Gomez Sal, J.A. Blanco, J.I. Espeso, J. Rodriguez Fernandez, *Phys. Rev. B*, **61**, 6821 (2000)
4. S. Majumdar, F.V. Sampathkumaran, St. Berger, M. Della Mea, H. Michor, E. Bauer, M. Brando, J. Hemberger, A. Loidl, *Solid State Commun.* **121**, 665 (2002)
5. A. Theumann, B. Coqblin, S.G. Magalhães, A.A. Schmidt, *Phys. Rev. B* **63**, 54409 (2001)
6. J.R. Iglesias, C. Lacroix, B. Coqblin, *Phys. Rev. B*, **56**, 54409 (1997)
7. A. Theumann, M. Vieira Gusmão, *Phys. Lett. A*, **105**, 311 (1984)
8. A. Theumann, *Phys. Rev. B* **33**, 559 (1986)
9. A.J. Bray, M.A. Moore, *J. Phys. C* **13**, 419 (1980)
10. R. Oppermann, A. Müller-Groeling, *Nucl. Phys. B* **401**, 507 (1993)
11. S. Kirkpatrick, D. Sherrington, *Phys. Rev. B* **17**, 4384 (1978)
12. M. Gabay, G. Toulouse, *Phys. Rev. Lett.* **47**, 201 (1981)
13. K.H. Fischer, J.A. Hertz, *Spin Glasses* 1st edn. (Cambridge University Press, Cambridge, 1991)
14. Ying-Jer Kao, G.S. Grest, K. Levin, J. Brooke, T.F. Rosenbaum, G. Aeppli, *Phys. Rev. B* **64**, 060402(R) (2001)
15. J.L. van Hemmen, *Phys. Rev. Lett.* **49**, 409 (1982)