Spin glass freezing in Kondo lattice compounds

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Abstract

It is presented a theory that describes a spin glass phase at finite temperatures in Kondo lattice systems with an additional RKKY interaction represented by long range, random couplings among localized spins like in the Sherrington- Kirkpatrick (SK) spin glass model. The problem is studied within the functional integral formalism where the spin operators are represented by bilinear combinations of fermionic (anticommuting) Grassmann variables. The Kondo and spin glass transitions are both described with the mean field like static ansatz that reproduces good results in the two well known limits. At high temperatures and low values of the Kondo coupling there is a paramagnetic (disordered) phase with vanishing Kondo and spin glass order parameters. By lowering the temperature a second order transition line is found at $T_{SG}$ to a spin glass phase. For larger values of the Kondo coupling there is a second order transition line at roughly $T_k$ to a Kondo ordered state. For $T < T_{SG}$ the transition between the Kondo and spin glass phases becomes first order.
1. Introduction

The antiferromagnetic s-f exchange coupling of conduction electrons to localized spins in heavy fermion rare-earth systems is responsible for two competing effects: the screening of the localized moments due to the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction among magnetic impurities which may induce a long-range magnetic (antiferromagnetic or ferromagnetic) ordering or eventually a spin glass magnetic ordering. The Doniach diagram[1] gives a good description of this competition: the Neel temperature $T_N$ is firstly increasing with increasing the absolute value of the exchange interaction constant $J_k$, then it is passing through a maximum and finally it tends to zero at the ”quantum critical point” (QCP). Such a decrease of $T_N$ down to the QCP has been observed in many Cerium compounds, such asCeAl₂, CeAg or CeRh₂Si₂, under pressure. Above the QCP, there exists a very strong heavy fermion character, but several possible behaviours, i.e. the classical Fermi liquid one with eventually a reduced Kondo temperature[2, 3] or different Non-Fermi-Liquid (NFL) ones, have been observed in Cerium or Ytterbium compounds[4, 5].

But, in the case of disordered Cerium alloys, the disorder can yield a Spin Glass (SG) phase in addition to the NFL behaviour at low temperatures around the QCP. The magnetic phase diagram of CeNi₁₋ₓCux has been extensively studied[6, 7]. CeCu is antiferromagnetic below 3.5 K and CeNi is a non magnetic compound with an intermediate valence. The low temperature antiferromagnetic phase changes, around $x = 0.8$, to a ferromagnetic one which finally disappears around $x = 0.2$. At higher temperatures, a
Spin Glass state is deduced from all measured bulk properties, such as for example the ac susceptibility; for example, for $x = 0.6$, the SG state exists between 2 K and the Curie temperature $T_c = 1.1K$. At $x = 0.2$, there exists below 6 K only a SG state which transforms to the intermediate valence CeNi, after passing probably through a Kondo lattice system. Thus, in the $CeNi_{1-x}Cu_x$ system, there appears a SG phase at finite temperatures above the ferromagnetic order and finally a SG-Kondo transition occurs for small $x$ values.

Another disordered Cerium system, namely $CeCoGe_{3-x}Si_x$ alloys, has been also studied for different $x$ values, by different experimental techniques including muon spin relaxation\cite{8, 9}. The compound $CeCoGe_3$ is antiferromagnetic below 21 K and $CeCoSi_3$ is an intermediate valence compound; the QCP of these alloys lies around $x = 1.5$. The muon spin relaxation experiments in the quantum critical region ($x = 1.1$ to 1.5) show that a fraction of Ce ions experience random f-f indirect exchange interactions, which causes frustration of some Ce spins in the system. So, for $x = 1.1$ and $x = 1.2$, frustrated moments of Cerium freeze like in a spin glass while the other Ce moments form a disordered antiferromagnetic state. Thus, near the QCP, a spin glass state can exist in these alloys, in addition to the observed NFL behaviour. So, a striking novel behaviour, i.e. the appearance of a spin glass state at finite temperatures in some disordered Cerium alloys, has been observed and a SG-Kondo transition is developing with increasing $x$ around the QCP.

The aim of our paper is to present a theoretical model that describes the spin glass-Kondo phase transitions, and that we do by studying a sys-
tem Hamiltonian that couples the localized spins of a Kondo lattice with an additional long range random interaction, like in the Sherrington-Kirkpatrick spin glass model [10]. A similar Hamiltonian has been considered in [11] to describe NFL behaviour and a QCP in some heavy fermions compounds, although the relevant approximations differ in this work and ours. The authors in [11] are primarily interested in the description of the QCP at $T = 0$, then they solve first for the Kondo effect by decoupling the conduction electrons bath into independent conduction electron "reservoirs", with no communication between the reservoirs at different sites.

During the course of our work, another paper using the same Hamiltonian has been proposed [12]. The representation of Popov and Fedotov eliminates the unwanted spin states but the approximations involved are in fact different from those used in our work. They study essentially the spin glass state and they finally obtain a second order SG transition with a transition temperature depressed by the Kondo effect, in second order perturbation theory.

In the present paper we take a different approach: the localized spins of the Kondo lattice will be effectively immersed in a common bath of conduction electrons and the Kondo effect will be studied in a quantum static approximation that is basically equivalent to the mean field decoupling scheme [3, 13]. The spin operators are represented by bilinear combinations of fermionic creation and destruction operators, for the localized f-electrons, and the spin glass transition will be studied within the static approximation. This deserves some special discussion. In the Ising quantum spin glass (QSG) model [14], the spin operator $S_i^z$ commutes with the particle number operator $n_{is}$ and the static Ansatz gives the exact answer, as the problem is
essentially classic. When we add to the fermionic Ising QSG a s-d exchange coupling of the localized spins to the conduction band electrons the problem ceases to be exactly soluble and the static Ansatz is just an approximation, that we consider justified to describe a transition at finite temperature. It has been shown in [15] that the exact numerical solution of Bray and Moore’s equations [16] gives for the spin-spin correlation function $Q(\tau)$ roughly its constant classical value at finite temperature, what justifies the use of the static Ansatz of [16] at not very low temperatures in the Heisenberg spin glass.

We consider then the static Ansatz which corresponds to an approximation similar to mean field theory, where by neglecting time fluctuations we can provide a description of the phase transitions occurring at finite temperature.

We use functional integral techniques where the spin operators are represented by bilinear combinations of fermionic (anticommuting) Grassmann fields. As we show in the next section, this method is ideally suited to describe a Kondo lattice transition, and it has been recently applied by two of us to the study of fermionic Ising spin glasses with local BCS pairing [17]. Recent work [18] also showed the existence of several characteristic temperatures in the Ising fermionic model, with the de Almeida-Thouless instability [19] occurring at a temperature lower than the spin glass transition temperature.

This paper is organized as follows: in Sect.2 we describe the model and relevant results, we reserve Sect.3 for discussions and conclusion, while the detailed mathematical calculations are left for the Appendix.
2. The model and results

We consider a Kondo lattice system with localized spins $\vec{S}_i$ at sites $i = 1 \cdots N$, coupled to the electrons of the conduction band via a s-d exchange interaction. It is necessary to introduce explicitly the resultant RKKY interaction by means of a random, long range coupling among localized spins like in the Sherrington Kirkpatrick (SK) model for a spin glass. To describe the Kondo effect in a mean-field-like theory it is sufficient to keep only the spin-flip terms [3] in the exchange Hamiltonian, while the spin glass interaction is represented by the quantum Ising Hamiltonian where only interact the $z$-components of the localized spins [11, 14, 17].

The Hamiltonian of the model is:

$$\mathcal{H} - \mu_c N_c - \mu_f N_f = \mathcal{H}_k - \mu_c N_c - \mu_f N_f + \mathcal{H}_{SG}$$

(1)

$$\mathcal{H}_k - \mu_c N_c - \mu_f N_f = \sum_{k,\sigma} \epsilon_k n_{k\sigma} + \epsilon_0 \sum_{i,\sigma} n_{i\sigma}^f + J_k \sum_i \left[ S_{fi}^+ s_{ci}^- + S_{fi}^- s_{ci}^+ \right]$$

(2)

$$\mathcal{H}_{SG} = -\sum_{ij} J_{ij} S_{fi}^z S_{fj}^z$$

(3)

where $J_k > 0$,

$$S_{fi}^+ = f_{i\uparrow}^\dagger f_{i\downarrow} \quad ; \quad s_{ci}^+ = d_{i\uparrow}^\dagger d_{i\downarrow}$$

(4)

$$S_{fi}^- = f_{i\downarrow}^\dagger f_{i\uparrow} \quad ; \quad s_{ci}^- = d_{i\downarrow}^\dagger d_{i\uparrow}$$

$$S_{fi}^z = \frac{1}{2} [ f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow} ]$$
and $f_{i\sigma}^+, f_{i\sigma}(d_{i\sigma}^+, d_{i\sigma})$ are creation and destruction operators for electrons with spin projection $\sigma = \uparrow$ or $\downarrow$ in the localized (conduction) band, that satisfy the standard fermion anticommutation rules. We also have $n_{k\sigma} = d_{k\sigma}^+ d_{k\sigma}$ where:

$$d_{k\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k} \cdot \vec{R}_i} d_{i\sigma}$$

$$d_{k\sigma}^+ = \frac{1}{\sqrt{N}} \sum_i e^{-i\vec{k} \cdot \vec{R}_i} d_{i\sigma}^+$$

The energies $\epsilon_0(\epsilon_k)$ are referred to the chemical potentials $\mu_f(\mu_c)$, respectively.

The coupling $J_{ij}$ in eq.(3) is an independent random variable with the gaussian distribution

$$P(J_{ij}) = e^{-J_{ij}^2 \frac{N}{32\pi J^2} \sqrt{N \over 32\pi J^2}}$$

Functional integration techniques have proved to be a suitable approach to describe phase transitions in disordered quantum mechanical many-particle systems [20]. The static approximation within this formulation consists in neglecting time fluctuations of the order parameter, and when it is combined with the neglect of space fluctuations it leads to the usual Hartree-Fock, mean field like approximation. When dealing with the Hamiltonian in Eq. (1)-Eq.(3), we notice that in the limiting case $J_k = 0$ we obtain a pure quantum Ising spin glass where the static approximation gives the exact result [14, 18], while for $J = 0$ we recover the mean field approximation that has been used successfully to describe the Kondo lattice [3, 13]. Then we consider that the use of the static approximation has an interpolation character and
will provide reliable results to describe critical behaviour at finite temperature \[15\] in systems that do not present a quantum critical point.

In the Lagrangian formulation \[17, 20\] the partition function is expressed as

\[
Z = \int D(\varphi^\dagger \varphi)(\psi^\dagger \psi) e^A
\]  

(7)

where the action \(A\) is given by

\[
A = \sum_{i,\sigma} \int_0^\beta d\tau \left\{ \left( \frac{\partial}{\partial \tau} \varphi^\dagger_{i\sigma} \right) \varphi_{i\sigma} + \left( \frac{\partial}{\partial \tau} \psi^\dagger_{i\sigma} \right) \psi_{i\sigma} \right\} - \int_0^\beta \mathcal{H}(\tau) d\tau
\]

(8)

In both expressions \(\varphi_{i\sigma}(\tau)\) and \(\psi_{i\sigma}(\tau)\) are anticommuting, complex Grassmann variables associated to the conduction and localized electrons fields, respectively, while \(\tau\) is an imaginary time and \(\beta\) the inverse absolute temperature.

We show in the Appendix that in the static, mean field like approximation the action \(A\) may be written:

\[
A = A_0 + A_K + A_{SG}
\]

(9)

with

\[
A_0 = \sum_{\omega, \sigma} \sum_{i,j} \left[ (i\omega - \beta \epsilon_0) \delta_{ij} \psi^\dagger_{i\sigma}(\omega) \psi_{i\sigma}(\omega) + (i\omega \delta_{ij} - \beta t_{ij}) \varphi^\dagger_{i\sigma}(\omega) \varphi_{j\sigma}(\omega) \right]
\]

(10)

where from Eq.(36)
\[ A_K = \frac{\beta J_k}{N} \sum_{\sigma} [\sum_{i,\omega} \psi_{i,\sigma}^+(\omega) \phi_{i,\sigma}(\omega)] [\sum_{i,\omega} \phi_{i,\sigma}^+ \psi_{i,\sigma}(\omega)] \] (11)

\[ A_{SG} = \sum_{i,j} J_{ij} S_i^z S_j^z \] (12)

and in the static approximation \[14, 17\]

\[ S_i^z = \frac{1}{2} \sum_{\sigma} \sum_{\omega} \psi_{i,\sigma}^+(\omega) \psi_{i,\sigma}(\omega) \] (13)

The sums are over fermion Matsubara frequencies \( \omega = (2n+1)\pi \).

The Kondo order is described by the complex order parameter

\[ \lambda_\sigma^+ = \frac{1}{N} \sum_{i,\omega} \langle \psi_{i,\sigma}^+(\omega) \phi_{i,\sigma}(\omega) \rangle \]

\[ \lambda_\sigma = \frac{1}{N} \sum_{i,\omega} \langle \phi_{i,\sigma}^+(\omega) \psi_{i,\sigma}(\omega) \rangle \] (14)

that in a mean field theory \[3, 13\] describes the correlations \( \lambda_\sigma^+ = \langle f_{i,\sigma}^t d_{i,\sigma} \rangle \) and \( \lambda_\sigma = \langle d_{i,\sigma}^t f_{i,\sigma} \rangle \) - Complex conjugation of Grassmann variables is defined through the transposition rule \[20\] \( (\psi^\dagger \varphi)^\dagger = \varphi^\dagger \psi \).

We show in the Appendix that standard manipulations give for the averaged free energy within a replica symmetric theory:

\[ \beta F = 2\beta J_k \lambda^2 + \frac{1}{2} \beta^2 J^2 (\overline{\lambda^2 + 2q\overline{\lambda}}) - \beta \Omega \] (15)
where
\[
\beta \Omega = \lim_{n \to 0} \frac{1}{Nn} \left\{ \int_{-\infty}^{+\infty} \prod_j N_j \, dz_j \prod_j \int_{-\infty}^{+\infty} D\varepsilon_{\alpha j} \exp \left( \sum_{\omega,\sigma} \ln |G_{ij\sigma}^{-1}(\omega)| \right) - 1 \right\} \tag{16}
\]
and the order parameters \(q, \chi\), and \(\lambda\) must be taken at their saddle point value. Here \(q\) is the SG order parameter \([14, 17]\) and the static susceptibility is \(\chi = \beta \chi\). We use the notation \(Dx = \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\).

The function \(G_{ij\sigma\alpha}(\omega)\) in Eq. (14) is the time Fourier transform of the Green’s function \(G_{ij\sigma}(\tau) = i \langle Tf_{i\sigma}(\tau)f_{j\sigma}^\dagger(0) \rangle\) for the localized electrons in the presence of random fields \(z_j\) and \(\varepsilon_{\alpha j}\) at every site, and from Eq. (57) satisfies the equation
\[
G_{ij\sigma\alpha}^{-1}(\omega) = [i\omega - \beta \varepsilon_0 - \sigma h_{j\alpha}] \delta_{ij} - \beta^2 J^2 \kappa_{ij}(\omega) \tag{17}
\]
where
\[
h_{j\alpha} = \sqrt{2q\beta J z_j} + \sqrt{2\chi \beta J \varepsilon_{\alpha j}} \tag{18}
\]
while \(\gamma_{ij}(\omega)\) is the time Fourier transform of the conduction electron Green’s function \(\gamma_{ij}(\tau) = i \langle Td_{i\sigma}(\tau)d_{j\sigma}^\dagger(0) \rangle\) and is given by
\[
\gamma_{ij}^{-1} = [i\omega - \beta \mu c] \delta_{ij} - \beta t_{ij} \tag{19}
\]

We obtained in Eq. (17) the Green’s function for the f-electrons in a Kondo lattice \([13]\), but now in the presence of a random field \(h_j\) at every site that prevents us from proceeding with the calculation. In the pure SG limit \(J_k = 0\) the Green’s function in Eq. (17) is local and the integrals in Eq. (14) reduce to a one site problem, while in the Kondo limit \(J = 0\) the random fields vanish and the integrals separate in reciprocal space. We adopt here a
decoupling approximation that is reminiscent of the model with independent "reservoirs" of electrons considered in [11]. We replace the Green's function $G_{ij\sigma}(\omega, \{h_1\ldots h_j\ldots h_{N\alpha}\})$ by the Green's functions $\Gamma_{\mu\nu\sigma}(\omega, h_j\alpha)$, $j = 1\ldots N$, of $N$ independent Kondo lattices, each one with a "uniform" field $h_j\alpha$ at every site $\mu, \nu$, by means of the approximation:

$$\ln |G_{ij\sigma}(\omega, \{h_1\ldots h_N\})| \approx \frac{1}{N} \sum_j \ln |\Gamma_{\mu\nu\sigma}^{-1}(\omega, h_j\alpha)|$$  \hspace{1cm} (20)

where $\Gamma_{\mu\nu\sigma}(\omega, h_j\alpha)$ is the f-electron Green's function for a fictitous Kondo lattice that has a uniform field $h_j\alpha$ at every site $\mu, \nu$ and satisfies the equation:

$$\Gamma_{\mu\nu\sigma}^{-1}(\omega, h_j) = [i\omega - \beta\epsilon_0 - \sigma h_j\alpha]\delta_{\mu\nu} - \beta^2 J^2_k \chi^2 \gamma_{\mu\nu}$$ \hspace{1cm} (21)

where, from Eq. (19):

$$\gamma_{\mu\nu}(\omega) = \frac{1}{N} \sum_k \frac{1}{i\omega - \beta\epsilon_k} e^{i\vec{k} \cdot \vec{R}_{\mu\nu}}$$ \hspace{1cm} (22)

Now Eq. (21) may be easily solved by a Fourier transformation with the result:

$$\ln |\Gamma_{\mu\nu\sigma}^{-1}(\omega, h_j\alpha)| = \sum_{\vec{k}} \ln |\Gamma_{\vec{k}\sigma}^{-1}(\omega, h_j\alpha)|$$ \hspace{1cm} (23)

where

$$\Gamma_{\vec{k}\sigma}^{-1}(\omega, h_j\alpha) = [i\omega - \beta\epsilon_0 - \sigma h_j\alpha] - \beta^2 J^2_k \chi^2 \frac{1}{i\omega - \beta\epsilon_k}.$$ \hspace{1cm} (24)

We may now introduce Eq. (20) and Eq. (23) in Eq. (16), the integrals over the fields separate and we obtain

$$\beta\Omega = \int_{-\infty}^{+\infty} Dz \ln \left\{ \int_{-\infty}^{+\infty} D\epsilon \exp \left( \sum_{\sigma} \frac{1}{N} \sum_{\vec{k}} S_\sigma(\vec{k}, h) \right) \right\}$$ \hspace{1cm} (25)
with

$$ S_\sigma(\mathbf{k}, h) = \sum_\omega \ln [\Gamma^{-1}_k(\omega, h)] $$

(26)

and \( h \) is given in Eq. (18), with \( z \) and \( \varepsilon \) in place of \( z_j \) and \( \varepsilon_{j\alpha} \).

The sum over the fermion frequencies is performed in the standard way by integrating in the complex plane, with the result:

$$ S_\sigma(\mathbf{k}, h) = \ln [(1 + e^{-\omega_{\sigma^+}})(1 + e^{-\omega_{\sigma^-}})] $$

(27)

where

$$ \omega_{\sigma^\pm} = \frac{1}{2} [\beta \varepsilon_k + \sigma h] \pm \left\{ \frac{1}{4} (\beta \varepsilon_k - \sigma h)^2 + (\beta J_k \lambda)^2 \right\}^{\frac{1}{2}}. $$

(28)

We consider \( \varepsilon_0 = 0 \) that corresponds to an average occupation \( \langle n_F \rangle = 1 \), per site.

Replacing sums by integrals, in the approximation of a constant density of states for the conduction band electrons, \( \rho(\epsilon) = \rho = \frac{1}{2D} \) for \(-D < \epsilon < D\), we obtain from Eq. (25) to Eq. (27) the final expression for the free energy in Eq. (15):

$$ \beta F = 2\beta J_k \lambda^2 + \frac{1}{2} \beta^2 J^2 (\chi^2 + 2q\chi) - \int_{-\infty}^{+\infty} Dz \ln \{\int_{-\infty}^{+\infty} D\epsilon e^{E(h)}\} $$

(29)

with

$$ E(h) = \frac{1}{\beta D} \int_{-\beta D}^{+\beta D} dx \ln \left\{ \frac{\cosh (x + h)}{2} + \cosh (\sqrt{\Delta}) \right\}, $$

(30)

$$ \Delta = \frac{1}{4} (x - h)^2 + (\beta J_k \lambda)^2 $$

(31)

and from Eq. (18) we have \( h = \beta J[\sqrt{2q}z + \sqrt{2\chi} \varepsilon] \). The saddle point equations for the SG order parameters are:

$$ q = \int_{-\infty}^{+\infty} Dz \left\{ \frac{D\varepsilon e^{E(h)}}{\int D\varepsilon e^{E(h)}} \right\}^2 $$

(32)
\[ \bar{\chi} = \int_{-\infty}^{+\infty} Dz \int_{\mathbb{R}} D\xi e^E \{ \int D\xi \frac{\partial}{\partial h} [e^E \frac{\partial E}{\partial h}] \} \]  

while we obtain for the Kondo order parameter \( \lambda \)

\[ 4\beta J_k \lambda \{1 - \frac{\beta J_k}{4} \int_{-\infty}^{+\infty} Dz \int_{\mathbb{R}} D\xi e^E \int D\xi e^E \times \frac{1}{\beta D} \int_{-\beta D}^{+\beta D} dx \frac{1}{\cosh \left( \frac{x}{2} \right) + \cosh \left( \frac{\sqrt{\Delta}}{\sqrt{\Delta}} \right)} \} = 0 \]  

The numerical solution of the saddle point equations as a function of \( T \) and \( J \) provides us with the phase diagram in Fig.1, that we discuss in the next section.

3. Conclusions

We study in this paper the phase transitions in a system represented by a Hamiltonian that couples the localized spins of a Kondo lattice [3, 13] with random, long range interactions, like in the SK model for a spin glass [10].

Using functional integrals techniques and a static, replica symmetric Ansatz for the Kondo and spin glass order parameters, we derive a mean field expression for the free energy and the saddle point equations for the order parameters. The Kondo and spin glass transitions are both described with the mean field like static ansatz that reproduces good results in two well known limits: when \( J_k = 0 \) we recover the exact solution for the quantum Ising spin glass [14, 18] while for \( J = 0 \) we recover the mean field results for the Kondo lattice [3, 13]. The use of the static ansatz is justified at finite
temperatures\[15\]. Numerical solution of the saddle-point equations allow us to draw the magnetic phase diagram in the $J_k vs T$ plane, for fixed value of $J$, presented in Fig.1.

Figure 1 shows three different phases. At high temperatures, the "normal" phase is paramagnetic with vanishing Kondo and spin glass order parameters, i.e. $\lambda = q = 0$. When temperature is lowered, for not too large values of the ratio $J_K / J$, a second-order transition line is found at $T = T_{SG}$ to a spin glass phase with $q > 0$ and $\lambda = 0$. Finally, for large values of the ratio $J_K / J$, we recover the "Kondo" phase with a non-zero $\lambda$ value and $q = 0$: the transition line from the paramagnetic phase to the Kondo phase for temperatures larger than $T_{SG}$ is a second-order one and occurs at a temperature very close to the one-impurity Kondo temperature $T_K$. On the other hand, the transition line from the spin-glass phase to the Kondo phase, for temperatures smaller than $T_{SG}$, is a first-order one and it ends at $J_K^c$ at $T = 0$. When the temperature is lowered, the transition temperature does not vary very much with the value of $J_K / J$; the separation between the spin-glass and the Kondo phases departs completely from the behaviour of $T_K$ and looks like the separation between the magnetic and Kondo phases when these two phases are considered\[21\]. We can also remark that we get here only "pure" Kondo or SG phases and never a mixed SG-Kondo phase with the two order parameters different from zero; this result is probably connected to the approximations used here to treat the starting Hamiltonian.

The diagram shown in figure 1 can explain the magnetic phase diagram observed above the Curie temperature for the $CeNi_{1-x}Cu_x$ for small $x$. 
values when there is a transition from a spin-glass state to a Kondo state and then to the intermediate valence compound CeNi; however, there is no experimental information on the precise nature of the SG-Kondo transition and our model cannot be checked from that point of view. There is also probably a SG-Kondo transition in the $CeCoGe_{3-x}Si_x$ alloys, but there the experimental situation is even more complicate than in the preceding case. An unsolved basic question concerns also the existence or not of a ”mixed” SG-Kondo phase in Cerium disordered alloys and this problem is worth of being studied experimentally in more detail. Thus, further experimental work is necessary, but our model yields a new striking point in the behaviour of heavy fermion disordered alloys in the vicinity of the quantum critical point.

Appendix

We present here a detailed derivation of the main equations of the paper. By introducing eqs. (1)-(3) in eq. (8) we obtain for the s-d exchange part of the action:

$$A_K = -\beta J_k \sum_i \sum_{w,w'} \sum_{\sigma} \psi_{i\sigma}^\dagger (w) \psi_{i-\sigma} (w' + \Omega) \varphi_{i-\sigma}^\dagger (w') \varphi_{i\sigma} (w - \Omega)$$

(35)

where $w = (2n + 1)\pi$ and $\Omega = 2n\pi$. In the mean field spirit we want to introduce the spatially uniform and static Kondo order parameter in eq. (14), then we take $\Omega = 0$, re-order the operators and separate the sites in eq.(35) with the introduction of a $N^{-1}$ factor, which gives:

$$A_K \approx +\frac{\beta J_k}{N} \sum_{\sigma} \sum_{i,w} \psi_{i\sigma}^\dagger (w) \varphi_{i\sigma} (w) \sum_{j,w'} \varphi_{j-\sigma}^\dagger (w') \psi_{j-\sigma} (w'),$$

(36)
that is eq. (11).

We find it convenient to introduce the Kondo order parameters in eq. (14) by means of the identity

\begin{equation}
\begin{aligned}
e^{A_k} &= \int_{-\infty}^{\infty} \Pi_\sigma d\lambda^\dagger_\sigma d\lambda_\sigma \delta[\lambda^\dagger_\sigma N - \sum_{j,w} \psi^\dagger_{j\sigma}(w)\varphi_{j\sigma}(w)] \delta \times [\lambda_\sigma N - \sum_{j,w} \varphi^\dagger_{j\sigma}(w)\psi_{j\sigma}(w)] e^{\beta J_k N[\lambda^\dagger_\sigma \lambda_\sigma + \lambda^\dagger_\sigma \lambda_\sigma]},
\end{aligned}
\end{equation}

and using the integral representation of the \(\delta\)-funtion:

\begin{equation}
\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} du e^{iu(x-x_0)}
\end{equation}

we may write the partition function by combining eq. (7) to eq. (13):

\begin{equation}
Z = \int_{-\infty}^{\infty} \Pi_\sigma d\lambda^\dagger_\sigma d\lambda_\sigma \int_{-\infty}^{\infty} \Pi_\sigma \frac{du_\sigma dv_\sigma}{(2\pi)^2} N \sum_\sigma \left\{ \beta J_k \lambda^\dagger_\sigma \lambda_\sigma - i[\lambda^\dagger_\sigma u_\sigma + \lambda_\sigma v_\sigma] \right\} Z_{\text{eff}}
\end{equation}

where

\begin{equation}
Z_{\text{eff}} = \int D(\psi^\dagger \psi) \int D(\varphi^\dagger \varphi) e^{A_0 + A_{SG}} \times e^{\sum_\sigma \left[ i[u_\sigma \sum_{j,w} \varphi^\dagger_{j\sigma}(w)\psi_{j\sigma}(w) + u_\sigma \sum_{j,w} \psi^\dagger_{j\sigma}(w)\varphi_{j\sigma}(w)] \right]}
\end{equation}

The saddle point values of \(\lambda_\sigma, \lambda^\dagger_\sigma, u_\sigma, u^\dagger_\sigma\) are obtained by extremizing the exponent in eq. (40):

\begin{align*}
\beta J_k \lambda^\dagger_{-\sigma} &= iv_\sigma \\
\beta J_k \lambda_{-\sigma} &= iu_\sigma
\end{align*}
\[
\lambda^\dagger_\sigma = \frac{1}{N} \sum_{j,w} \langle \psi^\dagger_{j\sigma}(w) \varphi_{i\sigma}(w) \rangle \\
\lambda_\sigma = \frac{1}{N} \sum_{j,w} \langle \varphi^\dagger_{i\sigma}(w) \psi_{j\sigma}(w) \rangle
\] (41)

where \( \langle \ldots \rangle = \int D(\psi^\dagger \psi) D(\varphi^\dagger \varphi) e^{A_{eff}}(\ldots) \) from eq.(40). Introducing the saddle point values of eq.(41) into eq.(39), we obtain:

\[
Z = e^{-2N\beta J_k} Z_{eff}.
\] (42)

From eq.(39), \( Z_{eff} \) is now the integral of a quadratic form in the \( \varphi^\dagger, \varphi \) variables, that can be integrated out to give:

\[
Z_{eff} = Z^0_d Z_{SG}
\] (43)

where \( Z^0_d \) is the partition function of the free conducting electrons:

\[
\ln (Z^0_d) = 2 \sum_w \log |\gamma^{-1}_{ij}(w)|,
\] (44)

and

\[
\gamma^{-1}_{ij}(w) = iw \delta_{ij} - \beta t_{ij},
\] (45)

is the inverse Green’s function for the d-electrons. The quantity \( Z_{SG} \) in eq.(43) is the partition function for the localized f-electrons:

\[
Z_{SG} = \int D(\psi^\dagger \psi) e^{u_{i,j} \sum_{i,j} g^{-1}_{ij}(w) \psi^\dagger_{i\sigma}(w) \psi_{j\sigma}(w)} + A_{SG}
\] (46)

where the inverse Green’s function for the localized, non-interacting f-electrons is now modified by the Kondo interaction:

\[
g^{-1}_{ij}(w) = (iw - \beta \varepsilon_0) \delta_{ij} - \beta^2 J^2_k \lambda^\dagger \lambda \gamma_{ij}(w)
\] (47)
and $A_{SG}$ is given in eq. (12).

The interesting part of the free energy is given by:

$$\beta F = -\frac{1}{N} \langle \ln (Z/Z_0) \rangle$$  \hfill (48)

where the double bracket indicates a configurational average over the random variables $J_{ij}$, with the distribution probability in eq. (16). Using the replica method we obtain from eq. (42) and eq. (43):

$$\beta F = 2\beta J_k \lambda^\dagger \lambda - \lim_{n \to 0} \frac{1}{Nn} [Z_n(SG) - 1]$$  \hfill (49)

where $\alpha = 1 \ldots n$ is the replica index and:

$$Z_n(SG) = \langle \langle Z_n^{SG} \rangle \rangle = \int \prod_{\alpha}^n D(\psi^\dagger \psi) \exp \{ \sum_{w,\sigma,i,j} g_{ij}^{-1}(w) \sum_{\alpha} \psi^\dagger_{i\sigma\alpha}(w) \psi_{j\sigma\alpha}(w) \} \times \prod_{i,j} \langle \langle e^{\beta J_{ij}} \sum_{\alpha} S_{i\alpha} S_{j\alpha} \rangle \rangle$$  \hfill (50)

The operators $S_{i\alpha}$ are bilinear combinations of $\psi^\dagger_{i\sigma\alpha}(w)$, $\psi_{i\sigma\alpha}(w)$ from eq. (13), then after performing the average in eq. (50) we must use standard manipulations with gaussian identities [16,17] to linearize the exponent in eq. (50). We obtain:

$$Z_n(SG) = \int \prod_{\alpha,\beta} dq_{\alpha\beta} e^{-\frac{1}{2} (\beta J)^2 N \sum_{\alpha,\beta} q_{\alpha\beta}^2} \Lambda(\{q_{\alpha\beta}\})$$  \hfill (51)

where

$$\Lambda(\{q_{\alpha\beta}\}) = \int D(\psi^\dagger \psi) \exp \{ \sum_{i,j} \sum_{w,\sigma,\alpha} g_{ij}^{-1}(w) \psi^\dagger_{i\sigma\alpha}(w) \psi_{j\sigma\alpha}(w) + \beta^2 J^2 \sum_{\alpha,\beta} q_{\alpha\beta} \sum_i S_{i\alpha} S_{j\alpha} \}$$  \hfill (52)
We obtain for $Z_n(SG)$ at the replica symmetric saddle point:

$$q_{\alpha \neq \beta} = q$$

$$q_{\alpha \alpha} = q + \chi$$

(53)

$$Z_n(SG) \approx e^{-\frac{1}{2}[(\beta J)^2 N (\chi^2 + 2q\chi)]} \Lambda(q, \chi)$$

(54)

where

$$\Lambda(q, \chi) = \int_{-\infty}^{\infty} \prod_j Dz_j \prod_\alpha \int_{-\infty}^{\infty} \prod_j D\xi_{\alpha j} I_\alpha(q, \chi, \{z_j\}, \{\xi_{\alpha j}\})$$

(55)

and

$$I_\alpha(q, \chi, \{z_j\}, \{\xi_{\alpha j}\}) = \int D(\psi_{\alpha}^\dagger \psi_{\alpha}) \exp \left\{ \sum_{w, \sigma} \sum_{i,j} G_{ij\sigma\alpha}^{-1}(w) \psi_{i\sigma\alpha}^\dagger (w) \psi_{j\sigma\alpha} (w) \right\}$$

$$= e^{\sum_{w, \sigma} \ln |G_{ij\sigma\alpha}^{-1}(w)|},$$

(56)

where

$$G_{ij\sigma\alpha}^{-1}(w) = g_{ij}^{-1}(w) - \delta_{ij}\sigma[\sqrt{2q}\beta J z_j + \sqrt{2\chi}\beta J \xi_{\alpha j}].$$

(57)

Introducing Eq.(56) and Eq.(55) in to Eq.(54), we obtain from Eq.(49) the expression for the free energy in Eq.(13) of the main text.
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Figure captions

**Figure 1:** Phase diagram in the $T - J_k$ plane as a function of $T/J$ and $J_k/J$ for fixed $J = 0.05D$, where D is the conduction bandwidth. The dotted line represents the “pure” Kondo temperature $T_k$. 
