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SPIN-GLASS TRANSITION IN KONDO LATTICE WITH QUENCHED DISORDER

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We use the Popov – Fedotov representation of spin operators to construct an effective action for a Kondo lattice model with quenched disorder at finite temperatures. We study the competition between the Kondo effect and frozen spin order in Ising-like spin glass. We present the derivation of new mean-field equations for the spin-glass order parameter and analyze the effects of screening of localized spins by conduction electrons on the spin-glass phase transition.

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One of the most interesting questions of physics of heavy-fermion compounds is the competition between Kondo screening of localized spins by conduction electrons (CE) and ordering of these spins due to Ruderman – Kittel – Kasuya – Yosida (RKKY) interaction (see, e.g. [1]). The screening is attributed to the Kondo effect - the resonance scattering of an electron on a magnetic atom with simultaneous change of the spin projection. In dilute alloys such a scattering results in the sharp resonance at Fermi level with characteristic energy width $\epsilon \sim T_K \sim \epsilon_F \exp(-\alpha^{-1})$, where T_K is Kondo temperature, J is a coupling constant, ρ is a density of states of CE on the Fermi level and $\alpha = \rho J$. As it was recently discussed (see, e.g. [2, 3]), such a competition can be responsible for the Non-Fermi-liquid behaviour observed in some heavy fermion compounds. Most of such a materials share two characteristics: proximity to magnetic region of appropriate phase diagram (usually temperature vs. pressure or chemical composition), and disorder due to chemical substitution. In many respects the concentrated Kondo systems, namely the lattice of magnetic atoms interacting with CE "bath" (Kondo lattice (KL)) show striking similarities with dilute Kondo systems. The Kondo temperature in these systems is a characteristic crossover temperature at which spins transform their local properties to some itinerant Fermi-liquid behaviour determining low temperature regime of heavy-fermion compounds. Non-Fermi-liquid behaviour in heavy-fermion system is mainly attributed then to reducing the Kondo temperature possibly even suppressing it to zero. In turn, magnetic or spin glass (SG) transition can also be suppressed due to interplay between Kondo scattering and spin-spin interaction. Thus, such an interplay can result in quantum phase transition [2] when both Kondo and magnetic temperatures are equal to zero at some finite doping. The role of chemical substitution in this case is to "tune" the Fermi level of metallic system providing sharp Kondo resonance.

The problem of competition between RKKY and Kondo interaction in clean system was studied for the first time by Doniach [4] in the "Kondo necklace" model. The transition typically takes place between a paramagnetic metal and magnetic (usually AFM) metal. In this case there are two possibilities: the compound will have long range magnetic order when the RKKY interaction is sufficiently large compared with the Kondo interaction, or the compound will be paramagnetic due to the quenching of magnetic moments of the rare earth atoms and the ground state has the features of Kondo-singlet state. Nevertheless, in the region $T^M_{\rm RKKY} \sim T_K$ the competition between magnetic and Kondo interaction results in dramatically change of "naive" Doniach diagram (see [5]). Namely, both Kondo and magnetic temperatures are strongly suppressed and spin-liquid state (e.g of Resonance Valence Bond type [6]) occurs.

The goal of this letter is to present some results concerning the competition between Kondo effect and Ising-like SG transition which is in many aspects similar to the magnetic instability. We study mechanisms of suppressing the SG transition and effects of screening in disordered environment. In this paper we consider the high temperature regime of KL model. We leave aside the issue of the ground state properties and especially the question whether Non-Fermi-liquid behaviour is a generic feature of vicinity to quantum phase transition for future publication.

The Hamiltonian of KL model with additional quenched randomness of exchange interaction between localized spins is given by

$$H_{KL} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_i \left(\mathbf{s}_i \mathbf{S}_i + \frac{1}{4} n_i N_i \right) - \sum_{ij} I_{ij} \left(S^z_i S^z_j + \lambda S^+_i S^-_j \right). \qquad (1)$$

The system under consideration is a periodic lattice of magnetic atoms modeled by f – orbitals interacting with metallic background spin density operator $\mathbf{s}_i = \frac{1}{2} c^\dagger_{i\alpha} \sigma_{\alpha\alpha'} c_{i\alpha'}$. The first term in the Hamiltonian (1) describes kinetic energy of CE, the second stands for Kondo coupling ($J > 0$). We denote $n_i = \sum_\sigma c^\dagger_{i,\sigma} c_{i,\sigma}$ as the CE density operator. The identity $N_i = 1$ describes the half-filled f-electron shell. Quenched independent random variables I_{ij} with distribution $P(I_{ij}) \sim \exp(-I^2_{ij} N/2I^2)$ stand for direct spin-spin interaction [7]. We assume that this random interaction is of RKKY origin [1)], namely, for d-dimensional system $I \sim \alpha^2 \epsilon_F l^{-d}$, l is a lattice constant in magnetic sublattice. The magnetic effects can also be included in our approach by introducing nonzero standard deviation $\Delta I = \bar{I}_{\rm RKKY}$ into the distribution $P(I_{ij})$, which, in turn, can result in the additional competition between SG and AFM (or, rarely FM) states. For simplicity we neglect these effects in present letter concentrating on the interplay between Kondo interaction and effects of bond disorder. Since indirect RKKY interaction through CE is mostly determined by "fast" electrons with characteristic energies $\epsilon \sim \epsilon_F \gg T_K$ we neglect also the Kondo renormalizations of RKKY exchange.

As it well-known for a long time, the spin $S = 1/2$ matrices can be exactly replaced by bilinear combination of Fermi operators

$$S^z_i = \frac{1}{2}(f^\dagger_{i\uparrow} f_{i\uparrow} - f^\dagger_{i\downarrow} f_{i\downarrow}), \quad S^+_i = f^\dagger_{i\uparrow} f_{i\downarrow}, \quad S^-_i = f^\dagger_{i\downarrow} f_{i\uparrow}.$$

Nevertheless, most of fermionic representations of spin are not free of constraint problem. For this reason, the dimensionality of space in which these operators act is always greater

[1)] It has been pointed out in [8], that the presence of nonmagnetic impurities makes RKKY interaction a random interaction even in the case of regular arrangement of magnetic moments.

than the dimensionality of the spin matrices. Elimination of unphysical states is a serious problem which makes the diagrammatic techniques quite complicated. Moreover, in most cases, the analytical continuation of Feynman diagrams becomes extremely uneasy. To avoid the main part of difficulties related to constraint, the new representation for spin operators was proposed in well-forgotten paper of Popov and Fedotov [9]. In this representation the partition function of the problem containing spin operators (H_S) then can be easily expressed in terms of new fermions with imaginary chemical potential (H_S^f):

$$Z_S = \mathrm{Tr}\; e^{-\beta H_S} = i^N \mathrm{Tr}\; \exp\{-\beta(H_S^f + i\pi N_f/2\beta)\}, \quad N_f = \sum_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma}, \quad \beta = 1/T.$$

As a result, there is no constraint, the unphysical states are eliminated and standard Matsubara – Abrikosov – Gor'kov diagrammatic technique is obtained [9 – 11].

We sketch our derivation of the effective action and of resulting mean field equations for KL model in order to explicit the approximations made and the physics underlying these approximations. To construct the path integral representation for the partition function, the new Grassmann variables $c_{i\sigma}^\dagger \to \bar{\Psi}_{i\sigma}$, $c_{i\sigma} \to \Psi_{i\sigma}$ for CE with chemical potential μ and $f_{i\alpha}^\dagger \to \bar{a}_{i\alpha}$, $f_{i\alpha} \to a_{i\alpha}$ for Popov – Fedotov spin operators ($S = 1/2$) are introduced. The Euclidean action for the KL model is given by

$$\mathcal{A} = \int_0^\beta d\tau \left(\sum_{i\alpha} \left[\bar{\Psi}_{i\alpha}(\tau)(\partial_\tau + \mu)\Psi_{i\alpha}(\tau) + \bar{a}_{i\alpha}(\tau)(\partial_\tau - i\pi T/2)a_{i\alpha}(\tau) \right] - H_{int}(\tau) \right), \quad (2)$$

where the generalized Grassmann fields satisfy the following boundary conditions: $\Psi_{i\alpha}(\beta) = -\Psi_{i\alpha}(0)$, $\bar{\Psi}_{i\alpha}(\beta) = -\bar{\Psi}_{i\alpha}(0)$, $a_{i\alpha}(\beta) = i a_{i\alpha}(0)$, $\bar{a}_{i\alpha}(\beta) = -i\bar{a}_{i\alpha}(0)$.

In this paper we consider $\lambda = 0$ which corresponds to Sherrington – Kirkpatrik [12] spin-glass model. Such an anisotropy of RKKY interaction can be associated e.g. with lattice geometry. In the case of Ising-like model the dynamical fluctuations in spin subsystem appear only due to interaction with conduction electrons and in high temperature regime $T \sim T_{\mathrm{SG}}$ can be neglected. To study the influence of Kondo-scattering on SG transition temperature T_{SG} we use standard replica trick $\Psi_i(\tau) \to v_i^a(\tau)$, $a_i(\tau) \to \varphi_i^a(\tau)$, $a = 1, ..., n$. Then, the free energy of the model can be calculated (see, e.g. [13]) by taking the formal limit $n \to 0$ in

$$< Z^n >_{av} = \prod \int dI_{ij} P(I_{ij}) \prod D[\varphi_{i,\sigma}^a v_{i,\sigma}^a] \exp\left(\mathcal{A}_0[v^a, \varphi^a] - \int_0^\beta d\tau H_{int}(\tau) \right), \quad (3)$$

where $\mathcal{A}_0$ is corresponding to noninteracting fermions.

As we already mentioned, for considering the competition between Kondo scattering and trend of disorder we assume that the magnetic temperature $T_{\mathrm{RKKY}}^M \ll T^*$, where T^* stands for characteristic temperature corresponding to the Kondo temperature in a lattice. This assumption allows one to decouple the Kondo interaction term $H_i^K = -\frac{J}{2}\bar{v}_{i,\sigma}^a \varphi_{i,\sigma}^a \bar{\varphi}_{i,\sigma'}^a v_{i,\sigma'}^a$ in each site by the replica-dependent Hubbard – Stratonovich field ψ_i^a [14]. Performing the average over random potential in Eq.(3) results in

$$< Z^n >_{av} = \prod \int D[v^a, \varphi^a, \psi^a] \exp\left(\mathcal{A}_0 + \frac{I^2}{4N}\mathrm{Tr}[X^2] + \right.$$

$$\left. + \int_0^\beta d\tau \sum_{i,a,\sigma} \left\{ \psi_i^a \bar{v}_{i\sigma}^a \varphi_{i\sigma}^a + \psi_i^{a*} \bar{\varphi}_{i\sigma}^a v_{i\sigma}^a - \frac{2}{J}|\psi_i^a|^2 \right\} \right) \quad (4)$$

with

$$X^{ab}(\tau,\tau') = \sum_i \sum_{\sigma,\sigma'} \bar{\varphi}^a_{i,\sigma}(\tau)\sigma\varphi^a_{i,\sigma}(\tau)\bar{\varphi}^b_{i,\sigma'}(\tau')\sigma'\varphi^b_{i,\sigma'}(\tau').$$

The next step is to perform the Gaussian integration over the replica-dependent Grassmann field v^a describing CE and to decouple the eight-fermion term $\mathrm{Tr}[X^2]$ with the help of Q matrices (see details in [10]). As a result, the partition function is given by:

$$< Z^n >_{av} = \int D[Q] \exp\left(-\frac{1}{4}(\beta I)^2 N \mathrm{Tr}[Q^2] + \right.$$

$$\left. + \sum_i \ln\left\{\prod \int D[\varphi^a,\psi^a] \exp\left[\sum_a \sum_{\{\omega\}} \bar{\varphi}^a_{i\sigma}\mathcal{G}_a^{-1}\varphi^a_{i\sigma} + \frac{1}{2}(\beta I)^2 \mathrm{Tr}[QX]\right]\right\}\right), \qquad (5)$$

where $\mathcal{G}^{-1}$ is inverse Green function for Popov – Fedotov fermions depending on Matsubara frequences $\omega_n = 2\pi T(n+1/4)$ (see details in [9])

$$\mathcal{G}_a^{-1} = i\omega_{n_1}\delta_{\omega_{n_1},\omega_{n_2}} - T\sum_\epsilon \psi_i^{a*}(\epsilon_l+\omega_{n_1})G_0(-i\nabla_i,\epsilon_l)\psi_i^a(\epsilon_l+\omega_{n_2}) \qquad (6)$$

and $G_0(-i\nabla,\epsilon_l) = (i\epsilon_l - \varepsilon(-i\nabla)+\mu)^{-1}$ stands for CE Greens function, $\epsilon_l = 2\pi T(l+1/2)$.

We are still left with a term of fourth order residing in $\mathrm{Tr}[QX]$ and can not evaluate the Grassmann integral directly. Consequently, the second decoupling is needed. To perform it, we stress that we do not intend to deal with dynamical behaviour here confining ourselves by high temperature regime in the vicinity of SG transition such that the lowest Matsubara frequency is sufficient. Assuming this and recalling that the spatial fluctuations are suppressed by the choice of infinite range interaction [12], one can consider Q as a constant saddle point matrix under condition $Q = Q^T$. The elements of this matrix will later be determined self-consistently from the saddle point condition. Assuming that the elements of Q are $Q^{aa}_{SP} = \tilde{q}$ and $Q^{a\neq b}_{SP} = q$ one can decouple the $\mathrm{Tr}[QX]$ term by introducing replica-independent z and replica-dependent y^a fields and map KL problem with disorder onto effective one-site interacting spin system coupled with external local replica-dependent magnetic field:

$$< Z^n >_{av} = \exp\left(-\frac{1}{4}(\beta I)^2 N(n\tilde{q}^2 + n(n-1)q^2) + \right.$$

$$\left. + \sum_i \ln\left[\prod \int D[\varphi^a,\psi^a] \int_z^G \int_{y^a}^G \exp(\mathcal{A}[\varphi^a,\psi^a,y^a,z])\right]\right), \qquad (7)$$

where $\int_z^G f(z)$ denotes $\int_{-\infty}^{\infty} dz/\sqrt{2\pi}\exp(-z^2/2)f(z)$,

$$\mathcal{A}[\varphi^a,\psi^a,y^a,z] = \sum_{a,\sigma} \bar{\varphi}^a_\sigma\left[\mathcal{G}_a^{-1} - \sigma H(y^a,z)\right]\varphi^a_\sigma - \frac{2}{J}\sum_\omega |\psi^a(\omega)|^2 \qquad (8)$$

and $H(y^a,z) = I\sqrt{q}z + I\sqrt{\tilde{q}-q}y^a$ is effective local magnetic field. Note, that the variable $q = < S_i^a S_i^b >$ corresponds to Edwards – Anderson SG order parameter when the limit $n \to 0$ is taken. Nevertheless, the diagonal element $\tilde{q}$ can be set neither zero nor one, in contrast to the classical Ising glass theory because of dynamical effects due to the interaction with CE "bath". To take into account this interaction we include replica dependent magnetic field into bare Green's function $\mathcal{G}^a_{0\sigma} = (i\omega_n - \sigma H(y^a, z))^{-1}$ and perform the integration over Popov – Fedotov Grassmann variables with the help of the expression

$$\mathrm{Tr}\ln\left(\mathcal{G}_a^{-1} - \sigma H\right) = \ln\left(2\cosh(\beta H)\right) + \mathrm{Tr}\sum_{m=1}^{\infty}\frac{(-1)^{m+1}}{m}\left(\mathcal{G}^a_{0\sigma}(H)\Sigma(\psi^a)\right)^m \qquad (9)$$

where $\Sigma(\psi^a) = -T\sum_\epsilon \psi_i^{a*}(\epsilon+\omega_{n_1})G_0(-i\nabla_i,\epsilon)\psi_i^a(\epsilon+\omega_{n_2})$ depends on the variable ψ "responsible" for Kondo interaction. Calculating the first term in expansion (9) one gets the following expression for the effective "bosonic" action in the one loop approximation

$$\mathcal{A}[\psi^a, H] = \ln\left(2\cosh(\beta H(y^a,z))\right) - \frac{2}{J}\sum_n\left[1 - J\Pi(i\Omega_n, H(y^a,z))\right]|\psi^a|^2 - O(|\psi^a|^4). \quad (10)$$

The polarization operator Π in the limit $T, H \ll \epsilon_F$ is given by:

$$\Pi(i\Omega_n, H) = -\beta^{-1}\sum_{n,\mathbf{k},\sigma} G_0(\mathbf{k}, i\epsilon_n + i\Omega_n)\mathcal{G}_{0\sigma}(i\epsilon_n, H) \overset{\Omega_n=0}{\longrightarrow}$$

$$\overset{\Omega_n=0}{\longrightarrow} \rho(0)\left[\ln\left(\frac{\epsilon_F}{\sqrt{H^2+\pi^2\beta^{-2}/4}}\right) + \frac{\pi}{2\cosh(\beta H)} + O\left(\frac{H^2}{\epsilon_F^2}\right)\right]. \qquad (11)$$

When $H = 0$, the coefficient in front of $|\psi^a|^2$ in (10) changes its sign at $T^* \sim \sim \epsilon_F\exp(-\alpha^{-1})$. This is a manifestation of single-impurity Kondo effect (see, e.g. [14, 15]).

One can now perform the Gaussian integration over ψ^a fields in (7) by stationary phase method

$$\int D[\psi^a]\exp(\delta\mathcal{A}[\psi^a]) = \exp\left(-\mathrm{Tr}\ln\left[1 - J\Pi(i\Omega_n, H(y^a,z))\right]\right).$$

After the last step, namely integration over replica dependent field y^a the limit $n \to 0$ can be taken. The free energy per site $f = \beta^{-1}\lim_{n\to 0}(1 - \langle Z^n\rangle_{av})/nN$ is given by

$$\beta f(\tilde{q}, q) = \frac{1}{4}(\beta I)^2\left(\tilde{q}^2 - q^2\right) - \int_z^G \ln\left(\int_y^G \frac{2\cosh(\beta H(y,z))}{1 - J\Pi(0, H(y,z))}\right). \qquad (12)$$

New equations for q, $\tilde{q}$ are determined by conditions $\partial f(\tilde{q},q)/\partial\tilde{q} = 0$, $\partial f(\tilde{q},q)/\partial q = 0$:

$$\frac{1}{2}(\beta I)^2\tilde{q} = \int_z^G \frac{\partial\ln\mathcal{F}}{\partial\tilde{q}}, \quad \frac{1}{2}(\beta I)^2 q = -\int_z^G\frac{\partial\ln\mathcal{F}}{\partial q}, \quad \mathcal{F} = \int_y^G\frac{2\cosh(\beta H(y,z))}{1 - J\Pi(0, H(y,z))}. \qquad (13)$$

The Eq. (12), (13) contain the key result of the paper. They represent the solution of KL problem with quenched disorder on a replica symmetrical level. To demonstrate some interesting physical effects, described by these equations let us consider the case $T \sim T_{SG} \geq T^*$ (Kondo high temperature limit). Since $H(y^a, z)$ is dynamical variable, we break the parametrical region of H to several pieces. First, when $H \gg T, T^*$, the logarithm in (11) is cut by H and there are no temperature dependent Kondo corrections to the mean field equations. This corresponds to the limit $T^* \ll I$ providing frozen spins and preventing them from resonance scattering [2]. Nevertheless, when $T^* \sim I$, the region $H \leq T$ becomes very important. We calculate $\mathcal{F}$ expanding the r.h.s of (12) up to $(H/T)^2$

$$\ln(C\mathcal{F}_{z,\tilde{q},q}) = -\frac{1}{2}\ln\left(1+\gamma u^2 r^2\right) + \frac{u^2}{2}\frac{r^2 - q\gamma z^2}{1+\gamma u^2 r^2} + \ln\left[\cosh\left(\frac{uz\sqrt{q}}{1+\gamma u^2 r^2}\right)\right]. \qquad (14)$$

We use the following short-hand notations: $u = \beta I$, $\gamma = 2c/\ln(T/T^*)$, $r^2 = \tilde{q} - q$, $C = 2c\alpha/\gamma$ with $c = \pi/4 + 2/\pi^2 \sim 1$. We note again that when $J = 0$, which corresponds to the absence of Kondo interaction,

$$\mathcal{F}(z,\tilde{q},q) = \exp\left(\frac{1}{2}(\beta I)^2(\tilde{q}-q)\right)\cosh(\beta I z\sqrt{q})$$

and standard Sherrington – Kirkpatrik equation [12] takes place, providing, e.g. an exact identity $\tilde{q} = 1$.

In the vicinity of the phase transition point Eq.(13) reads:

$$\tilde{q} = 1 - \frac{2c}{\ln(T/T^*)} + O\left(\frac{1}{\ln^2(T/T^*)}\right),$$

$$q = \int_z^G \tanh^2\left(\frac{\beta I z\sqrt{q}}{1 + 2c(\beta I)^2(\tilde{q}-q)/\ln(T/T^*)}\right) + O\left(\frac{q}{\ln^2(T/T^*)}\right) \qquad (15)$$

These equations describe a second-order transition in SG Ising-like Sherrington – Kirkpatrik [3] system coupled with CE "bath" in the presence of Kondo-scattering. Taking the limit $q \to 0$ we estimate the temperature of SG transition $(T_{SG}/I)^2 = 1 - 4c/\ln(T_{SG}/T^*) - \ldots < 1$. Thus, the Kondo-scattering resonance results in depressing of SG transition temperature due to the screening effects in the same way as magnetic moments and one-site susceptibility are screened in single-impurity Kondo problem [15]. This screening shows up at large time scale $t \geq 1/T^*$ and affects both diagonal and nondiagonal elements of Q matrix. Moreover, $\tilde{q}$ becomes partially screened well above the SG transition point. Recalling that $H \sim Iy\sqrt{\tilde{q}}$ one can see that our assumption $H/T \leq 1$ is consistent with Eq.(15) even if $T \sim T_{SG}$. It is necessary to note, that a growing SG order parameter in Eq.(10-11) suppresses Kondo effect as well as providing a broader validity domain for Eq.(15). We leave the self-consistent analysis of Eq.(12), (15) for a future detailed publication.

In conclusion, we have considered the Kondo high temperature limit (in a sence of $T > T^*$) of a KL model with quenched disorder. We derived new mean field equations for SG transition in the presence of strong Kondo-scattering and have shown that the partial screening of both diagonal and nondiagonal elements of Q matrix takes place. As a result, the temperature of SG transition is strongly suppressed when Ising and Kondo interactions are of the same order of magnitude.

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[2] We also note, that when $T^* \gg I$ the SG transition does not happen.

[3] When an Ising system described by (1) with nearest neighbor interaction is treated with mean field theory, equations identical to (13) are obtained with $\sqrt{Z}I$ replacing I, where Z is average number of neighbors.

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