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Spin correlations in Kondo lattices

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Abstract

Effective action and free energy functional is derived for nearly antiferromagnetic (AFM) Kondo lattice that takes into account the interplay between the nonlocal modes of AFM and spin-liquid type and local Kondo-like interaction. The modified Doniach's diagram is constructed on this basis.

Keywords: Kondo lattice; Spin liquid; Spin glass

Competition between the one-site Kondo-type correlations and the indirect inter-site exchange is the source of heavy fermion phenomenon and unconventional antiferromagnetism in Kondo lattice (KL). Kondo effect with a characteristic energy scale T_K tends to screen the local moments, whereas the indirect inter-site exchange I binds these moments into antiferromagnetic (AFM) collective state [1]. The trend of spin-liquid (SL) ordering is the third type of correlation which modifies essentially the magnetic phase diagram of KL in a critical region $T_K \sim I$ of Doniach's diagram [2]. All the above theories appeal to the mean-field approximations that violate the local gauge invariance both in Kondo and SL channel. In this paper, a mean-field description of transitions from a paramagnetic state to the correlated spin states in KL does not violate the local constraint for spin-fermion operators. The Popov–Fedotov representation of spin operators [3] that satisfies the local constraint is used in the construction of generalized Doniach's diagram where there exists a mutual influence of Kondo, AFM, and SL correlations.

The Hamiltonian of the KL model is $H = \sum_{\mathbf{k}\sigma} \varepsilon_k n_{\mathbf{k}\sigma} + (J/4)\sum_{\mathbf{j}}(4\mathbf{S_j s_j} + N_{\mathbf{j}} n_{\mathbf{j}})$. Here $n_{\mathbf{j}} = \sum_\sigma c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma}$ and $\mathbf{s_j} = \sum_\sigma \frac{1}{2} c^\dagger_{\mathbf{j}\sigma}\tau_{\sigma\sigma'} c_{\mathbf{j}\sigma'}$, where τ are the Pauli matrices and $c_{\mathbf{j}\sigma} = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}\exp(\mathrm{i}\mathbf{kR}_j)$. To include in the Doniach's diagram all the relevant spin correlations, the spin part of free energy $\mathsf{F}_s(T)$ is calculated in a critical region of temperatures slightly exceeding all the characteristic energy scales of the KL, i.e. T_N (Neel temperature), T_K (Kondo temperature) and T_s (the temperature of cross-over to the SL state). Integrating the high-energy states $\sim\varepsilon_F$ in conduction band results in the appearance of indirect RKKY exchange $H' = \sum_{\mathbf{jl}} I_{jl}(\mathbf{S_j S_l})$. The same renormalization procedure results in the enhancement of sf-exchange constant $J \to \tilde{J} \approx \varepsilon_F/\ln(T/T_K)$ [4].

The spin $S = \frac{1}{2}$ operators are represented as combinations of fermion operators $S^z_{\mathbf{j}} = (f^\dagger_{\mathbf{j}\uparrow} f_{\mathbf{j}\uparrow} - f^\dagger_{\mathbf{j}\downarrow} f_{\mathbf{j}\downarrow})/2$, $S^+_{\mathbf{j}} = f^\dagger_{\mathbf{j}\uparrow} f_{\mathbf{j}\downarrow}$, $S^-_{\mathbf{j}} = f^\dagger_{\mathbf{j}\downarrow} f_{\mathbf{j}\uparrow}$. These operators should obey the constraint $N_{\mathbf{j}} = \sum_\sigma f^\dagger_{\mathbf{j}\sigma} f_{\mathbf{j}\sigma} = 1$. According to Popov and Fedotov [3], the constraint is taken into account by adding a Lagrange term with a fixed imaginary chemical potential $-\mathrm{i}\pi T/2$ to the Hamiltonian without changing the spin part of partition function Z. The latter is represented in terms of path integral, and the effective action A in this integral is given by

$$\mathsf{A} = \sum_{n\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\varepsilon_n) G_n^{-1} c_{\mathbf{k}\sigma}(\varepsilon_n) + \sum_{mj\sigma} \bar{f}_{\mathbf{j}\sigma}(\omega_m) D_m^{-1} f_{\mathbf{j}\sigma}(\omega_m) - \frac{2}{\tilde{J}}\mathrm{Tr}|\phi|^2 - \mathrm{Tr}\frac{1}{I_{\mathbf{q}}}\mathbf{Y_q Y_{-q}} - \frac{1}{I}\mathrm{Tr}\, W_{\mathbf{Rr}} W_{\mathbf{R},-\mathbf{r}} - \mathrm{Tr}\, \bar{f}_{j\sigma}\phi_j G_0(\mathbf{r})\bar{\phi}_l f_{l\sigma}.$$

Here Green's functions (GF) for bare quasiparticles are $G_n^{-1}(k) = \mathrm{i}\varepsilon_n - \varepsilon_k + \mu$, $D_m^{-1} = \mathrm{i}\omega_m$, and the Matsubara frequencies are $\omega_m = 2\pi T(m + \frac{1}{4})$ for spin semi-fermions and $\varepsilon_n = 2\pi T(n + \frac{1}{2})$ for conduction electrons. The spin

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correlations in the inter-site RKKY term are treated in terms of vector Bose fields $\mathbf{Y}$ (AFM mode) and scalar field W (SL RVB mode). $\mathbf{R} = (\mathbf{R}_j + \mathbf{R}_l)/2$ and $\mathbf{r} = \mathbf{R}_j - \mathbf{R}_l$ are the coordinates of RVB field. Two modes result in a free energy with two local minima reflecting the instabilities against AFM at vector $\mathbf{Q}$ and homogeneous SL. Near these points one can pick up the classic part N of Neel field and use the eikonal approximation for SL, $\mathbf{Y} = (I_{\mathbf{q}}/2\sqrt{T})\mathsf{N}\delta_{\mathbf{q},\mathbf{Q}} + \tilde{\mathbf{Y}}_{\mathbf{q}}$, $W_{\mathbf{R},\mathbf{r}} = I\Delta(\mathbf{r})\exp(i\mathbf{r}\cdot\mathbf{A}(\mathbf{R}))$. Kondo field ϕ screens the Neel moment N and enhances SL correlations. Expanding the free energy around the minima, the self-consistent equations for N and Δ are obtained:

$$\mathsf{N} = \tanh\left(\frac{I_{\mathbf{Q}}\mathsf{N}}{2T}\right)\left[1 - \frac{\delta}{\ln(T/T_{\mathrm{K}})}\frac{\cosh^2(I_{\mathbf{Q}}\mathsf{N}/2T)}{\cosh^2(I_{\mathbf{Q}}\mathsf{N}/T)}\right],$$

$$\Delta = -\sum_{\mathbf{q}} v(\mathbf{q})\left[\tanh\left(\frac{I(\mathbf{q})\Delta}{T}\right) + a_{\mathrm{sl}}\frac{I_{\mathbf{q}}\Delta}{T\ln(T/T_{\mathrm{K}})}\right],$$

$$v(\mathbf{q}) = I_{\mathbf{q}}/I.$$

The results of numerical solution of these equations are presented in Fig. 1. Based on these results the following scenario of unconventional AFM in KL can be proposed. In a critical region of Doniach's diagram marked by hatched line, Kondo screening suppresses Neel temperature, T_{N} (upper insert) but enhance T_{sl}. As a result, SL order increases *above* T_{K} and magnetic order can be realized as a localized magnetism with reduced moments ($T_{\mathrm{N}} > T_{\mathrm{sl}}$) or magnetically ordered SL ($T_{\mathrm{sl}} > T_{\mathrm{N}}$).

Proximity of three characteristic temperatures, T_{K}, T_{sl} and T_{N} means that only one of them determines the local minimum of the free energy, and this is, in fact T_{N}, whereas T_{sl} and T_{K} are merely characteristic crossover temperatures. The crossover is described beyond the mean-field approximation. In our model, the nonlocal SL modes arise as a result of inter-site spinon exchange via interference of Kondo clouds around distant sites in KL. Then, instead of standard Neel equation for magnetic susceptibility $\chi_{\mathbf{Q}}^{-1}(T) = \chi_0^{-1}(T) + \tilde{I}_{\mathbf{Q}}$, where $\chi_0(T) = 1/4T$ is a Curie susceptibility of spin $\frac{1}{2}$, one has a new equation for magnetic instability $\chi_{\mathbf{Q}}^{-1}(T) = \chi_{\mathrm{sl}}^{-1}(T) + \tilde{I}_{\mathbf{Q}}$, where $\chi_{\mathrm{sl}}^{-1}(T)$ is spinon susceptibility with slower than $1/T$ temperature dependence. The magnetic phase transition at $\tilde{T}_{\mathrm{N}} < T_{\mathrm{N}}$ in a hatched region of Doniach's diagram characterizes magnetic instability of SL in KL.

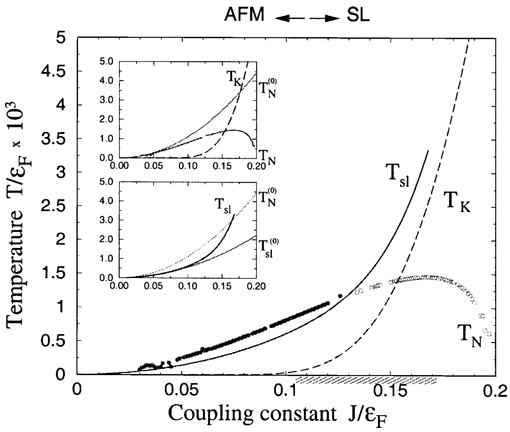

Fig. 1. Reconstructed Doniach's diagram.

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