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Correlations between Kondo clouds in nearly antiferromagnetic Kondo lattices

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Abstract

We discuss a novel fluctuational mechanism explaining the physics of nearly antiferromagnetic Kondo lattices (KL). The effective action for KL model is expressed in terms of Bose operators responsible for paramagnetic excitations and semi-bosonic fields describing the dynamic Kondo clouds created by conduction electrons around local spin. The gauge invariant resonance valence bond theory of interacting Kondo clouds describes the spin liquid with strong critical fluctuations imitating itinerant fluctuation magnetism of Moriya type.

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The problem of competition between Ruderman–Kittel–Kasuya–Yosida (RKKY) magnetic exchange and Kondo correlations [1] is one of the most interesting problem of heavy fermion physics. Recent experiments unambiguously show that such a competition is responsible for unusual properties of integer valent heavy fermion compounds, e.g. quantum critical behavior [2], unconventional antiferromagnetism [3] and superconductivity [4]. It is known that strong competition between inter-site (magnetic, spin glass) and on-site (Kondo) correlations results in suppression of the local magnetism enhancing the tendency to a spin liquid RVB crossover. We discuss in this paper a novel fluctuational mechanism responsible for the physics of the nonmagnetic state in Kondo lattices (KL).

The KL Hamiltonian is

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_j \left(\mathbf{S}_j \mathbf{s}_j + \frac{1}{4} N_j n_j \right). \qquad (1)$$

Here the local electron and spin density operators for conduction electrons in a site j are defined as $n_j = \sum_{j\sigma} c^\dagger_{j\sigma} c_{j\sigma}$, $\mathbf{s}_j = \sum_\sigma \frac{1}{2} c^\dagger_{j\sigma} \hat{\tau}_{\sigma\sigma'} c_{j\sigma'}$, where $\hat{\tau}$ are the Pauli matrices and $c_{j\sigma} = \sum_k c_{k\sigma} \exp(\mathrm{i}kj)$. Applying the standard procedure of exclusion of the "fast" electronic degrees of freedom we come to the effective Hamiltonian describing both the local Kondo correlations and inter-site RKKY exchange:

$$\tilde{H} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \tilde{J} \sum_j \mathbf{s}_j \mathbf{S}_i - \sum_{jl} I_{jl} \mathbf{S}_j \mathbf{S}_l. \qquad (2)$$

We consider the antiferromagnetic sign of RKKY exchange as the most interesting possibility. The spin operators in Eq. (2) are represented as a bi-products of Fermi operators $\mathbf{S}_j = \sum_\sigma \frac{1}{2} f^\dagger_{j\sigma} \hat{\sigma}_{\sigma\sigma'} f_{j\sigma'}$. To exclude the spurious empty and doubly occupied states appearing in the extended Fock space, the *fixed imaginary chemical potential* is introduced [5]. This procedure properly casts the statistics of spins which actually corresponds to neither Fermi, nor Bose "exclusion principle". We adopt the definition of the auxiliary f-operators as "semi-fermions" in accordance with Ref. [6]. To calculate the effective action corresponding to the Hamiltonian (2) we use two different decoupling schemes for local and nonlocal interaction. The first one is known as

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Newns–Read procedure [7] allowing one to decouple the Kondo term $\bar{c}_{i\sigma} f_{i\sigma} \bar{f}_{i\sigma'} c_{i\sigma'}$ with the help of *local complex spinless* field ϕ_i which affects one conduction electron and one semi-fermion. The Heisenberg-like term with long-range RKKY interaction is decoupled by *local vector real* field $\mathbf{\Phi}$ describing the paramagnons [8]. As a result, effective action describing low-energy physics of KL acquires the form

$$A_{\mathrm{int}} = -\mathrm{Tr}\left(\frac{2|\phi|^2}{\tilde{J}} + \frac{\mathbf{\Phi}^2}{I_{\mathbf{q}}}\right) - \mathrm{Tr}\,\bar{f}_{j\sigma}\phi_j G^0_{\mathbf{r}}\,\bar{\phi}_l f_{l\sigma}, \quad (3)$$

where $G^0_{\mathbf{r}}$ denotes the Green's function of conduction electrons.

Following the scenario formulated in Ref. [8], we calculate the correlation function $K(\omega, \mathbf{q}) = \langle \phi_{\mathbf{q},\omega} \phi_{\mathbf{q},\omega} \rangle$. In a single-site approximation, it is given by the following equation:

$$K^{-1}_{\mathrm{loc}}(\omega) \approx \frac{-\mathrm{i}\omega}{\gamma T} + \ln\frac{\{T, \omega\}}{T_K}. \quad (4)$$

This equation is obtained by analytical continuation of $K(\mathrm{i}\omega_n)$ to the real axis in a region of small $\omega \ll \varepsilon_{\mathrm{F}}$; $\gamma = \pi/8$. Non-local corrections to this function due to the second-order processes result in appearance of dispersion:

$$K^{-1}(\omega, \mathbf{q}) = K^{-1}_{\mathrm{loc}} + \alpha q^2. \quad (5)$$

Here q is dimensionless parameter in the units of lattice spacing R, $\alpha \sim (T/\varepsilon_{\mathrm{F}})^2$. In accordance with our anticipation, $K(\omega, q)$ has no singularities at $\omega \sim T_K$. Instead it has a purely imaginary pole, i.e. describes relaxation of Kondo clouds.

We evaluate the fluctuational corrections to the spin susceptibility. In conventional scenarios of magnetic phase transition, the single-loop diagram describes the magnetic instability at $T = T_{\mathrm{N}}$ and critical fluctuations in a vicinity of Néel point. Two next diagrams (Fig. 1) describe the vertex corrections (Kondo screening of on-site exchange coupling) and interference of Kondo clouds, respectively. The latter diagram together with the higher-order contributions of the same sort describe the processes responsible for a crossover from localized magnetism to itinerant-like fluctuational spin-liquid-type magnetism. The temperature dependence of static magnetic susceptibility $\chi^{-1}(T) = \Theta + T^{\lambda}$ is nonuniversal in spite of the fact that we are in a region of critical AFM fluctuations. The power λ is a function of ε_{F} and R. In other words it may vary with changing the experimental control parameters (e.g., pressure or impurity concentration). The Kondo-fluctuations depress T_{N} to temperatures well below mean-field value T^0_{N}. Magnetic instabilities at $T \ll T^0_{\mathrm{N}}$ in this scenario are the instabilities of the spin liquid, but the power-law $\chi(T)$ dependence differs from that in a quantum critical point regime.

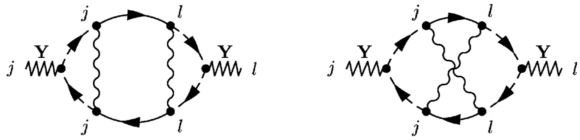

Fig. 1. Diagrams describing local (Curie-type) and nonlocal corrections to magnetic susceptibility $\chi(T)$. Solid line denotes conduction electrons, dashed and wiggly lines stand for semi-fermions and spins, respectively, wavy line denotes $\langle \phi\phi \rangle$ correlator, j, l are site indexes.

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