



Stabilization of spin liquid in Kondo lattice: High temperature regime

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Abstract

The mechanism explaining the key role of AFM correlations in formation of the heavy fermion state is offered. It is shown that in the case of $(T^* - T_N)/T_N \ll 1$, the critical spin fluctuations transform the mean-field second-order transition to RVB state into the crossover from high-temperature paramagnetic behavior of localized spins to strongly correlated spin liquid with quasi itinerant character of susceptibility. Thus the spin-liquid state *by its origin* is close to magnetic instability, so either short-range or long-range AFM order should arise at low T .

Keywords: Spin liquid; Magnetic instability

It was shown in [1] that the spin-liquid state of resonating valence bond (RVB) type can be stabilized by the Kondo scattering against the antiferromagnetic (AFM) ordering in 3D Kondo lattices at high enough temperatures $T^* > T_K$, provided the Kondo temperature T_K is close to the mean-field (MF) Neel temperature T_N . This stabilization is due to the fact that the Kondo scattering screens dynamically the local moments and, thus, suppresses the magnetic order, whereas the spin-liquid correlations which result in the singlet RVB are left intact by this scattering. The theory was based on the MF description of RVB state which, as is known [2], results in second-order-type transition from paramagnetic state to RVB phase. However, since the transition to the spin-liquid state takes place close to the point of AFM instability, the critical fluctuations influence essentially the character of spin-liquid transition. The description of this influence is the main subject of the present paper.

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We start with a standard Kondo lattice Hamiltonian

$$H_{\text{eff}} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J_{\text{st}} \sum_i c_{i\sigma}^\dagger c_{i\sigma'} f_{i\sigma}^\dagger f_{i\sigma'} \quad (1)$$

Here ε_k is the band level of conduction electron $c_{k\sigma}$, and the operator of localized f-spin is represented via fermionic operators, $S_i = \frac{1}{2} f_{i\sigma}^\dagger \hat{\sigma} f_{i\sigma'}$, where $\hat{\sigma}$ is the Pauli matrix. At $T > T_K$ the non-crossing approximation for the Kondo scattering processes is valid, and this Hamiltonian can be transformed into effective RKKY-type Hamiltonian for spin variables only,

$$H_{\text{RKKY}} = I_{\text{ss}} \sum_{ij} f_{i\sigma}^\dagger f_{j\sigma} f_{i\sigma'}^\dagger f_{j\sigma'} \quad (2)$$

where $I_{\text{ss}} \sim \tilde{J}_{\text{st}}^2(T^*)/\varepsilon_F$ is the indirect RKKY exchange interaction with the sf-vertices $\tilde{J}_{\text{st}}(T^*)$ enhanced by the Kondo scattering which is taken into account in a high-temperature approximation of perturbation theory [1]. The Kondo processes are “quenched” at some temperature $T^* > T_K$ which characterizes the onset of spin-liquid RVB state described by the variables $b_{ij} = \sum_{\sigma} f_{i\sigma}^\dagger f_{j\sigma}$ under the constraint $\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = 1$. If one introduces the

MF parameter $\Delta = \langle b_{ij} \rangle$ in the Hamiltonian (2), the temperature T^* is determined as $T^* = I_{ss}(2zN)^{-1} \sum_{\mathbf{k}} \varphi^2(\mathbf{k})$, where $\varphi(\mathbf{k})$ is a lattice structure factor with the coordination number z . Just this temperature was shown in [1] to become higher than T_N in a critical region $T_K \sim T_N$ of the Doniach state diagram.

Since the inequality $(T^* - T_N)/T_N \ll 1$ is valid for the MF solution, the closeness to AFM instability should be taken into account. This closeness enriches the phase diagram of 3D spin-liquid in comparison with the MF scenario of homogeneous RVB state formation [1]. We consider here the Kondo lattice with AFM-type RKKY interaction for the nearest neighbors which could result in commensurate ordering with AFM wave vector \mathbf{Q} at $T = T_N$ provided the RVB state was not realized at higher temperature T^* . This means that the denominator of the static susceptibility

$$\chi_Q = \chi_0(T)[1 - \chi_0(T)I(\mathbf{Q})]^{-1} \quad (3)$$

is close to zero at $T \approx T^*$. Here $\chi_0(T) = \langle \mathbf{S}_Q \cdot \mathbf{S}_{-Q} \rangle_{\omega=0} = C/T$ is the Curie susceptibility of free localized spin. Below T^* the latter acquires dispersion, begins to deviate gradually from Curie law, and finally takes the form

$$\chi_{0Q}(T) = N^{-1} \sum_{\mathbf{k}} (n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{Q}})(t_{\mathbf{k}+\mathbf{Q}} - t_{\mathbf{k}})^{-1}, \quad (4)$$

where $n_{\mathbf{k}}$ is the Fermi distribution function for the RVB excitations which are characterized by the dispersion law $t_{\mathbf{k}}$. This deviation is shown schematically by the solid curves in Fig. 1. The zero-temperature limit of these curves can be estimated as $\chi_{0Q}^{-1}(0) = \alpha T^*$, where α is the numerical coefficient whose value depends on the character of phase transition. This value can be either lower or higher than $T_N = CI(\mathbf{Q})$.

In the first case (curve 1 in Fig. 1), the point \tilde{T}_N where χ_{0Q}^{-1} crosses the dotted line, corresponds to AFM transition. However, the character of this transition differs from that of the localized spins. According to our scenario, the spin subsystem in the Kondo lattice bypasses the magnetic instability at $T = T_N$ to order at essentially lesser temperature \tilde{T}_N . However, within the interval $T_N > T > \tilde{T}_N$ the localized spins are transformed into spin liquid,

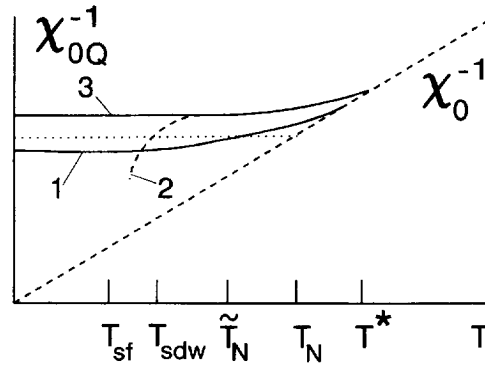


Fig. 1. Static magnetic susceptibility of RVB spin liquid.

and, as a result, the magnetic order reminds rather the itinerant AFM of conduction electrons with modulated spin density and small moments.

Since the spinon band is always half-filled because of the constraint, the nesting condition with the same wave vector \mathbf{Q} can be realized for some geometries of the Fermi surface. In this case, χ_{0Q}^{-1} logarithmically diverges, $\chi_{0Q} \sim \Delta^{-1} \ln \Delta/T$, so the SDW-type magnetism appears at T_{SDW} (curve 2).

Next possibility occurs when the curve χ_{0Q}^{-1} does not intersect T_N but comes close enough to it (curve 3). In this case we meet the peculiar situation when the paramagnon-type excitations can develop in the absence of itinerant electrons because the spin excitations have their own Fermi-type continuum in a spin-liquid state. Then, the spin-fluctuation order which reminds that for itinerant electrons [3] can occur at some temperature T_{sf} . If these fluctuations are too weak to provide the long-range order, the short-range magnetic correlations characterized by the vector \mathbf{Q} persist at low temperatures. Thus, we see that the model grasps the whole variety of peculiar magnetic states with tiny itinerant-like moments which are known for the heavy-fermion materials.

The AFM spin fluctuations also influence the character of transition from the paramagnetic state to the RVB state. It is known that the second-order transition at $T = T^*$ is the artifact of the MF approximation, which violates the gauge invariance of the Hamiltonian (1), and the real situation is that of crossover type. Our approach demonstrates

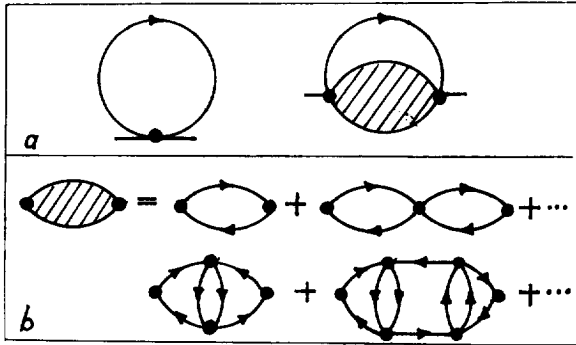


Fig. 2. Self-energy part of spinon Green's function (a) and dynamic susceptibility with vertex corrections (b).

that the real phase transition in Kondo lattice is *always* magnetic phase transition, and the spin-liquid-type correlations only change the character of this transformation.

To show this, we consider the MF self-energy Σ_{ij} of the temperature spinon Green's function $G_{ij}(\tau) = -\langle T_{\tau} f_{i\sigma}(\tau) f_{j\sigma}^{\dagger}(0) \rangle$ corrected by the critical AFM fluctuations (Fig. 2(a)). Here the lines stand for the Fourier-transformed G_{ij} , full dots correspond to $I(\mathbf{Q})$, the loop means spin susceptibility, $\chi_{\mathbf{Q}}(\varepsilon_n)$, whose static part is given by (3). The latter correction, $\delta\Sigma_p$, inserts retardation into $G_p(\omega_m)$ and "opens" the system of equations which determine the spinon correlators for the influence of critical fluctuations. The correction $\delta\Sigma_p$ corresponds to the mode-mode coupling term in the free energy functional, $\delta\mathcal{F}_{\mathbf{Q}} = J^2(\mathbf{Q}) M_{\mathbf{Q}}^{\text{AFM}} M_{\mathbf{Q}}^{\text{RVB}}$ where $M_{\mathbf{Q}}^X$ means the spin density fluctuations of localized ($X = \text{AFM}$) and itinerant ($X = \text{RVB}$) type.

To find $\chi_{\mathbf{q}}(\varepsilon_n)$ for \mathbf{q} close to \mathbf{Q} one should take into account that the RVB continuum exists at temperature $T > T^* > T_N$ but still in the critical region of AFM instability as a "virtual" continuum of spinon, particle-hole pairs with the gap Ω_0 and nonzero damping γ . These excitations give both static ($\delta\chi_{0\mathbf{q}}$) and dynamical ($\delta\chi_{\mathbf{q}}(\varepsilon_n)$) contributions in a simple spinon loop and, correspondingly, in the RPA equation for $\chi_{\mathbf{Q}}(\varepsilon_n)$. The vertex corrections in

γ/Ω_0 should be also taken into account (Fig. 2(b)). The static contribution is responsible for initial deviation of $\chi_{0\mathbf{Q}}(T)$ (Fig. 1) from the Curie law, and the calculation of dynamics reminds formally that was offered in Ref. [4] for the 2D Heisenberg model at finite temperatures. Our spinon-pair excitations with the gap play the same role as the Schwinger bosons in [4]. So, we come to the similar result: the relaxation mode appears in $\chi_{\mathbf{q}}(\Omega)$ (Ω is the frequency analytically continued to the real axis),

$$\chi^{-1}(\mathbf{q}, \Omega) \sim \gamma + (qD\gamma^{-1/2})^2 - i\Omega, \quad (5)$$

where D is a sort of diffusion coefficient.

In conclusion, we have found that the RVB-type excitations appear in the Kondo lattice at high temperature, first, as a relaxation mode in susceptibility due to closeness of T^* to T_N . These excitations evolve into fermi-type particle-hole pairs with lowering temperature, and, eventually, the magnetic order of itinerant-like character arises at $\tilde{T}_N \ll T^*, T_K$. The relaxation regime is extended in T in comparison with standard critical regime for the localized moments, and even can persist at $T \rightarrow 0$. The theory predicts the presence of inelastic neutron scattering at $\Omega \approx \Omega_0$ and $\mathbf{q} \approx \mathbf{Q}$. The small magnetic moments correspond to modulation of spin-liquid density. This picture correlates with the experimental observations for CeRu_2Si_2 and CeCu_6 [5].

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