Mean Field Description of Kondo-Stabilized Spin Liquid in Kondo Lattice with Heavy Fermions

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Abstract

Microscopic mechanism of forming the spin liquid of neutral fermions in Kondo lattices with nearly integer valence of the f-electrons in presented. It is shown that the competition between the Kondo scattering and the indirect exchange interaction can result in stabilization of a state with separated spin and charge excitations with a Fermi-type spectrum for both of them. The origin of strong antiferromagnetic fluctuations is briefly discussed.
1. The well-known Doniach dichotomy \[1\] for the ground state of the Kondo lattice offers the antiferromagnetic state at small values of effective coupling parameter \(\alpha = J_{sf}/\varepsilon_F\) and the nonmagnetic "Kondo-singlet" state at large values of \(\alpha\) as the ground states of the system. Here \(J_{sf}\) is the on-site \(sf\)-exchange integral and \(\varepsilon_F\) is the energy characterizing the width of conduction electron band. The critical region where two regimes compete is determined by the condition \(\alpha^2 c_0 \approx \exp(-1/2\alpha c_0)\), or, in other terms, \(T_N \approx T_K\) where \(T_{N,K}\) are the Neel and Kondo temperatures, respectively. We show in this paper that the third possibility can be realized at \(\alpha \sim \alpha_c\): the Kondo-stabilized spin liquid state of the RVB type is formed instead of the Kondo singlet state. This neutral spin-fermi liquid interacts strongly with charged conduction electrons, the low-temperature thermodynamics is determined mainly by the spin-component of this two-component Fermi liquid, whereas the conduction electrons with enhanced effective masses are responsible for the charge transport and diamagnetic properties of the system in accordance with the phenomenological picture offered in \([2, 3, 4]\).

The idea of Kondo-type stabilization mechanism of the resonance valence bond state was offered in \([5]\). Coleman and Andrei described a picture of resonating valence bonds linked up with the electrons in a layer of \(T_K\) around the Fermi energy. However, the introduction of the Kondo-type mean field resulted in charge transfer from the low-energy conduction electrons to the neutral fermi excitations originating from the f spins. Thus they obtained a "charged spin liquid" like that considered in the mean-field slave-boson theory \([6]\). The general arguments against such a procedure were presented in \([4]\), and here we show that formation of spin liquid can prevent the system from forming the Kondo singlets, and the Fermi liquid with neutral spin and charged electron components is formed instead.

2. We start with a standard Kondo lattice Hamiltonian \(H_{eff}\) which can be derived from the general Anderson lattice model in the case of nearly integer valence.

\[
H_{eff} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J_{sf} \sum_i S_i S_i .
\] (1)

Here \(\varepsilon_k\) is the band level of conduction electron, \(S_i\) and \(s_i = c_{i\sigma}^\dagger \hat{\sigma} c_{i\sigma}\) are the operator of localized f spin and conduction electron spin, respectively, \(\hat{\sigma}\) is the Pauli matrix.

To consider this strongly coupled electron liquid in a controllable way, we start from the high temperature region \(T > T_K\) where the non-crossing approximation (NCA) is acceptable and logarithmic perturbation theory is valid. We study the competition between the homogeneous RVB \([3, 4]\) and Neel ordering within the mean field approximation by using the Abrikosov pseudofermion operator representation (see, e.g., \([3]\)) for the f-spins, \(S_i = f_{i\alpha}^\dagger \hat{\sigma}_{\alpha\beta} f_{i\beta}\). Then the on-site and intersite contributions of the indirect RKKY inter-
action to the self energy part of the pseudofermion temperature Green’s function $F(i\epsilon_n)$ are given by the diagrams of fig.1a and 1b, respectively. Here the dashed and full lines stand for the pseudofermion and conduction electron propagators, hatched squares and crosshatched rectangles symbolize the sf- and ff vertex parts renormalized by the multiple on-site electron-spin scattering. First of these diagrams describes the standard molecular field due to the indirect RKKY interaction acting on the spin in a site $i$, and second one corresponds to the ”anomalous” RVB-type correlations. The polarization operator in the diagram 1a is taken in a nearest neighbor approximation,

$$
\Pi_{q}(i\omega_n) = \Pi_R(i\omega_n)S(q)
$$

where $S(q) = \sum_1 \exp iqR_{jl}$ is a structure factor, $R_{jl} = |R_j - R_l|$. The possibility of commensurate magnetic order with the antiferromagnetic vector $Q$ such that $QR = \pi$ and $J(R) \equiv J_{ij} = J_{sf}^2\Pi_R(0)$ is suggested.

We consider the renormalization of these diagrams by the on-site Kondo scattering at $T > T_K$. According to the NCA approach, this scattering processes renormalize independently the vertices $\Gamma$ belonging to different cites $(i,j)$, and this renormalization should be taken in the logarithmic approximation where the maximum energy variable in the argument of the vertex part is retained. This energy is determined by the characteristic frequencies of the electron Green’s function $G(i\epsilon_m)$ entering the polarization operator $\Pi_R(i\omega_n)$ in the RKKY interaction.

Within the mean-field approach the transition temperatures $T_N$ and $T_{RVB}$ are found from the self-consistent equations for the temperature Green’s functions with the self-energy parts shown in figs.1(a,b). These approximations are obtained in a static approximation for RKKY interaction. It was found by Doniach [1] that the Kondo scattering destroys the magnetic order in a Kondo lattice at least at $\alpha > \alpha_c$, and the ”Kondo singlet” state can be formed in this strong coupling limit. Later it was recognized [5] that one can expect the stabilization of RVB phase instead of the hypothetical Kondo singlet phase provided the inequality $|T_{RVB} - T_N| \ll T_K$ is valid. Here we shall see that this inequality is realized in a critical region $\alpha \approx \alpha_c$ of the Doniach’s phase diagram where $T_N \approx T_K$ and the Kondo scattering nearly screens out the localized moments thus reducing the Neel molecular field

$$
B_N(T) = \lambda_1 \tilde{J}(R,T)\langle S_z \rangle
$$

where $\lambda_1$ is the numerical factor determined by the lattice geometry.

To find the molecular field $B_N(T)$ renormalized by the Kondo scattering one should first estimate the effective exchange integral $\tilde{J}(T)$ entering the self-energy parts of Figs
1(a,b) (the hatched squares),
\[ \tilde{J}(R, T) = T \sum_n G^2(R, \varepsilon_n) \Gamma^2(\varepsilon_n, T) \] (4)
where the asymptotic expression for the Green’s function in a coordinate representation for \( p_F R \gg 1 \) and the spherical Fermi surface has the form
\[ G(R, \varepsilon) = -\frac{v_F}{2\pi p_F R} \exp(-\frac{|\varepsilon| R}{v_F} + i p_F R \text{sgn}\varepsilon), \] (5)
the vertex part
\[ \Gamma(\varepsilon) = J_{sf} \left( 1 - 2\alpha \ln \frac{\varepsilon}{\text{max}\{\varepsilon, T\}} \right)^{-1} \] (6)
is the Kondo-enhanced sf-exchange integral. The simple calculation give
\[ \tilde{J}(R, T) \approx \Phi(p_F R) \alpha^2 \varepsilon_f \int T^{\varepsilon_F} d\varepsilon \exp\left(-\frac{\varepsilon F}{p_F R} \right) \left[ 1 + 2\alpha \ln \frac{\varepsilon}{\varepsilon F} \right]^2 \] (7)
where \( \Phi(x) \) is the oscillatory RKKY function.

In spite of the enhancement of the indirect exchange at \( T > T_K \), the Kondo scattering eventually suppresses the AFM ordering because the same Kondo processes screen the localized spin entering the molecular field (3). The screening factor (the insert \( K(T) \) at fig.1b) has the form
\[ K(T) = 1 - \frac{\varepsilon F}{\ln \frac{T}{T_K}} \] (8)
within the logarithmic perturbation theory (see, e.g., [5]) and formally turns into zero at \( T^* = T_K(\varepsilon_{F, s}^{(s)})^{1/\alpha} > T_K \). However, this function should be corrected for the exact solution of the on-site Kondo problem [6], so the local spins are only partially screened at \( T \) approaching \( T_K \), \( [K(T_K) \approx 0.37] \). Nevertheless, the molecular field is diminished essentially in comparison with the pure Heisenberg exchange \( J_{ij} \).

The spin screening is absent for the RVB molecular field \( B_{RVB} \). To find this field one should calculate the self-energy part of Fig.1b in a static approximation \( \Pi_q(i\omega_n) \to \Pi_q(0) \). Then the field \( B_{RVB} \) is given by the equation (see, e.g., [3, 4, 6])
\[ B_{RVB}(T) = \lambda_2 \tilde{J}(R, T) \Delta_{RVB} \] (9)
where \( \Delta_{RVB} = \sum_\sigma < f_{i\sigma}^+ f_{j\sigma}^\sigma >, \) is the “anomalous” RVB correlator. The homogeneous RVB state possesses the fermi-type excitation spectrum with a dispersion \( u(k) = \dots \)
\[ \lambda_2 \tilde{J}(R, T) \Delta_{RVB} S(k) \] To find the mean-field transition temperature \( T_{RVB} \) one should solve a self-consistent equation

\[
\Delta_{RVB} = (zN)^{-1} \sum_k S(k) \tanh \frac{\lambda_2 \tilde{J}(R, T) \Delta_{RVB} S(k)}{2T} \tag{10}
\]

(cf.\[5\]). Here \( z \) is the coordination number. If the lattice geometry is such that several coordination spheres \( (m) \) give \( \Phi(k_F R^{(m)}) \) of negative sign and comparable values, then the RVB molecular field has the form \[10\]

\[ B_{RVB}(T) = \lambda_2 \Delta_{RVB} \sum_m \tilde{J}(R_m, T) S^{(m)}(k) \]. \tag{11} \]

where \( m \) is the number of coordination sphere. To simplify the numerical calculations we used the approximation \( B_{RVB}(T) \approx \lambda_2 \tilde{J}(R_1, T) \Delta_{RVB} S^{(1)}(k) \) where \( \lambda_2 \) is a numerical factor.

Then, the molecular fields \( B_N(T) \) and \( B_{RVB}(T) \) are given by

\[
B_N(T) \approx B_N^0(T) K(T/T_K) \ln^{-n}(T/T_K),
\]

\[
B_{RVB}(T) \approx B_{RVB}^0(T) \ln^{-n}(T/T_K).
\]

where index \( (0) \) stands for a ”pure” Heisenberg interaction \( J_{ij} \) without Kondo renormalization. In the convolution procedure of eqs.\[4,7\] the logarithmic enhancement is partially ”integrated out”, and \( n \) is close to 1 for the reasonable values of the model parameters. When comparing these equations we find that exchange enhancement favors both Neel and RVB states but the spin screening influences only Neel field thus weakening the trend to the AFM ordering. The possible contribution of several coordination spheres in \( B_{RVB} \) \[11\] is an additional factor stabilizing the spin-liquid state, because the staggered Neel field possesses the definite antiferromagnetic vector \( \mathbf{Q} \). We have taken this possibility into account by varying the factor \( \lambda_2 \) in \( B_{RVB} \).

The phase diagram \( (T_N, T_{RVB} vs \alpha) \) depends also on the form of the electron Fermi surface which influences the coordinate dependence of the function \( \Phi(x) \). We calculated the transition temperatures for the spherical and cylindrical Fermi surfaces with \( \Phi(x) \approx \pi x^{-3} \cos 2x \) and \( \Phi(x) \approx -2x^{-2} \sin 2x \), respectively, and found that the region of existence of the RVB phase is larger in the latter case which is close to the real situation in CeRu\(_2\)Si\(_2\) \[11\].

The example of numerical solution of the mean field equation for \( T_N, T_{RVB} \) with cylindrical Fermi surface is presented in figure 2. Here again the index ”0” marks the transition temperatures for the bare Heisenberg interaction, \( T_N^0, T_{RVB}^0 \sim \varepsilon_F \alpha^2 \Phi(p_F R) \)
It is known that $T^0_N > T^0_{RVB}$ in a 3D case and the RVB state does not arise in three dimensions, but here we find the Kondo-processes change essentially the Doniach’s diagram ($T^0_N, T_K$ vs $\alpha$) \cite{1} in a critical region $\alpha \sim \alpha_c$. We have instead a modified diagram ($T_N, T_{RVB}$ vs $\alpha$) with a wide region of spin liquid phase overcoming the magnetic phase and arising instead of the Kondo-singlet phase.

The critical region is characterized by the temperature sequence $T_{RVB} > T_N > T_K$, all of them being of the same order. This means, firstly, that the spins entering the RVB pairs are screened essentially by the Kondo interaction, and, secondly, that the neutral spin liquid is close to the antiferromagnetic instability. On the other hand, the Kondo scattering is “quenched” at $T \approx T_{RVB} > T_K$. This means that the Kondo singlet state is not formed in this case, so the Kondo mean field $\langle c^+_i f_i \rangle$ which could glue together the spin and charge excitations \cite{5, 6} equals zero. Then, the Kondo temperature is no more the singular point of the theory, and we can transit to the low-temperature region $T < T_K$ where the two-component Fermi liquid occurs. This liquid contains the slow electrons with the energy $\varepsilon < T_K$ which interact strongly with the neutral spin fermions with the energy scaled by $T_{RVB}$. The coupling constant can be estimated as $\sim J(T_{RVB})$. Just this picture was offered in \cite{2, 3, 4} for description of the heavy fermion state in the rare-earth intermetallicides with nearly integer valence (see also \cite{12, 13}.

3. In conclusion, we obtained that the Kondo processes in Kondo lattices at $T$ above $T_K$ prevent the system from forming the Neel state in a critical region $\alpha \sim \alpha_c$ of the Doniach diagram. The same processes stabilize the spin liquid state which, in turn, results in binding the spins in the RVB pairs and quenching the Kondo processes at $T \sim T_{RVB}$. At low temperature we have a two-component Fermi liquid of strongly interacting spin and charge fermions instead of the Kondo singlet, and $T_{RVB}$ plays the role of characteristic temperature of the heavy fermion behavior. However, since $T_{RVB}$ is close to $T_N$, the AFM fluctuations should be strong in this spin liquid, and the magnetic order can be restored under small external influences.

There are many essential effects which are left beyond the mean-field approximation. First of all, the mean-field approximation introducing the average $\Delta_{RVB}$ violates the gauge invariance of the Hamiltonian (\cite{1}) (see, e.g., \cite{14}). The fluctuations of the phase of pseudofermions should result in transformation of an abrupt phase transition described by equation (\cite{10}) into a smooth crossover. It is known \cite{14, 11} that the homogeneous fluctuations of the gauge field in a 2D $t-J$ model (chirality fluctuations) result in infrared singularity of the gauge field fluctuation correlator. In a 3D sf-exchange model the RVB transition is close to the antiferromagnetic instability according to the phase diagram of fig.2, hence the phase fluctuations should be essentially inhomogeneous. Thus, we believe that the influence of the gauge fluctuations is not so destructive for the RVB pairs as in
the 2D case, and the spin-charge separation persists in the heavy fermion systems at low temperatures.

When the retardation effects (the frequency dependence of the polarization operator) are taken into account in the diagram 1b, the "polaron renormalization" $\sim \alpha^2 \omega \ln \frac{\omega}{T}$ and the damping $\sim \alpha^2 T$ of the spin-fermion spectrum arise at $T < T_{RVB}$. The spin fermions, in turn, should influence noticeably the electron spectrum [2, 3, 13, 15]. One should hope, however, that these processes will not change in principle the picture of forming the two-component quantum liquid consisting of charged electrons and neutral spin fermions with different effective masses which share the responsibility for the thermodynamic and transport properties of the heavy fermion systems.

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Figure captions

Fig.1. Self-energy parts for the pseudofermion Green’s functions $G_{ii}$ (a) and $G_{ij}$ (b).

Fig.2. Modified Doniach diagram for competing Neel and RVB phases calculated with the values of $z = 6$, $\lambda_1/\lambda_2 = 2.1$, $p_FR = 2.88$. $\alpha_{c0}$ and $\alpha_c$ are the critical points where the AFM solution disappears in Doniach’s and modified Doniach’s pictures, respectively.