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On the spin origin of heavy fermions in rare earth intermetallides

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Abstract

Microscopic arguments are presented in favor of a spin nature of the heavy fermions in Kondo lattices with nearly integer valence of the f-elections. It is shown that the competition between the Kondo scattering and the indirect exchange interaction can result in stabilization of a spin-liquid state with a Fermi-type spectrum both for neutral spin and charged electron excitations. The origin of strong antiferromagnetic fluctuations is briefly discussed.

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 non-magnetic 'Kondo-singlet' state at large values of α. Here J_{sf} in the on-site sf-exchange integral and ε_F is the energy characterizing the width of the conduction electron band. The critical region where two regimes compete is determined by the condition $\alpha_c^2 \approx \exp(-1/2\alpha_c)$, or, in other terms, $T_N \approx T_K$ where $T_{N,K}$ are the Néel 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 single state. This neutral spin-fermi liquid interacts strongly with charged conduction electrons, the low-temperature thermodynamics are 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 Ref. [2].

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The idea of a Kondo-type stabilization mechanism of the resonance valence bond state was offered in Ref. [3] although 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. The general arguments against such a procedure were presented in Ref. [2], and here we show that formation of the spin liquid prevents the system from forming the Kondo singlet.

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.

$$H_{eff} = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + J_{sf} \sum_i s_i S_i \,. \tag{1}$$

Here ε_k is the band level of conduction electron, S_i and $s_i = c^+_{i\sigma}\hat{\sigma}c_{i\sigma}$ are the operators of localized f spin and conduction electron spin, respectively; $\hat{\sigma}$ is the Pauli matrix.

To consider a 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 RVB and Néel ordering within the mean field approxi-

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mation by using the Abrikosov pseudofermion operator representation (see, e.g. Ref. [4]) for the f-spins, $S_i = f^{+}_{i\alpha}\hat{\sigma}_{\alpha\beta} f_{i\beta}$. Then T_N and T_{RVB} can be found from the self-consistent equations for the temperature Green's functions with the self-energy parts reduced as shown in Fig. 1(a,b). Here the dashed and full lines stand for the pseudofermion and conduction electron propagators. According to the NCA approach, the Kondo scattering processes renormalize independently the vertices Γ belonging to different sites (i, j). Within the logarithmic approximation we leave only the maximum energy variable in the argument of the vertex part which is determined by the interplay between the characteristic energies of the pseudofermion propagator $G(i\epsilon_n)$ and the polarization operator $\Pi_q(i\omega_m) = N^{-1} \Sigma_{jl}\, \Pi_{i-1}(i\omega) \exp i\boldsymbol{qR}_{jl}$ in the RKKY interaction. The case of commensurate spin order with the AFM vector $\boldsymbol{Q}$ such that $\boldsymbol{QR}_{ij} = \pi$ is considered. The effective coupling constant is $J_{ij} = J^2_{sf}\Pi_{i-j}$.

The approximations corresponding to the diagrams Fig. 1(a,b) are expressed as

$$\Sigma^{(N)}_{ii}(i\varepsilon_n) \simeq T \sum_m \sum_j [\Gamma^2\Pi_{ij}]_{i\omega_m} \sum_\sigma \sigma G^\sigma_{jj}(i\epsilon_n - i\omega_m)$$

$$\Rightarrow \tilde{J}^2_1 \varepsilon_f^{-1} \langle S_z \rangle\,, \tag{2}$$

$$\Sigma^{(RVB)}_{ij}(i\varepsilon_n) \simeq T \sum_m [\Gamma^2\Pi_{ij}]_{i\omega_m} \sum_\sigma G^\sigma_{ij}(i\varepsilon_n - i\omega_m)$$

$$\Rightarrow \tilde{J}^2_2 \varepsilon_f^{-1} \langle \Delta_{RVB} \rangle\,. \tag{3}$$

Here [...] stands for the convolution operation over internal frequencies in Γ and Π. Such a reduction is possible only when the main energy dependence of $\Pi_{i-j}(i\omega_m)$ is determined by the low frequencies $\omega < T_{RVB}$. These approximations work well for large enough R, such that $p_F R \gg 1$.

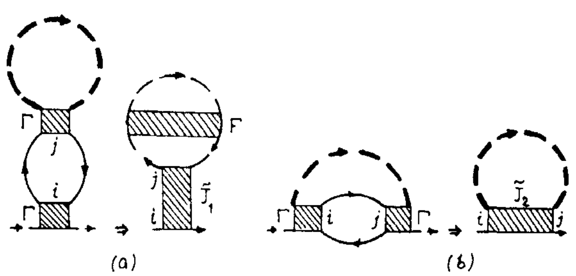

Fig. 1. Self-energy parts for the pseudofermion Green's functions G_{ii} (a) and G_{ij} (b).

The first of these diagrams with the bare vertices $\Gamma \to J_{sf}$ gives a standard expression for Néel temperature $T^0_N/\varepsilon_F = z\lambda_1\alpha^2\Phi(p_F R)$ of RKKY type. Here z is the coordination number, $\Phi(x)$ is the oscillating RKKY function. $R = |\boldsymbol{R}_{ij}|$. λ_1 is the numerical factor determined by the lattice geometry. The second one describes the mean-field solution for the 'anomalous' propagator describing the RVB pair of spins belonging to the sites i and j connected by the AFM exchange interaction. These homogeneous RVB states [3,5] possess the fermi-type spectrum with a dispersion $u(k) = \Delta_{RVB}\alpha^2\varepsilon_F S(\boldsymbol{k})$ where $\Delta_{RVB} = \Sigma_\sigma \langle f^{+}_{i\sigma} f_{j\sigma}\rangle$, $S(\boldsymbol{k})$ is the structure factor for a given coordination sphere. Then we have for bare transition temperature T^0_{RVB} the simple expression $T^0_{RVB}/\varepsilon_F = z\lambda_2\alpha^2\Phi(p_F R)$. Usually the numerical coefficient $\lambda_1 > \lambda_2$ in 2D and 3D lattices, and this is the reason why the RVB state is not realized.

However, in the case of $\alpha \geqslant \alpha_c$ where the condition $T_{RVB} - T_N \ll T_K$ is valid, one can expect effective stabilization of the RVB state by the Kondo processes which renormalizes the vertices $J_{sf} \to \Gamma \sim \varepsilon_F \ln^{-1}(T/T_K)$ and dresses the pseudofermion Green's functions G. Such stabilization is due to the fact that the Kondo scattering influences the on-site and intersite spin propagators differently. First, the logarithmic Kondo corrections results in enhancement of the effective on-site exchange Γ, and this enhancement favors both Néel and RVB ordering. On the other hand, the Kondo scattering eventually kills the AFM order due to the spin screening. This screening is given by the vertex insert in the spin-fermion bubble of the diagram Fig. 1(a) [6] for the AFM molecular field B_N and is characterized by the function $F(T/T_K)$ which is taken in the logarithmic approximation [6] corrected for the exact solution [4] at $T \to T_K$. However, the screening does not influence the RVB mean field B_{RVB} (Fig. 1(b)). As a result, we have $B_N(T) \simeq B^0_N(T)F(T/T_K) \ln^{-n} T/T_K$, $B_{RVB}(T) \simeq B^0_{RVB}(T) \ln^{-n} T/T_K$. The exponent $n = 2$ for 'pure' Heisenberg interaction J_{ij}. However, in the convolution procedure of Eqs. (2), (3) the logarithmic enhancement is partially 'integrated out', and n is close to 1 for the reasonable values of the model parameters. In addition, the renormalization of the Green's function G^σ_{ij} results in a sort of 'polaron shift' and temperature-dependent damping of the RVB propagator. The anisotropy of the Fermi surface also favors the RVB state.

The example of numerical solution of the mean field equation for transition temperatures is presented in Fig. 2. Here the cylindrical Fermi surface for conduction electrons (which is close to that realized in

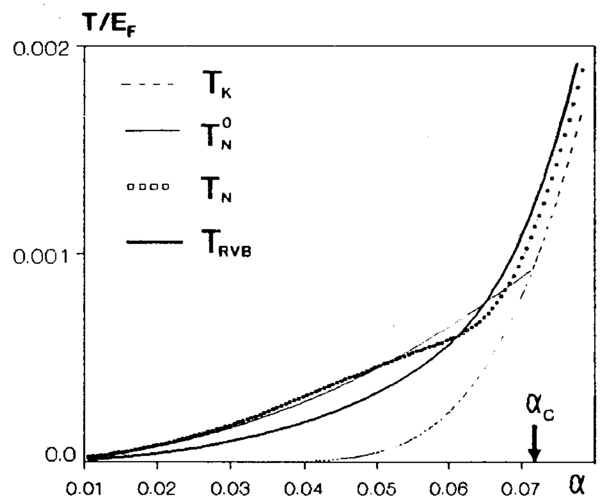

Fig. 2. Modified Doniach diagram for competing Néel and RVB phases calculated with the values of $z = 6$, $\lambda_1/\lambda_2 = 2.1$, $p_F R = 2.88$. α_c is the critical point where the AFM solution disappears in standard Doniach's picture. In the modified diagram, the AFM solution exists only for Kondo-enhanced T_N exceeding T_{RVB}.

$CeRu_2Si_2$ [7]) was used in the calculation of the RKKY function $\Phi(x)$. This example shows that the RVB ordering overcomes the Néel ordering at $T > T_K$ and $\alpha \sim \alpha_c$. This means that the Kondo singlet state does not occur in this case, so the Kondo mean field $\langle c_i^+ f_i \rangle = 0$. The polaron shift which was not taken into account in this solution also favors the RVB state (see Ref. [3]).

In conclusion, we found that the Kondo processes in Kondo lattices at T above T_K prevent the system from forming the Néel 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 $T \sim R_{RVB}$. Thus 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.

Beyond the mean-field approximation strong interaction between two components of the Fermi liquid arises due to the interaction with the gauge field [5] which transform the phase transition into crossover. 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.

Acknowledgements

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