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Anisotropic Kondo lattice without Nozieres exhaustion effect

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Abstract

The properties of layered Anderson/Kondo lattices with metallic electrons confined in 2D xy planes and local spins in insulating layers forming chains in z direction are studied. Each spin possesses its own 2D Kondo cloud, so that the Nozieres' exhaustion problem does not arise. The excitation spectrum is gapless both in charge and spin sectors. Possible experimental realizations of the model are briefly discussed.

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An exhaustion principle formulated by Nozieres [1] claims that the number of spin degrees of freedom provided by conduction electrons in a Kondo lattice (KL) is not enough for screening N_i localized spins when N_i is comparable with the number of sites N in the KL [2]. Here we propose a model, which possesses the generic properties of KL, but is not subject to the exhaustion principle limitations. Possible physical realizations of this model are layered systems formed by 2D metallic layers interlaid by insulating layers containing magnetic centers, which are stacked in chains (see Fig. 1).

Such systems are described by an anisotropic Kondo lattice Hamiltonian

$$H_{\text{int}}^{cd} = \sum_{j,l=1,k,k'}^{N_i} J_{\mathbf{k}\mathbf{k}'} \mathbf{s}_{ll',\mathbf{k}\mathbf{k}'} (\mathbf{S}_j + \mathbf{S}_{j+1}), \tag{1}$$

where N_i magnetic sites characterized by spins S_i are distributed in L layers, so that the concentration of magnetic ions in each layer $n_i = N_i/L \leqslant n = N/L$. Each magnetic center is in exchange contact $J_{kk'}$ with two adjacent metallic layers, and the Kondo clouds are formed

below/above the points of this contact due to Kondo screening by itinerant spins $\mathbf{s}_{ll',\mathbf{kk}'} = \frac{1}{2}c^{\dagger}_{l,\mathbf{k}\sigma}\tau_{\sigma\sigma'}c_{l',\mathbf{k}'\sigma'}$ where $l' = l, l \pm 1$. Now one has *L* Fermi reservoirs with capacity *n*, and this capacity is enough to screen each magnetic site. The model may be treated in terms of the Doniach's dichotomy, where the superposition of Kondo clouds competes with indirect interlayer exchange.

Integrating out the high-energy part of electron bands in 2D layers, we come to an effective spin Hamiltonian for an array of chains with RKKY-like spin–spin interaction mediated by the in-plain electrons:

$$H_{\rm int}^{dd} = -I \sum_{j,\sigma\sigma'} d_{j\sigma}^{\dagger} d_{j+1,\sigma} d_{j+1,\sigma'}^{\dagger} d_{j\sigma'}.$$
 (2)

 $I \sim J^2 \chi_{j,j+1}$, where $\chi_{j,j+1}^c = N^{-1} \sum_{\mathbf{q}} \chi_c(\mathbf{q}) \exp i(q_z a_z)$ is the Fourier transform of the spin susceptibility of 2D electrons in metallic layers, and a_z is the distance between adjacent magnetic sites in z direction. As a result the magnetic subsystem is formed by an array of 1D spin chains. Thus, the spin liquid correlations arise in 1D chains at low T and compete with Kondo screening. These correlations play the same part as the antiferromagnetic (AF) correlations in conventional Doniach dichotomy in Kondo lattices.

To describe this dichotomy we adopt the functional integration method of Ref. [3]. We decouple the Euclidean

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Fig. 1. (a) Layered lattice of spatially separated charges in planes and spins in chains. (b) A fragment of a chain with Kondo clouds formed as "shadows" in metallic layers.

action of the model (1), (2)

$$A = \int_0^\beta \mathrm{d}\tau \left[\sum_j (\bar{c}G_0^{-1}c + \bar{d}D_0^{-1}d) - H_{\mathrm{int}}^{cd} - H_{\mathrm{int}}^{dd} \right]$$
(3)

by means of the Hubbard–Stratonovich scheme in terms of the fields $\Delta_{j,j\pm 1} \rightarrow \sum_{\sigma} (d_{j\sigma}^{\dagger} d_{l\pm 1,\sigma} + \text{c.c}), \quad \phi_l \rightarrow \sum_{k\sigma} (c_{l-1,k\sigma}^{\dagger} (d_{j,\sigma} + d_{j+1,\sigma}) + \text{c.c}) \quad [3,4].$ Here, $G_0^{-1} = \partial_{\tau} - \varepsilon(-i\nabla) + \mu$ and $D_{\text{loc}}^{-1} = \partial_{\tau} - i\pi/(2\beta)$ are the bare inverse single particle Green functions (GF) for conduction electrons and local spins, respectively, $\beta = 1/T$. The field ϕ describes the single-site Kondo screening and the field Δ represents the spinon propagation in the spin liquid regime along the 1D spin chain with AF coupling. The single occupancy constraint $d_{j\uparrow}^{\dagger} d_{j\uparrow} + d_{j\downarrow}^{\dagger} d_{j\downarrow} = 1$ is preserved at each site in the chain by the semi-fermionic transformation [5]. These two fields resolve the Doniach's dichotomy, because the long-range AF order is absent in 1D. We appeal to the uniform resonance valence bond (RVB) spin liquid state [4] and treat the spinon modes as fluctuations around the homogeneous solution in a *nn*-approximation, $\Delta_{j,j\pm 1} \rightarrow \Delta_{j,j\pm 1}^u - \bar{\Delta}$ with $\bar{\Delta}^2(\beta) = \beta^{-1} \int_0^\beta \Delta(\tau) \Delta(-\tau) \, d\tau$. The action in these terms is

$$A_{\rm eff} = \sum_{jl,\omega_n} \left(\frac{|\phi_{l,l}(\omega_n)|^2}{\tilde{J}_{lj}} + \frac{|\Delta_{j,j+1}(\omega_n)|^2}{I} \right) + \operatorname{Tr} \log(G_0^{-1}) + \operatorname{Tr} \log(D^{-1}(\Delta) + G_0 \phi_{l,l}^* \phi_{l,l\pm 1} + \text{c.c})$$
(4)

The spin and charge sectors are separated in $A_{\rm eff}$.

The last term in Eq. (4) may be represented as a loop expansion. Analysis of this expansion shows that the KL remains in a weak Kondo screening regime even at $T \rightarrow 0$ since the spin subsystem transforms into a quasi 1D spin liquid existing in the array of spin chains at $T \sim T^* \approx 8J^2/E_F$ [6], where the spin susceptibility of a chain, $\langle \Delta^+ \Delta^- \rangle_{\omega=0} \sim \overline{\Delta}^2$, acquires the Pauli form. The screening results in reduction of the sound velocity of spin excita-

tions, $\hbar v = \tilde{I}a_z$ with $\tilde{I} = I[1 + I/\bar{\Delta}\ln(\bar{\Delta}/T_K)]^{-1}$. As to the in-plane charge excitations, the formation of Kondo clouds is quenched at $T \gg T_K$, so instead of a coherent Fermi liquid regime, $\langle \phi^+ \phi^- \rangle_{\omega \to 0}$ behaves as a relaxation mode $\sim [-i\omega/\Gamma + \alpha q^2 + \ln(\bar{\Delta}/T_K)]^{-1}$ (Γ, α are the numerical constants).

The characteristic features of a two-component electron/ spin liquid predetermine the thermodynamics of the KL. The logarithmic corrections $\sim \ln^{-1}(T^*/T)$ are expected in the low-*T* Pauli-like susceptibility of isotropic spin chains, whereas the logarithmic corrections to the susceptibility of charged layers are quenched as $\ln \overline{\Delta}/T_K$. The overdamped relaxation mode should be seen as a quasielastic peak in χ_0 . The 1D spinons contribute to the linear-*T* term in specific heat thus mimicking the heavy-fermion behavior, while the contribution of Kondo clouds is frozen at low *T*.

To conclude, the layered KL possess unique properties of Fermi liquid behavior in xy plane and spin liquid behavior in z plane, which are straightforwardly manifested in the magnetic response. One may point out the class of layered conducting/magnetic hybrid molecular solids as an object for the application of above theory. These crystals are formed by alternating metallic cationic layers and insulating magnetic anionic layers with radicals $[N(CN)_2]^-$ as building blocks and transition metal ions (e.g., Mn) attached to these radicals as carriers of localized spins [7]. Organic cations with magnetic ions in such systems form ordered stacks. The problem is in preparing metallic layers with large enough Fermi surface to make Kondo screening effective and to find insulating networks with large enough distance between the magnetic ions.

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