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Phase diagrams and properties of the ground state of the anisotropic Kondo lattice model

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The properties of the half-filled Kondo lattice model with anisotropic intersubsystem exchange interaction J_{XY} and J_Z are discussed. The phase diagram and ground state characteristics of the system are determined within a variational mean-field approximation for the case of rectangular density of states (DOS) for itinerant electrons. The ground state phase diagram is found to exhibit five different phases: Kondo singlet state, two planar antiferromagnetic phases, and two Ising antiferromagnetic (Néel) phases.

Key words: *Kondo lattice; exchange interaction; phase diagram*

1. Introduction

The Kondo lattice model (KLM) is one of the most common models for heavy fermion materials, Kondo insulators and also for manganites (in its ferromagnetic version). In the model, charge fluctuations for localized electrons are suppressed, which leads to a coupled electron–spin system. Crucial for physics of this system is a strong competition between demagnetization resulting from the Kondo effect and magnetism, which tends to yield magnetic orderings. Up to now, most of the studies of this model focused on the case of isotropic exchange interaction [1–6].

In this paper, we present some of our results concerning the case of the Kondo lattice model (KLM) with anisotropic exchange couplings J_{XY} and J_Z. The model is defined by the following Hamiltonian:

$$H = \sum_{\langle ij\rangle\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_i J_Z S^z_i \sigma^z_i + \frac{1}{2} J_{XY} \left(S^{+}_i \sigma^{-}_i + S^{-}_i \sigma^{+}_i \right) \quad (1)$$

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where S_i^α and σ_i^α are the spin operators for localized *d* electrons at *i*th site and those for itinerant *c* electrons, respectively:

$$S_i^\mu = \frac{1}{2}\sum_{\sigma\sigma'} d_{i\sigma}^+ \tau_{\sigma\sigma'}^\mu d_{i\sigma'}, \qquad \sigma_i^\mu = \frac{1}{2}\sum_{\sigma\sigma'} c_{i\sigma}^+ \tau_{\sigma\sigma'}^\mu c_{i\sigma'}$$

with the Pauli matrices $\tau_{\sigma\sigma'}^\mu$, and with a local constraint $d_{i\uparrow}^+ d_{i\uparrow} + d_{i\downarrow}^+ d_{i\downarrow} = 1$, such that every d orbital is always occupied by just one electron. The bandwidth parameter *D* of c electron band is defined by $2D = 2zt$, where *z* is the number of nearest neighbours (nn).

We performed a detailed analysis of the phase diagrams and thermodynamic properties of model (1) for *d*-dimensional hypercubic lattices and arbitrary, positive and negative J_{XY} and J_Z [7]. In the analysis, we used an extended mean-field approximation (MFA-HFA), analogous to that used in the treatment of the isotropic Kondo lattice model [2, 4]. Below, we only quote the main results of this investigation, concentrating on the case of a half-filled electron band. We restrict our analysis to the pure phases and assume rectangular density of states (DOS) for c electron band.

Considered phases are characterised by the following order parameters:

- planar antiferromagnetic (AF_{XY})

$$\sigma_Q^{XY} \neq 0, \qquad S_Q^{XY} \neq 0$$

where

$$\sigma_Q^{XY} = \frac{1}{2N}\sum_i \left\langle \sigma_{ic}^+ \right\rangle e^{-iQR_i}, \qquad S_Q^{XY} = \frac{1}{2N}\sum_i \left\langle S_{id}^+ \right\rangle e^{-iQR_i}$$

$$\sigma_{ic}^+ = c_{i\uparrow}^+ c_{i\downarrow}, \qquad S_{id}^+ = d_{i\uparrow}^+ d_{i\downarrow}, \qquad \vec{Q} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$$

- uniaxial AF state (AF_Z)

$$\sigma_Q^z \neq 0, \qquad S_Q^z \neq 0$$

where

$$\sigma_Q^z = \frac{1}{N}\sum_i \left\langle 2\sigma_{ic}^z \right\rangle e^{-iQR_i}, \qquad S_Q^z = \frac{1}{N}\sum_i \left\langle 2S_{id}^z \right\rangle e^{-iQR_i}$$

- Kondo state (K)

$$\lambda = \frac{1}{2N}\sum_i \left(\left\langle d_{i\sigma}^+ c_{i\sigma} \right\rangle + hc \right) = \frac{1}{2N}\sum_k \left(\left\langle d_{k\sigma}^+ c_{k\sigma} \right\rangle + hc \right)$$

2. Results and discussion

The ground state phase diagram of the considered model calculated for rectangular density of states (DOS) is shown in Fig. 1. In the next two figures, the plots of the order parameters and the quasi-particle gaps in the excitation spectrum as a function of increasing interactions are presented: in Fig. 2 as a function of $J_{XY}/2D$ for $J_Z = 0$, whereas Fig. 3 as a function of $J_Z/2D$ for $J_{XY}/2D = 0.14$.

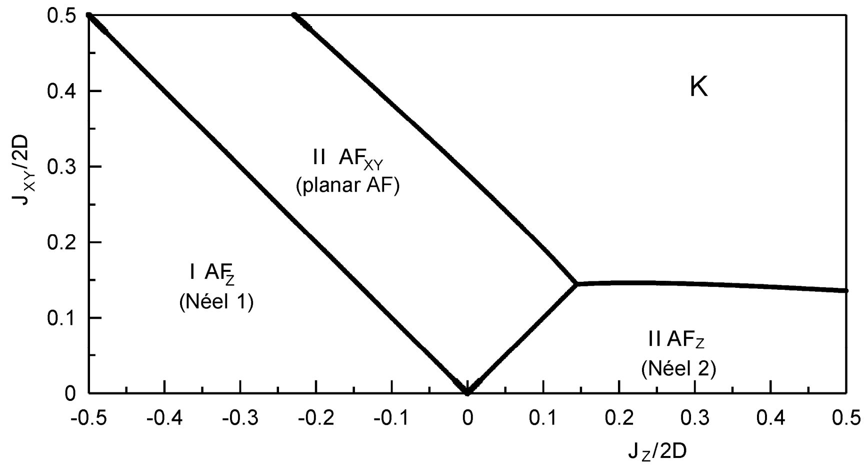

Fig. 1. Ground state phase diagram of the anisotropic Kondo lattice model at half-filling, plotted as a function of $J_{XY}/2D$ and $J_Z/2D$, for rectangular DOS

The diagram in Fig. 1 has been derived for $J_{XY} \geq 0$ and consists of four phases: K Kondo singlet state, I AF_Z Néel 1 (Ising AF with parallel sublattice uniaxial magnetizations of spins and electrons), II AF_Z Néel 2 (Ising AF with antiparallel sublattice magnetizations) and II AF_{XY} (planar AF with antiparallel sublattice *XY* magnetization).

For $J_{XY} \leq 0$ the diagram has the same form with the replacement of II AF_{XY} by I AF_{XY} (planar antiferromagnet with parallel sublattice *XY* magnetizations of spins and electrons).

Let us shortly point out the main conclusions:

- For small values of JXY/2D and JZ/2D the ground states are AFXY, if |JXY|>|JZ| and AFZ if |JXY|<|JZ|, for both signs of JXY and JZ.
- For |JXY|>|JZ| with increasing |JXY|/2D the system exhibits a transition from AFXY to Kondo state at (|JXY|/2D)c. The value (|JXY|/2D)c depends on the strength of JZ: JZ > 0 reduces this critical value, whereas JZ < 0 enhances it (cf. Fig. 1).
- For 0 < |JXY|<|JZ|, the system remains in the I AFZ state for any |JZ|/2D, if JZ < 0, whereas for JZ > 0 the increase of |JZ|/2D yields a transition II AFZ → K, at the critical value (|JXY|/2D)c which slowly decreases with increasing JZ/2D (cf. Fig. 1).

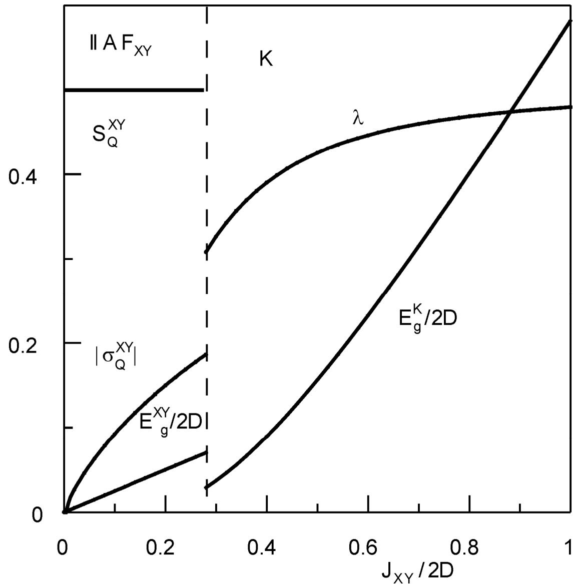

Fig. 2. Variation of the II AF$_{XY}$ and Kondo (K) order parameters and the quasiparticle gap at T = 0 as a function of $J_{XY}/2D$ for J_Z = 0

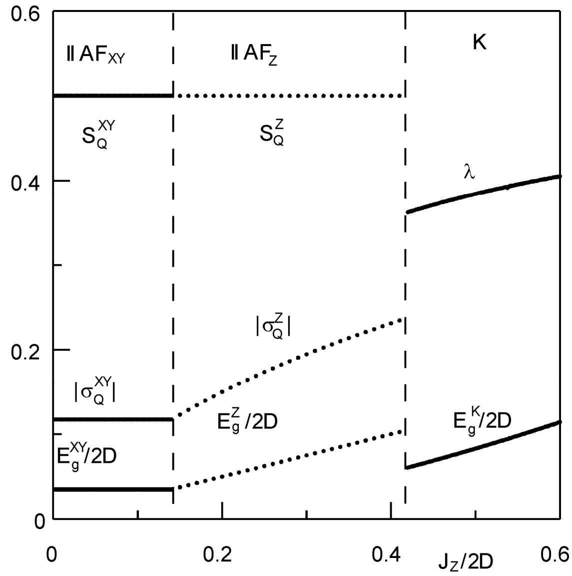

Fig. 3. Variation of the II AF$_{XY}$, II AF$_Z$ and Kondo (K) order parameters and the quasiparticle gap at T = 0 as a function of $J_Z/2D$ for $J_{XY}/2D$ = 0.14

• In the considered case of half filled electron band at T = 0 all phases are nonmetallic, with the quasi-particle gaps: $E_g = |J_Z S_Q^z|$, for AF$_Z$ states, $E_g = |J_{XY} S_Q^{XY}|$, for

AF_{XY} states and $E_g = \sqrt{D^2 + X^2} - D$, where $X = (2J_{XY} + J_Z)\lambda$, for K state. Notice a sharp decrease of the gap at the transitions from AF_{XY} and AF_Z to Kondo state (cf. Figs. 2 and 3).

• With increasing $J_Z/2D$ ($-\infty < J_Z/2D < \infty$) for fixed $J_{XY}/2D > 0$ one can observe the following sequences of transitions (cf. Figs. 1, 3):

$$\text{I AF}_Z \to \text{AF}_{XY} \to \text{II AF}_Z \to \text{K}, \quad \text{if} \quad |J_{XY}|2D < (J_{XY}/2D)_0$$

$$\text{I AF}_Z \to \text{AF}_{XY} \to \text{K}, \quad \text{if} \quad |J_{XY}|/2D > (J_{XY}/2D)_0,$$

where $(J_{XY}/2D)_0 \approx 0.145$ for a rectangular DOS.

Our present studies of model (1) concentrate on the effects of external magnetic field and take into consideration mixed ordered phases.

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