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Spiral magnetic order, non-uniform states and electron correlations in the conducting transition metal systems

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ABSTRACT

The ground-state magnetic phase diagram is calculated within the Hubbard and *s-d* exchange (Kondo) models for square and simple cubic lattices vs. band filling and interaction parameter. The difference of the results owing to the presence of localized moments in the latter model is discussed. We employ a generalized Hartree-Fock approximation (HFA) to treat commensurate ferromagnetic (FM), antiferromagnetic (AFM), and incommensurate (spiral) magnetic phases. The electron correlations are taken into account within the Hubbard model by using the Kotliar-Ruckenstein slave boson approximation (SBA). The main advantage of this approach is a correct qualitative description of the paramagnetic phase: its energy becomes considerably lower as compared with HFA, and the gain in the energy of magnetic phases is substantially reduced.

1. Introduction

Magnetic properties of strongly correlated transition-metal systems and their relation to doping, lattice geometry and band structure are still extensively investigated. The general result of these investigations is the existence of first-order transition between various commensurate and incommensurate magnetic states which invokes a phase separation (first discussed by Visscher [1]).

To describe the properties of such systems one uses many-electron models like the Hubbard, *s-d* exchange (Kondo) and Anderson lattice models. These are widely applied, *e.g.*, for high-T_c cuprates and rare earth compounds. There exist some relations between these models in various parameter regions. The problem of local moments formation, *e.g.* within the Hubbard model, is very difficult and still under investigation [2]. On the other hand, in the *s-d* exchange model the localized moments (spins S) are explicitly present in the Hamiltonian (although they are screened in the Kondo regime).

In the present paper we perform an investigation of the magnetic phase diagram of the Anderson-Kondo lattice model for the square and simple cubic lattices including the phase separation, as well as non-collinear magnetic ordering, and trace these relations. We treat the influence of inter-orbital interaction on the spiral state formation, the difference of the Hubbard (one-orbital) and Anderson-Kondo lattice (two-orbital) models results being considered.

2. Theory

The theoretical investigation of spiral formation in itinerant systems is generally based (in minimal variant) on the non-degenerate Hubbard and Anderson models. Within the Hubbard model

$$\mathcal{H}_{\mathrm{H}} = \sum_{ij\sigma} t_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + U \sum_{i} n^{d}_{i\uparrow} n^{d}_{i\downarrow}, \tag{1}$$

the itinerant electrons demonstrate both transport and interaction induced magnetic properties. Here the matrix elements of the electron transfer are $t_{ij} = -t$ for the nearest neighbors (we assume $t > 0$), $d^{\dagger}_{i\sigma}$, $d_{i\sigma}$ are the electron creation and annihilation operators, respectively, i is the site number, $\sigma = \uparrow, \downarrow$ is the spin projection, the last term being responsible for the on-site Coulomb interaction of d-electrons, $n^{d}_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$.

In the case of the Anderson model transport and magnetic properties are separated between different systems, s and d correspondingly:

$$\mathcal{H}_{\mathrm{A}} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \epsilon_d \sum_{i\sigma} d^{\dagger}_{i\sigma} d_{i\sigma} + V \sum_{i\sigma} (c^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{i\sigma}) + U \sum_{i} n^{d}_{i\uparrow} n^{d}_{i\downarrow}, \tag{2}$$

$c^{\dagger}_{i\sigma}$, $c_{i\sigma}$ is creation/annihilation electron operator in itinerant ('*s*-electron') state at site i. ϵ_d is the energy of localized ('*d*-electron') electron state, V is on-site *s-d* hybridization providing the coupling between these subsystems. The total electron concentration in the system is

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$n = n_s + n_d$, where $n_s = \sum_\sigma \langle c^\dagger_{i\sigma} c_{i\sigma}\rangle$ and $n_d = \sum_\sigma \langle d^\dagger_{i\sigma} d_{i\sigma}\rangle$ are the occupation numbers for itinerant and localized states respectively.

Provided that the d-level is well below the Fermi energy and Coulomb interaction is sufficiently large ($|V| \ll \epsilon_F - \epsilon_d$, U), this model can be reduced by the Schrieffer-Wolf transformation [3] to the s-d exchange model with spin $S = 1/2$ and the negative exchange parameter

$$I = V^2[1/(\epsilon_d - \epsilon_F) - 1/(U + \epsilon_d - \epsilon_F)], \tag{3}$$

where ϵ_F is the Fermi level. The Hamiltonian of the latter model reads

$$\mathcal{H}_{s-d} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - I \sum_{i\sigma\sigma'} (\mathbf{S}_i \cdot \vec{\sigma}_{\sigma\sigma'}) c^\dagger_{i\sigma} c_{i\sigma'}, \tag{4}$$

$\mathbf{S}_i$ is localized spin operator, $\vec{\sigma}_{\sigma\sigma'}$ stands for Pauli matrices.

We consider ferromagnetic and antiferromagnetic, as well as spiral incommensurate magnetic order, with the magnetization $\mathbf{m}_i^{s,d} = \sum_{\sigma\sigma'} \langle (c, d)^\dagger_{i\sigma} \vec{\sigma}_{\sigma\sigma'} (c, d)_{i\sigma'}\rangle$ being modulated in the xy-plane with the wave vector $\mathbf{Q}$ [4]. After local rotation in spin space matching the average magnetization direction at different sites we have a hopping matrix, non-diagonal with respect to spin, $t_{ij}\delta_{\sigma\sigma'} \to t_{ij}^{\sigma\sigma'}$ [5].

The saddle-point expression for the spiral state grand canonical potential (per site) Ω has the form

$$\Omega = \Omega_f + \Omega_{bg}, \tag{5}$$

where Ω_f is a contribution from effective fermion Hamiltonian $\mathcal{H}_f$ describing their motion in the ground state in some effective field,

$$\Omega_f \equiv (1/N) \sum_{\mathbf{k}\nu} (E_\nu(\mathbf{k}) - \mu) f(E_\nu(\mathbf{k})) \tag{6}$$

where $E_\nu(\mathbf{k})$ are eigenvalues of $\mathcal{H}_f$, $f(E) = \theta(\mu - E)$ is the Fermi function at T=0, μ is the chemical potential, N is the lattice site number. Ω_{bg} is 'inner' effective field ('background') contribution to the grand canonical potential.

Within the Hubbard model we have

$$\mathcal{H}_f = \sum_{\sigma\sigma'\mathbf{k}} (z_\sigma z_{\sigma'} (e_+(\mathbf{k})\delta_{\sigma\sigma'} + e_-(\mathbf{k})\delta_{\sigma,-\sigma'}) + \delta_{\sigma\sigma'}\lambda_\sigma) d^\dagger_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma'}, \tag{7}$$

where

$$e_\pm(\mathbf{k}) = (1/2)(t_{\mathbf{k}+\mathbf{Q}/2} \pm t_{\mathbf{k}-\mathbf{Q}/2}), \tag{8}$$

$$t_{\mathbf{k}} = \sum_i \exp(i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)) t_{ij} \tag{9}$$

is the bare electron spectrum. The concrete expressions for the spectrum renormalization factors z^2_σ, λ_σ and Ω_{bg} depend on the approximation employed.

The resulting wave vector $\mathbf{Q}$ is determined by minimization of Ω over various spiral states at fixed μ which allows to take into account the phase separation possibility [4,6].

2.1. Hartree-Fock approximation

The generalized HFA for the Coulomb interaction in d-subsystem reads

$$U n_{d\uparrow} n_{d\downarrow} \to U n^d_{i\uparrow} \langle n_{d\downarrow}\rangle + U\langle n^d_{i\uparrow}\rangle n^d_{i\downarrow} - U\langle n^d_{i\uparrow}\rangle\langle n^d_{i\downarrow}\rangle. \tag{10}$$

The main shortcoming of HFA is the account of contributions of singly and doubly occupied states to $n^d_\sigma \equiv \langle n^d_{i,\sigma}\rangle$ in the equal way, which becomes incorrect at sufficiently large U.

Correlation-induced band narrowing is here absent, $z^2_\sigma = 1$ and $\lambda_\sigma = U n^d_{-\sigma}$ in Eq. (7),

$$\Omega_{bg} = -U n^d_\uparrow n^d_\downarrow. \tag{11}$$

In the case of the Anderson model we have

$$\mathcal{H}_f = \sum_{\sigma\sigma'\mathbf{k}} (e_+(\mathbf{k})\delta_{\sigma\sigma'} + e_-(\mathbf{k})\delta_{\sigma,-\sigma'}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma'} + V \sum_{\mathbf{k}\sigma} (c^\dagger_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} + d^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}) + \sum_{\mathbf{k}\sigma} (\epsilon_d + U n_{d,-\sigma}) d^\dagger_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma}, \tag{12}$$

so that two types of mixing are present: the hybridization V of s- and d-systems and spin flip terms proportional to $e_-(\mathbf{k})$.

2.2. The account of correlations: slave boson approximation

Besides HFA, we apply SBA [7] to the single-band Hubbard model. The idea of this approximation is extension of configuration space. This duplicates the standard description based on the Slater determinant wave functions (related to operators c, $c^\dagger$) by using the boson operators e_i, $p_{i\sigma}$, d_i and their conjugates which correspond to empty, singly occupied, and doubly occupied states respectively. The bosonic space construction is realized by requiring the presence of exactly one boson at any time,

$$e^\dagger_i e_i + p^\dagger_{i\uparrow} p_{i\uparrow} + p^\dagger_{i\downarrow} p_{i\downarrow} + d^\dagger_i d_i = 1. \tag{13}$$

Any on-site transition operator (Hubbard X operator [10]) has its counterpart in the slave boson language, *e.g.*, $X^{0\sigma}_i \sim \mathcal{P} e^\dagger_i p_{i\sigma} \mathcal{P}$ for any site i, $\mathcal{P}$ being the projection operator onto the corresponding subspace. The exact coherence of fermion and boson systems is established by the replacement [8]

$$c^\dagger_{i\sigma} c_{j\sigma'} \to g^{(1)}_{i\sigma} (p^\dagger_{i\sigma} e_j + d^\dagger_i p_{j,-\sigma'}) g^{(2)}_{j\sigma'} c^\dagger_{i\sigma} c_{j\sigma'}, \tag{14}$$

$g^{(1)}_{i\sigma}$ ($g^{(2)}_{i\sigma}$) being an operator equal to unity on the subspace defined by the equation $d^\dagger_i d_i + p^\dagger_{i,\sigma} p_{i,\sigma} = 1$ ($e^\dagger_i e_i + p^\dagger_{i,-\sigma} p_{i,-\sigma} = 1$) needed to reproduce HFA results at small U within the saddle-point approximation [7]. The consequence of this coherence is the connection of site occupation numbers in terms of fermions and bosons,

$$c^\dagger_{i\sigma} c_{i\sigma} = d^\dagger_i d_i + p^\dagger_{i\sigma} p_{i\sigma}. \tag{15}$$

The Hubbard on-site interaction becomes diagonal in the boson representation: $U n_{i\uparrow} n_{i\downarrow} = U X^{22}_i = U d^\dagger_i d_i$. Within the saddle-point approximation, the bosonic operators are replaced by site-independent c-numbers e, p_σ, d. This yields an improvement of the Hartree-Fock approximation, so that the corresponding effective field can be interpreted as a result of average many-electron site amplitudes satisfying Eq. (13). The partial electronic concentrations are parametrized by

$$n^d_\sigma = p^2_\sigma + d^2. \tag{16}$$

The subband narrowing is the c-number function of extremal bosonic fields,

$$z^2_\sigma = (1 - d^2 - p^2_\sigma)^{-1} (e p_\sigma + p_{\bar\sigma} d)^2 (1 - e^2 - p^2_{\bar\sigma})^{-1}. \tag{17}$$

The grand canonical background potential has the form

$$\Omega_{bg} = U d^2 - \sum_\sigma \lambda_\sigma (p^2_\sigma + d^2). \tag{18}$$

The impact of the occupation of site states on electron states manifests itself in two types of renormalizations of bare spectrum: (i) narrowing of the bare spectrum, similar to the Hubbard–I approximation [11], which is specified by the factor $z^2_\sigma \le 1$, (ii) the additional energy shift λ_σ which is an analogue of the Harris–Lange shift [12]. Both these quantities are essentially spin dependent, which allows one to study the magnetic states formation. Unlike HFA, in the slave-boson approach λ_σ cannot be expressed in terms of n and m only and is obtained from the saddle-point equation as

$$\lambda_\sigma = (ed - p_\uparrow p_\downarrow) \left[\Phi_\sigma \left(\frac{p_{\bar\sigma}/e}{e^2 + p^2_{\bar\sigma}} + \frac{d/p_\sigma}{p^2_\sigma + d^2} \right) + \Phi_{\bar\sigma}/(e p_\sigma) \right], \tag{19}$$

$$\Phi_\sigma \equiv \frac{e p_\sigma + p_{\bar\sigma} d}{(e^2 + p^2_{\bar\sigma})(p^2_\sigma + d^2)} \frac{1}{N} \sum_{\mathbf{k}\nu} f(E_\nu(\mathbf{k})) \frac{\partial E_\nu(\mathbf{k})}{\partial (z^2_\sigma)}. \tag{20}$$