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Properties of extended Hubbard models with anisotropic spin-exchange interaction

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The phase diagrams and electron orderings of the half-filled extended Hubbard models with anisotropic spin-exchange interactions ($J_\perp$, $J_{||}$) are studied. The cases of ferromagnetic ($J_\alpha < 0$) and antiferromagnetic ($J_\alpha > 0$) exchange couplings are considered for repulsive on-site interaction ($U \geq 0$). The analysis of these t–U–$J_{||}$–$J_\perp$ models is performed for d-dimensional hypercubic lattices including $d = 1$ and $d = \infty$ by means of the (broken symmetry) HFA supplemented, for $d = \infty$, by the slave-boson mean-field method. The basic features of the derived phase diagrams are discussed.

Key words: *phase diagram; Hubbard model; anisotropic spin exchange*

1. Introduction

The extended Hubbard model with anisotropic spin exchange interactions is a conceptually simple phenomenological model for studying correlations and for description of magnetism and other types of electron orderings in narrow band systems with easy-plane or easy-axis magnetic anisotropy.

The model Hamiltonian is of the form:

$$H = -\sum_{i,j,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_{i,j,\sigma} n_{i\uparrow} n_{i\downarrow} + (1/2) \sum_{i,j} {}' J_\perp \left(\sigma^+_i \sigma^-_j + hc \right) + \sum_{i,j} {}' J_{||} \sigma^z_i \sigma^z_j \tag{1}$$

where t is the single electron hopping integral, U is the on-site density interaction, $J_\perp$ and $J_{||}$ are XY and Z components of intersite magnetic exchange interaction, respectively, μ is the chemical potential, and Σ' restricts the summation to nearest neighbours (nn). The spin operators $\{\vec{\sigma}_i\}$ are defined by $\sigma^z_i = (1/2)(n_{i\uparrow} - n_{i\downarrow})$, $\sigma^+_i = c^+_{i\uparrow} c_{i\downarrow} = (\sigma^-_i)^+$.

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For strong on-site repulsion and isotropic antiferromagnetic exchange ($J_{||} = J_{\perp} = J > 0$) the model (1) was extensively studied in the context of high T_c superconductivity (HTS). Recently, such a model with transverse (*XY*-type) anisotropic exchange has been proposed by Japaridze et al. [1] as a suitable approach for description of narrow band systems with easy-plane magnetic anisotropy. In particular, the authors studied the weak-coupling ground-state phase diagram of the one-dimensional t–U–$J_{\perp}$ model at half filling ($n = 1$) using the continuum-limit (infinite band) field theory approach [1] as well as (for $U > 0$) the density-matrix renormalization group (DMRG) method [2].

The purpose of our research is an extension of those studies and discussion of the properties of the t–U–$J_{\perp}$–$J_{||}$ model in arbitrary dimension ($1 \le d \le \infty$), both at $T = 0$ and $T > 0$.We performed a detailed analysis of the phase diagrams and thermodynamic properties of this model for d-dimensional hypercubic lattices [3]. Preliminary results for the case $J_{||} = 0$, and $2 \le d \le\infty$ have been given in [4].

In the analysis, we have used the (broken symmetry) HFA supplemented for $d = \infty$ by the spin and charge rotationally invariant slave boson mean-field approach (SBMFA), analogous to that applied previously for the attractive Hubbard model [5] and the Penson–Kolb–Hubbard model [6]. In the following, we shortly summarize the results of our investigation of the model (1) obtained for $1 \le d \le\infty$ lattices in the case of exchange interactions $J_{||}$, $J_{\perp}$ of either sign and $U \ge 0$, and discuss basic features of the derived phase diagrams.

2. Summary of the results

In Figures 1–3 we show representative ground state diagrams of the model (1) at half-filling and $U \ge 0$ derived for lattice structures of various dimensions, including $d = 1$, $d = 2$ and $d = \infty$. Figures 1 are plotted for $J_{\perp} \neq 0$, $J_{||} = 0$, Figs. 2 – for $J_{||} \neq 0$, $J_{\perp} = 0$ and Fig. 3 for $J_{||} = J_{\perp} = J$.

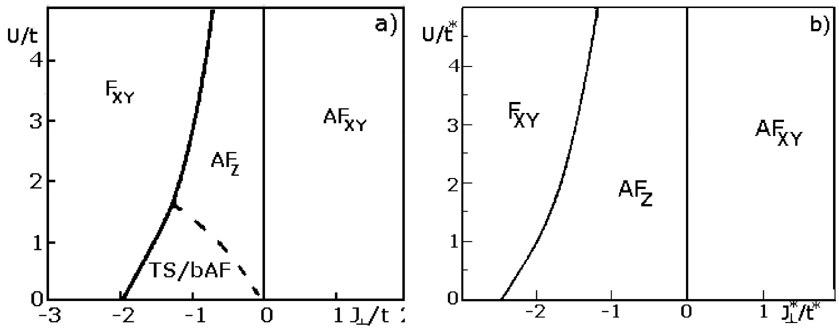

Fig. 1. Ground state phase diagrams of the half-filled t–U–$J_{\perp}$ ($J_{||} = 0$) model: a) for the 1 D chain, b) for $d = \infty$ hypercubic lattice, determined within the broken symmetry HFA. The SBMFA phase diagram for $d = \infty$ is almost identical to (b). In 1Fig. b: $t^* = td^{1/2}$, $J_{\perp}^* = J_{\perp}d$

For $d = \infty$ the diagrams involve exclusively site-located magnetic orderings (cf. Fig. 1b): uniaxial ferromagnetic (F_Z) phase, with $x_{F_Z} = (1/N)\sum_i \langle \sigma_i^Z \rangle \neq 0$, and antiferromagnetic (AF_Z) one, with $x_{AF_Z} = (1/N)\sum_i \langle \sigma_i^Z \rangle e^{i\vec{Q}\cdot\vec{R}_i} \neq 0$, as well as the planar ferromagnetic (F_{XY}) phase, with $x_{F_{XY}} = (1/N)\sum_i \langle \sigma_i^+ \rangle \neq 0$, and antiferromagnetic (AF_{XY}) one, with $x_{AF_{XY}} = (1/N)\sum_i \langle \sigma_i^+ \rangle e^{i\vec{Q}\cdot\vec{R}_i} \neq 0$. It is shown in Fig. 1b plotted for the case of $J_\perp \neq 0$, $J_\| = 0$.The diagram for $J_\| \neq 0$, $J_\perp = 0$ has exactly the same form as Fig. 1b if one makes the replacements: $J_\perp \to J_\|$, $F_{XY} \to F_Z$, $AF_Z \to AF_{XY}$ and $AF_{XY} \to AF_Z$. The phase diagrams for $d = \infty$ determined within SBMFA are almost identical to those obtained in HFA, although the values of the order parameters and the energy gaps in various phases can be substantially reduced by the correlation effects.

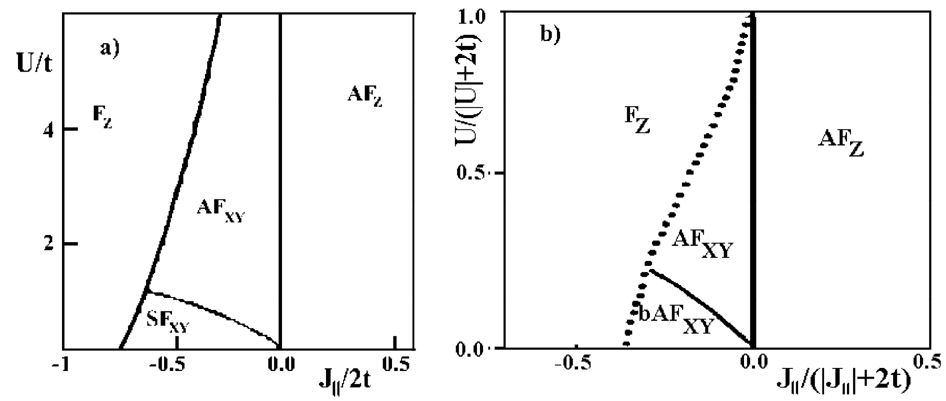

Fig. 2. Ground state phase diagrams of the half-filled t–U–$J_{||}$ ($J_\perp = 0$) model (a) for the $d = 2$SQ lattice determined within the (broken symmetry) HFA, and (b) for the 1D chain, obtained numerically, using level-crossing approach for finite-size clusters (L = 12)

For $d \leq 3$, the model can also exhibit various bond-located orderings. In the considered case of repulsive U, they are realized for ferromagnetic exchange interactions ($J_\alpha < 0$) in the weak/intermediate coupling regimes: in the case of t–U–$J_\perp$ model ($J_\| = 0$) this is the triplet superconductivity (TS) order for $d = 1$ (Fig. 1a), whereas for the t–U–$J_{||}$ model ($J_\perp = 0$) the bond AF_{XY} order (bAF_{XY}) for $d = 1$ (Fig. 2b) and the spin-flux (spin nematic) order (SF_{XY}) for $d = 2$ (Fig. 2a). The phase diagram of t–U–$J_{||}$ model for $d = 1$ shown in Fig. 2b has been obtained numerically using the level crossing approach for finite-size clusters, analogous to that applied previously for the Hubbard model with intersite Coulomb interaction by Nakamura [7]. The corresponding HFA diagram has a very similar form, except that close to the boundary line separating the AF_{XY} and bAF_{XY} states one finds a narrow regime of the mixed ordered phase: AF_{XY}+bAF_{XY}.

In any dimension, for anisotropic exchange interactions the transition at $T = 0$ to the ferromagnetic phases (F_{XY} and F_Z) is of the first order (except of $U = 0$ for $d = \infty$) and occurs only above some critical values of $|J_\alpha|/D$ ($J_\alpha < 0$, $\alpha = \perp, \|$) which for large U decrease with increasing U (Figs. 1–3). This is in obvious contrast with the properties of the antiferromagnetic phases (AF_{XY} and AF_Z), which at $T = 0$ and $U \geq 0$ are stable for any $J_\alpha > 0$ and exhibit smooth crossovers from the weak coupling limit to the local magnetic moment regime with increasing $J_\alpha > 0$.

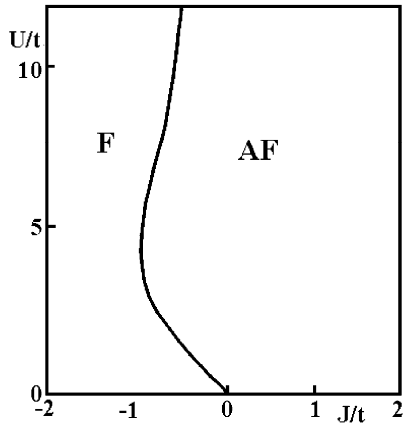

Fig. 3. Ground state diagram of the t–U–J model ($J = J_\perp = J_\|$) at half filling for $d = 2$ SQ lattice calculated within (broken symmetry) HFA. The line denotes first-order phase boundary

In Figure 4, we present the plots of order parameters with increasing $|J_\||$ at $T = 0$ for F_Z and AF_Z phases of the t–$J_\|$ model ($U = 0$) in $d = \infty$.

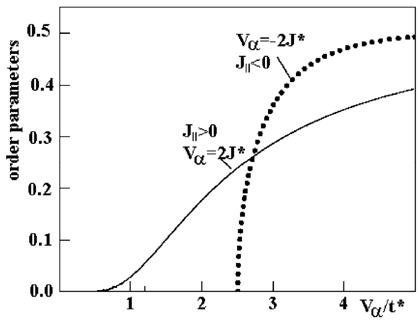

Fig. 4. The order parameters x_α at $T = 0$ as a function of the coupling parameters V_α for AF_Z phase of the t–$J_\| > 0$ model (solid curve, $V_\alpha = 2J^*$) as well as for the F_Z phase of the t–$J_\| < 0$ model (dotted curve, $V_\alpha = -2J^*$), calculated for the $d = \infty$ lattice ($J^* = J_\| d$, $t^* = td^{1/2}$, $J_\perp = 0$, $U = 0$)

Let us shortly summarize our findings concerning possible effects of anisotropic spin exchange interactions at half-filling.

(i) The XY spin exchange ($J_\perp$) can stabilize planar ferro- (antiferro) magnetic orderings with $x_{F_{XY}} \neq 0$ (for $J_\perp < 0$) and $x_{AF_{XY}} \neq 0$ (for $J_\perp > 0$), as well as the triplet superconductivity (TS), for $d = 1$ lattices in the weak/intermediate coupling regime and $J_\perp < 0$ (Fig. 1a), and the charge-flux (orbital AF) order for $d = 2$ lattices [3].

(ii) The longitudinal exchange ($J_{\|}$) favorize uniaxial ferro- (antiferro) magnetic orderings with $x_{F_Z} \neq 0$ (for $J_{||} < 0$), x_{AF_Z} (for $J_{\|} > 0$), as well as the bond AF_{XY} order in the weak/intermediate coupling limit and $J_{\|} < 0$ for $d = 1$, and the spin-flux (spin nematic) order for $d = 2$ lattice (Figs. 2a, b and Fig. 4).

(iii) In the case of isotropic spin exchange ($J_{||} = J_{\perp} = J$) and $U = 0$ the stable phase at $T = 0$ is the isotropic AF (F) state, for any $J > 0$ ($J < 0$), whereas $U > 0$ favourizes the AF phase and makes this state stable also in a definite range of $J < 0$ (cf. Fig. 3).

The problems studied are of relevance for various classes of narrow band magnetic materials including the transition metal and rare earth compounds, where the effects of exchange anisotropy can be important. Possible applications of the model considered include also unconventional superconductors showing close proximity of magnetic and superconducting orderings (see [1, 2] and references therein), e.g. (i) $(TMTSF)_2$ X family of organic materials (the Bechgaard salts), (ii) UGe_2, URhGe and $ZrZn_2$ (coexistence of TS with magnetic orderings), (iii) the ruthenate compounds: Sr_2RuO_4 (TS), $SrRuO_3$ (F), $SrRuYO_6$ (AF). Let us also mention the experimentally observed easy plane anisotropy of the spin exchange in Sr_2RuO_4.

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