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Properties of the extended Hubbard model with transverse (XY-type) spin-exchange interaction

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The properties of the extended Hubbard model with transverse (XY-type) spin-exchange intersite interaction ($J_\perp$) are studied. The cases of ferromagnetic and antiferromagnetic XY exchange are considered. The analysis of the model is performed for d-dimensional hypercubic lattices $2 \le d \le \infty$, by means of the (broken symmetry) Hartree – Fock approximation supplemented, for $d = \infty$, by the slave-boson mean-field method. The effects of phase fluctuations on T_c of XY phases for $d = 2$ lattices are estimated within the Kosterlitz – Thouless scenario. Qualitative differences between the properties of the ferromagnetic and antiferromagnetic XY phases are pointed out.

1 Introduction

The extended Hubbard model with anisotropic exchange interactions is an interesting (conceptually simple) phenomenological model for studying correlations and for description of magnetism and various other types of electron orderings in narrow band systems. The model Hamiltonian has the form:

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \tfrac{1}{2} \sum_{\langle i,j \rangle} J_\perp (\sigma^\dagger_i \sigma^-_j + hc) + \sum_{\langle i,j \rangle} J_\parallel \sigma^z_i \sigma^z_j \,, \tag{1}$$

where t is the single electron hopping integral, U is the on-site density interaction, $J_\perp$ and $J_\parallel$ are the XY and Z components of the intersite magnetic exchange interaction, respectively, the limit $\langle ij \rangle$ restricts the summation to nearest neighbors (nn).

The spin $\{\sigma_i\}$ operators are defined by $\sigma^z_i = (1/2)\,(n_{i\uparrow} - n_{i\downarrow})$, $\sigma^\dagger_i = c^\dagger_{i\uparrow} c_{i\downarrow} = (\sigma^-_i)^+$.

The model (1) was intensively studied in the context of high-T_c superconductivity (HTS) for strong on-site repulsion and isotropic antiferromagnetic exchange ($J_\parallel = J_\perp = J > 0$). Recently, the Hubbard model with transverse (XY-type) anisotropic exchange (of either sign) has been proposed by Japaridze et al. [1] as a suitable approach for description of narrow band systems with easy-plane magnetic anisotropy. The authors studied the weak-coupling ground-state phase diagram of the one-dimensional $t - U - J_\perp$ model ($J_\parallel = 0$) 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 work is extension of those studies and discussion of the properties of the $t - U - J_\perp$ model ($J_\parallel = 0$) in higher dimensions ($2 \le d \le \infty$) at $T \ge 0$. We performed a detailed analysis of the phase diagrams and thermodynamic properties of this model for d-dimensional hypercubic lattices and arbitrary, positive and negative U and $J_\perp$ [3]. In the analysis we have used the (broken symmetry) HFA supplemented for $t = 0$, by the variational approach, which treats the on-site interaction term exactly, and for

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$d = \infty$, by the (spin and charge rotationally invariant) slave-boson mean-field approach (SBMFA), analogous to that applied previously for the attractive Hubbard model [4] and the Penson–Kolb–Hubbard model [5]. Also, the effects of phase fluctuations on the critical temperatures of XY phases in two dimensions were estimated within the Kosterlitz–Thouless (K–T) scenario. Below we only quote the main results of this investigation, concentrating on the half-filled-band case for $2 \le d \le \infty$ lattices.

2 Results and discussion

(1) The ground-state diagrams of the half-filled $t-U-J_\perp$ model derived within the (broken symmetry) HFA are shown in Fig. 1 for the $d = \infty$ hypercubic lattice (Fig. 1a) and for rectangular density of states (DOS) (Fig. 1b). The diagrams consist of the planar ferromagnetic (F_{XY}) and antiferromagnetic (AF_{XY}) phases, the uniaxial antiferromagnetic (AF_Z) phase as well as the superconducting (SS) and CDW phases, described by the following order parameters:

$$x_{F_{XY}} = \frac{1}{N}\sum_i \langle \sigma_i^\dagger \rangle, \qquad x_{AF_{XY}} = \frac{1}{N}\sum_i e^{i\boldsymbol{QR}_i}\langle \sigma_i^\dagger \rangle, \qquad x_{AF_Z} = \frac{1}{N}\sum_i e^{iQR_i}\langle \sigma_i^z \rangle,$$

$$x_{SS} = \frac{1}{N}\sum_i \langle c_{i\uparrow}^+ c_{i\downarrow}^+ \rangle, \qquad x_{CDW} = \frac{1}{2N}\sum_{i,\sigma} e^{i\boldsymbol{QR}_i}\langle n_{i\sigma} \rangle.$$

For $n = 1$ the energies of SS and CDW phases are strictly degenerate and we denote the corresponding state as SS/CDW. Any deviation from $n = 1$ removes this degeneracy and stabilizes SS phase. The phase diagram for $d = \infty$ determined within SBMFA is almost identical to Fig. 1a, although the values of the order parameters and the energy gaps in various phases can be substantially reduced by the correlation effects. It is clearly seen in Fig. 2, where an example of the J^* dependences of the gap parameters for a fixed value of U/t^*, determined within HFA and SBMFA, is presented.

(2) The transition to the F_{XY} phase, which is favored by $J_\perp < 0$, is found to occur only above some critical value $|J_c|$ (cf. Fig. 1). This is in obvious contrast with the properties of AF_{XY} phase that at $T = 0$ and $U \ge 0$ exhibit a smooth crossover from the weak coupling limit to the local magnetic moment regime with increasing $J_\perp > 0$. The plots of order parameters with increasing $|J_\perp|$ for the F_{XY} and AF_{XY} phases of the $t-J_\perp$ model for $d = \infty$ and $n = 1$ are shown in Fig. 3. Repulsive on-site interaction U expands the range of stability of F_{XY} phase at $T = 0$ towards lower values of $|J_\perp|$. Moreover, the F_{XY} and AF_{XY} phases can survive also for attractive values of U ($0 < U < U_c$) (cf. Fig. 1).

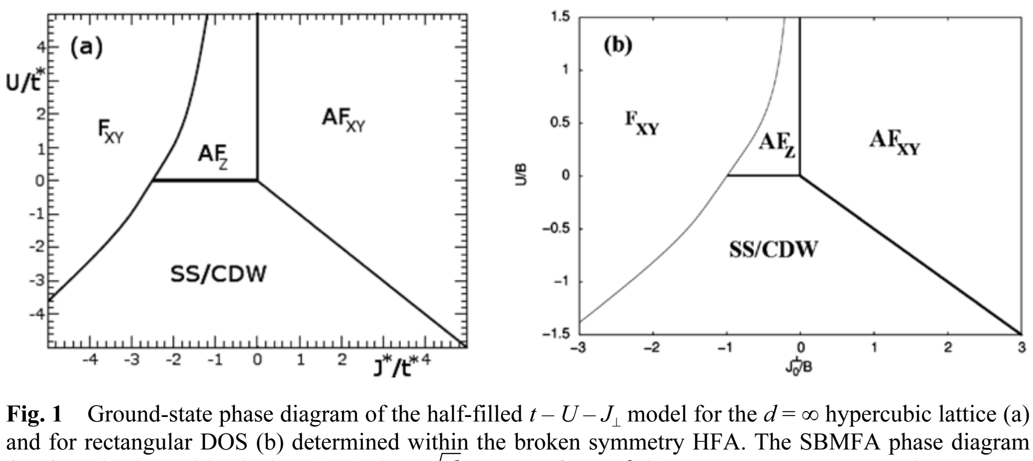

Fig. 1 Ground-state phase diagram of the half-filled $t-U-J_\perp$ model for the $d = \infty$ hypercubic lattice (a) and for rectangular DOS (b) determined within the broken symmetry HFA. The SBMFA phase diagram for $d = \infty$ is almost identical to (a). a) $t^* = t\sqrt{d}$, $J^* = J_0/2 = J_\perp d$; b) $J_0 = zJ_\perp$, $B = 2zt$, $z = 2d$.

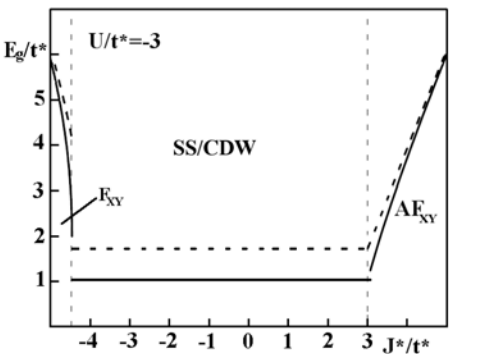

Fig. 2 J^* dependence of the gap in the excitation spectrum at $T = 0$ in the $t - U - J_\perp$ model calculated in the SBMFA (solid curves) and in the HFA (dashed curves) for $d = \infty$-hypercubic lattice, $U/t^* = -3$ and $n = 1$. The stability ranges of the different phases are indicated by the vertical dashed lines $t^* = t\sqrt{d}$, $J^* = J_\perp d$.

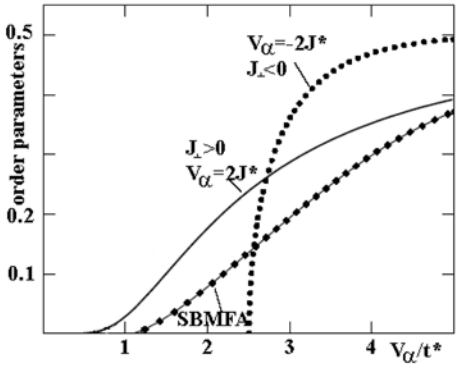

Fig. 3 Plots of the order parameters $x_\alpha = E_g^\alpha / V_\alpha$ at $T = 0$ as a function of the coupling parameters V_α for AF_{XY} phase of the $t - J_\perp > 0$ model (solid curve, $V_\alpha = 2J^*$, $U = 0$) as well as for the F_{XY} phase of the $t - J_\perp < 0$ model (dotted curve, $V_\alpha = -2J^*$, $U = 0$), calculated within the HFA, for the $d = \infty$ lattice, $n = 1$. For $d = \infty$ the plots of x_{AF} vs. V_α for the $t - J_\perp > 0$ model and the $t - U > 0$ model have the same form (solid curve). For the sake of comparison the SBMFA results for the AF phase of the $U > 0$ Hubbard model in $d = \infty$ are presented by the curve with diamonds ($V_\alpha = U$).

(3) For F_{XY} phase and $d < \infty$ there exists also a second characteristic value of $J_\perp / B$ that we call J_{c1} (in the case of alternating lattices $|J_{c1}| = 2t$ for $n = 1$, $U = 0$). For $|J_\perp| > |J_{c1}|$ the ground state is characterized by a nonzero minimal gap between the lower and higher quasiparticle band $E_g^m (T = 0) > 0$ and by the order parameter $x_{F_{XY}}$ that takes its maximum value (the same as in the zero bandwidth limit). On the contrary, for $\dfrac{|J_c|}{B} < \dfrac{|J_\perp|}{B} < \dfrac{|J_{c1}|}{B}$: $E_g^m \le 0$ and $x_{F_{XY}} < x_{F_{XY}}^{max}$ at $T = 0$ (cf. Fig. 4).

The energy gap E_g^m is reduced with increasing T and vanishes at some characteristic temperature, which we denote by T_m. In Fig. 4 we show the plots of T_c and T_m vs $B/|J_\perp|$ calculated for SC lattice and $n = 1$. As we see $T_c > T_m$ except at $B = 0$, and also for the strong ferromagnet phase $\left(\text{i.e. for } \dfrac{|J_\perp|}{B} > \dfrac{|J_c|}{B}\right)$ there exists a range of T where $E_g^m \le 0$.

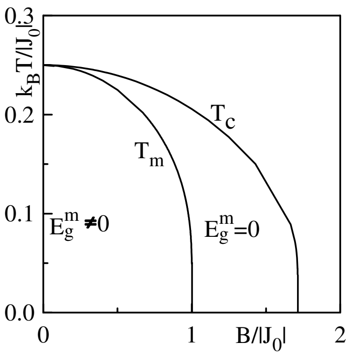

Fig. 4 Critical temperature T_c for F_{XY} ordering and the temperature T_m at which E_g^m vanishes, in the $t - J_\perp < 0$ model, plotted as a function of $B/|J_0|$ for $n = 1$. E_g^m is the gap between the lower and higher quasiparticle band, i.e. $E_g^m = \min E_k^+ - \max E_k^-$, SC lattice (HFA, $U = 0$, $J_0 = zJ_\perp$).

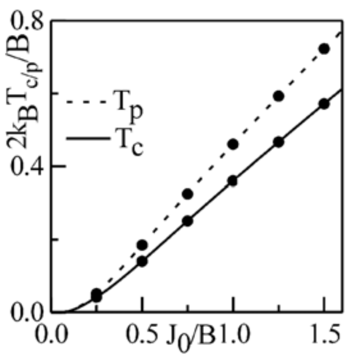

Fig. 5 The K–T critical temperature (T_c) and the HFA critical temperature (T_p) versus J_0/B for AF_{XY} phase of the $t - J_\perp > 0$ model. SQ lattice, $n = 1$ ($U = 0$, $J_0 = zJ_\perp$).

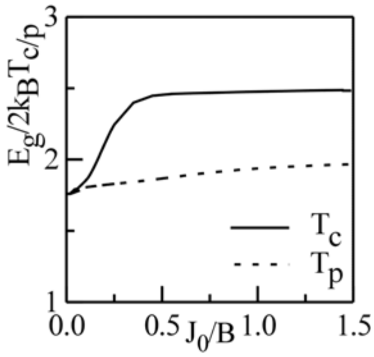

Fig. 6 Gap to critical temperature ratio $E_g(0)/2k_BT_{c/p}$ for AF_{XY} phase of the $t - J_\perp > 0$ model, plotted as a function of J_0/B for $n = 1$. Solid and dashed lines correspond to T_c and T_p, respectively. SQ lattice.

(4) There are strong effects of phase fluctuations on the F_{XY} and AF_{XY} phases in $d = 2$. Going beyond the HFA we have determined T_c for the $t - U - J_\perp$ model on a SQ lattice taking into account the phase fluctuations within the framework of the Kosterlitz–Thouless (K–T) scenario [6–8]. The T_c^{KT} has been obtained by calculating the helicity modulus ρ_s as a function of T and using the K–T relation for the universal jump of ρ_s at $T_c : k_BT_c = (\pi/2)\,\rho_s(T_c)$. As we see from Fig. 5 plotted for $J_\perp > 0$, $U = 0$ the K–T transition temperature T_c^{KT} can be substantially lower than T_c^{HFA} (denoted here by T_p), which in $d = 2$ gives only the estimation of the local magnetic moment formation temperature. Also, the phase fluctuations enhance the gap to critical temperature ratio $E_g(0)/2k_BT_c$ (cf. Fig. 6).

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