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Strongly Anisotropic $S = 1$ (Pseudo) Spin Systems: from Mean Field to Quantum Monte-Carlo

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The $S = 1$ pseudospin formalism was recently proposed to describe the charge degree of freedom in a model high-T$_c$ cuprate with the on-site Hilbert space reduced to the three effective valence centers, nominally Cu$^{1+;2+;3+}$. With small corrections the model becomes equivalent to a strongly anisotropic $S = 1$ quantum magnet in an external magnetic field. We have applied a generalized mean-field approach and quantum Monte-Carlo technique for the model 2D $S = 1$ system to find the ground state phase with its evolution under deviation from half-filling and different correlation functions. Special attention is given to the role played by the on-site correlation ("single-ion anisotropy").

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1. Introduction

These days spin algebra and spin Hamiltonians are used not only in the traditional fields of spin magnetism but in so-called pseudospin lattice systems with the on-site occupation constraint. For instance, the $S = 1$ pseudospin formalism was applied to study an extended Bose-Hubbard model (EHBM) with truncation of the on-site Hilbert space to the three lowest occupation states $n = 0, 1, 2$ (semi-hard-core bosons) considered to be three pseudospin states with $M_S = -1$, $M_S = 0$, $M_S = +1$, respectively (see Ref. [1] and references therein). At variance with quantum $s = 1/2$ systems the Hamiltonian of $S = 1$ spin lattices in general is characterized by several additional terms such as a single ion anisotropy that results in their rich phase diagrams. Recently we made use of the $S = 1$ pseudospin formalism to describe the charge degree of freedom in high-T$_c$ cuprates with the on-site Hilbert space reduced to only the three effective valence centers $[CuO_4]^{7-,6-,5-}$ (nominally Cu$^{1+;2+;3+}$) [2–5].

2. $S = 1$ (pseudo) spin Hamiltonian

The $S = 1$ spin algebra includes the eight nontrivial independent spin operators: spin-dipole moment **S** and five spin-quadrupole operators $Q_{ij} = (\frac{1}{2}\{S_i, S_j\} - \frac{2}{3}\delta_{ij})$ whose mean values define so-called spin-nematic order. Spin operators $S_\pm$ and $T_\pm = \{S_z, S_\pm\}$ change the pseudospin projection (and occupation number!) by ± 1, while $S^2_\pm$ changes the pseudospin projection by ± 2.

Hereafter in the paper we will focus on a simplified 2D $S = 1$ (pseudo) spin Hamiltonian with the nearest neighbor coupling and the only two-particle transport term (inter-site biquadratic anisotropy) as follows:

$$\hat{H} = \sum_i (\Delta S^2_{iz} - \mu S_{iz}) + V \sum_{\langle ij \rangle} S_{iz} S_{jz}$$

$$-t \sum_{\langle ij \rangle} (S^2_{i+} S^2_{j-} + S^2_{i-} S^2_{j+}), \qquad (1)$$

where $V > 0$, $t > 0$. The first single-site term in $\hat{H}$ describes the effects of a bare pseudo-spin splitting and relates with the on-site density-density interactions, or correlations: $\Delta = U/2$. The second term, or a pseudospin Zeeman coupling may be related with a pseudo-magnetic field $\| Z$ which acts as a chemical potential μ for boson systems with a boson density constraint:

$$\frac{1}{N} \sum_i \langle S_{iz} \rangle = n, \qquad (2)$$

where n is the deviation from a half-filling ($n = 0$). The third (Ising) term in $\hat{H}$ describes the effects of the short- and long-range inter-site density-density interactions. The last term in $\hat{H}$ describes the two-particle inter-site hopping. In the strong on-site attraction limit of the model (large easy-axis pseudospin on-site anisotropy) we arrive at the Hamiltonian of the hard-core, or local, bosons which was earlier considered to be a starting point for explanation of the cuprate high-T$_c$ superconductivity [6]. The spin counterpart of $\hat{H}$ corresponds to an anisotropic $S = 1$ magnet with a single ion (on-site) and two-ion (bilinear and biquadratic) symmetric anisotropy in an external magnetic field. It describes an interplay of the Zeeman, single-ion and two-ion anisotropic terms giving rise to a competition of an (anti)ferromagnetic order along Z-axis with an in-plane XY spin-nematic order. A remarkable feature of the Hamiltonian (1) is that the on-site pseudospin states $M = 0$ and $|M| = 1$ do not mix under the inter-site coupling. The model allows us to directly study a continuous transformation of the semi-hard-core bosons to the effective hard-core bosons formed by boson pairs under driving the correlation parameters $\Delta = U/2$ to large negative values ("negative-U model"). The simplified model can be directly applied to a description of bosonic systems with suppressed one-particle hopping.

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3. Mean-field approximation

To analyse the simplified model we start with a mean-field approximation (MFA) for 2D square lattice, however, at variance with a conventional classical MFA we made use of more correct approach that takes into account the quantum nature of the $S = 1$ (pseudo) spin states [7]. First we introduce a set of the on-site $S = 1$ coherent states

$$|\boldsymbol{c}\rangle = c_{-1}|-1\rangle + c_0|0\rangle + c_{+1}|+1\rangle, \tag{3}$$

where the c_M coefficients can be represented as follows

$$c_1 = \sin\frac{\theta}{2}\cos\frac{\phi}{2}\,\mathrm{e}^{-\mathrm{i}\frac{\alpha}{2}}, \quad c_0 = \cos\frac{\theta}{2}\,\mathrm{e}^{\mathrm{i}\frac{\beta}{2}},$$
$$c_{-1} = \sin\frac{\theta}{2}\sin\frac{\phi}{2}\,\mathrm{e}^{\mathrm{i}\frac{\alpha}{2}} \tag{4}$$

with $\theta, \phi, \alpha, \beta$ to be parameters defined by the minimization of the energy. The MFA energy can be written as follows

$$E = \frac{\Delta}{2}\sum_i(1-\cos\theta_i) - \frac{\mu}{2}\sum_i(1-\cos\theta_i)\cos\phi_i \tag{5}$$
$$+\frac{V}{4}\sum_{\langle ij\rangle}(1-\cos\theta_i)(1-\cos\theta_j)\cos\phi_i\cos\phi_j$$
$$-\frac{t}{8}\sum_{\langle ij\rangle}(1-\cos\theta_i)(1-\cos\theta_j)\sin\phi_i\sin\phi_j\cos(\alpha_i-\alpha_j).$$

It is worth noting that due to the absence of the one-particle inter-site hopping terms in Hamiltonian (1) the energy does not depend on phase parameter β, so the β remains undetermined. Below we denote $\delta = \Delta/t$ and $v = V/t$. In a two-sublattice A-B model we arrive at a high-temperature non-ordered (NO) phase and the five MFA uniform phases, two phases with nonzero local superfluid order parameter, or pseudospin nematic order $\langle S^2_{A,B\pm}\rangle \neq 0$ and three charge ordered phases with $\langle S^2_{A,B\pm}\rangle = 0$ but different types of the sublattice occupation (pseudospin S_z components):

Superfluid (SF) phase: $\langle S_{A,Bz}\rangle = n$, $\langle S^2_{A,Bz}\rangle = 1$, $\langle S^2_{A,B\pm}\rangle = \frac{\zeta}{2}\sqrt{1-n^2}e^{\pm i\alpha}$, uncertain factor $\zeta = \pm 1$.

Supersolid (SS) phase: $\langle S^2_{A,Bz}\rangle = 1$, $\langle S_{A,Bz}\rangle = n \mp \sqrt{1+n^2-\frac{4|n|\nu}{\sqrt{4\nu^2-1}}}$, $\langle S^2_{A,B\pm}\rangle = \frac{\zeta}{2}e^{\pm i\alpha}\left(\sqrt{|n|\sqrt{\frac{2\nu+1}{2\nu-1}}-n^2} \pm \operatorname{sgn} n\sqrt{|n|\sqrt{\frac{2\nu-1}{2\nu+1}}-n^2}\right)$.

Charge ordered COI phase: $\langle S_{Az}\rangle = 0$, $\langle S^2_{Az}\rangle = 0$, $\langle S_{Bz}\rangle = 2n$, $\langle S^2_{Bz}\rangle = 2|n|$, $(|n| \leqslant 0.5)$.

Charge ordered COII phase: $\langle S_{Az}\rangle = 2n - \operatorname{sgn} n$, $\langle S^2_{Az}\rangle = 1-2|n|$, $\langle S_{Bz}\rangle = \operatorname{sgn} n$, $\langle S^2_{Bz}\rangle = 1$, $(|n| \leqslant 0.5)$.

Charge ordered COIII phase: $\langle S_{Az}\rangle = \operatorname{sgn} n$, $\langle S^2_{Az}\rangle = 1$, $\langle S_{Bz}\rangle = 2n - \operatorname{sgn} n$, $\langle S^2_{Bz}\rangle = 2|n| - 1$, $(|n| \geqslant 0.5)$.

Interestingly, all the local order parameters do not depend on the correlation parameter Δ, while this parameter governs the energy of different phases. Taking into account the on-site correlations we arrive at very rich and intricate phase diagrams for the model system as compared with relatively simple phase diagrams for hard-

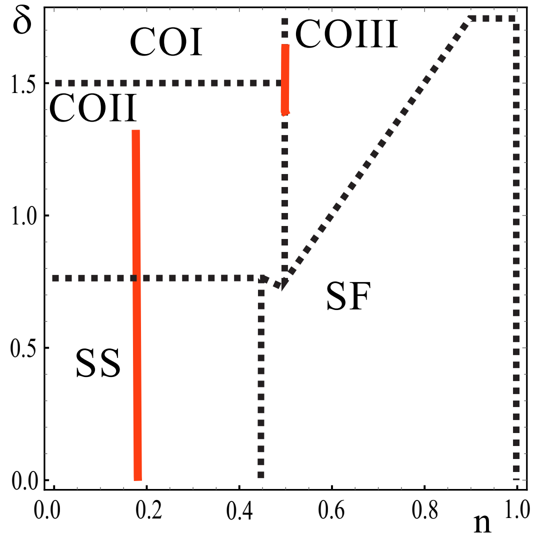

Fig. 1. The δ-n ground state phase diagrams for the model system given $V/t = 0.75$ (dotted lines are the MFA results, solid lines are the QMC results).

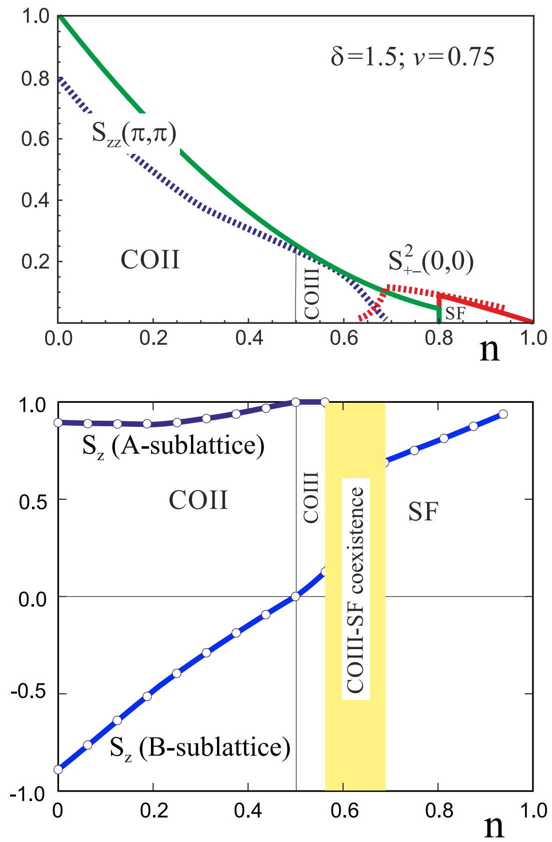

Fig. 2. Top panel: Correlation functions for the model S=1 pseudospin system given $\Delta/t = 1.5$, $V/t = 0.75$, solid lines are the MFA results, dotted lines are the QMC results. Bottom panel: QMC data for the sublattice S_z-components as functions of the deviation from the half-filling. Filling points to a COIII-SF coexistence phase typical for the first kind phase transition.

core bosons [6, 8]. In Fig. 1 (dotted curves) we present an example of the MFA $\delta - n$ phase diagrams calculated given $v = 0.75$. At half-filling $n = 0$ the positive values of the correlation parameter δ stabilize a limiting COI phase with $\langle S_{A,Bz}\rangle = \langle S^2_{A,Bz}\rangle = 0$, or a "parent Cu^{2+} phase" for a model cuprate, while positive values of v stabilize a limiting COII phase with $\langle S_{A,Bz}\rangle = \pm 1$; $\langle S^2_{A,Bz}\rangle = 1$, or a checkerboard "antiferromagnetic" order of pseudospins along z-axis, or a disproportionated Cu^{1+}-Cu^{3+} phase for a model cuprate. As a result of the competition between the on-site and inter-site correlations we arrive at a "starting" COI phase for $\delta > 2v$ or COII phase for $\delta \leqslant 2v$. At n=0.5 we see a transformation of the COI and COII phases into the COIII phase. The line of the first order phase transition COIII-SF in Fig. 1 corresponds to the equality of the respective energies. It is worth to note that the critical concentration n for the SS-SF, COI, COII-COIII transitions does not depend on the correlation parameter δ. In Fig. 2 (top panel, solid lines) we present the n-dependence of the correlation functions $S_{zz}(\pi,\pi)$=$\langle S_z, S_z\rangle$ (static structure factor) and $S^2_{+-}(0,0)$=$\langle S^2_+, S^2_-\rangle$ at δ=1.5, v=0.75, determining the long-range CO and SF orders, respectively, given $\Delta/t = 1.5$, that is in an immediate closeness to COII-COI phase transition for small n.

4. Quantum Monte-Carlo calculations

We have performed Quantum Monte-Carlo (QMC) [9] calculations for our model Hamiltonian (1). In Fig. 1 (solid lines) we compare the ground state $\delta - n$ phase diagram of our model 2D system calculated on square lattice 8×8 given $v = 0.75$ with that of calculated within MFA approach. As for simple hard-core counterpart [6,8], despite some qualitative agreement, we see rather large quantitative difference between two curves in Fig. 1. In particular, it concerns a clearly larger volume of the quantum SF phase that might be related with a sizeable suppression of quantum fluctuations within MFA approach. In Fig. 2 (top panel, two dotted lines) we present the QMC calculated static structure factor $S_{zz}(\pi,\pi)$ and the superfluid (pseudospin nematic) correlation function $S^2_{+-}(0,0)$. It is worth to note a semiquantitative agreement with the MFA data. Smaller value of the quantum structure factor $S_{zz}(\pi,\pi)$ at n=0 is believed to be a result of the pseudospin reduction due to quantum fluctuations. Bottom panel in Fig. 2 shows the n-dependence of the mean sublattice S_z values, S_{Az} and S_{Bz}, that clearly demonstrates the pseudospin quantum reduction effect within COII phase and specific features of the sublattice occupation, or "pseudo-magnetization" under COII-COIII-SF transformation.

5. Conclusions

A simplified 2D $S = 1$ pseudospin Hamiltonian with a two-particle transport term (pseudospin nematic coupling) was analyzed within a generalized MFA and QMC technique.

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References

[1] A.S. Moskvin, *JETP* **121**, 477 (2015).

[2] A.S. Moskvin, *Phys. Rev. B* **84**, 075116 (2011).

[3] A.S. Moskvin, *J. Phys.:Condens. Matter* **25**, 085601 (2013).

[4] A.S. Moskvin, *J. Phys.: Conf. Ser.* **592**, 012076 (2015).

[5] A.S. Moskvin, Yu.D. Panov, F.N. Rybakov, A.B. Borisov, *J. Supercond. Nov. Magn.* **30**, 43 (2017).

[6] R. Micnas, J. Ranninger, S. Robaszkiewicz, *Rev. Mod. Phys.* **62**, 113 (1990).

[7] N.A. Mikushina, A.S. Moskvin, *Phys. Lett. A* **302**, 8 (2002).

[8] G. Schmid, S. Todo, M. Troyer, A. Dorneich, *Phys. Rev. Lett.* **88**, 167208 (2002).

[9] V.G. Rousseau, *Phys. Rev. E* **78**, 056707 (2008).