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 (EHB) 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 $M_S = -1, 0, 1$, 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$_4$]$^{2−;6−;5−}$ (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 $\mathbf{S}$ and five spin-quadrupole operators $Q_{ij} = (\frac{1}{2}[S_i, S_j] − \frac{3}{4} \delta_{ij})$ whose mean values define so-called spin-nematic phase. Spin operators $S_{\pm}$ and $T_{\pm} = \{S_{\pm}, S_{\mp}\}$ change the pseudospin projection (and occupation numbers) by $\pm 1$, while $S_{\pm}$ changes the pseudospin projection by $\pm 2$.

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:

$$\hat{H} = -t \left( \sum_{\langle ij \rangle} (S_{iz}^2 - \mu S_{iz}) + V \sum_{\langle ij \rangle} S_{iz} S_{jz} \right).$$

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 $\mu$ for boson systems with a boson density constraint:

$$\frac{1}{N} \sum_i \langle S_{iz} \rangle = n,$$

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 intersite 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 or 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 $|M| \neq 1$ 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

$$|\psi \rangle = c_{-1}| -1 \rangle + c_0|0 \rangle + c_1|1 \rangle, \quad (3)$$

where the $c_M$ coefficients can be represented as follows

$$c_1 = \sin \frac{\theta}{2} \cos \phi e^{i \frac{\phi}{2}}, \quad c_0 = \cos \frac{\theta}{2} e^{i \frac{\phi}{2}},$$

$$c_{-1} = \sin \frac{\theta}{2} \sin \phi e^{i \frac{\phi}{2}} \quad (4)$$

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

$$E = \frac{\Delta}{2} \sum_i (1 - \cos \theta_i) - \frac{\mu}{2} \sum_i (1 - \cos \theta_i) \cos \phi_i \quad (5)$$

$$+ \frac{V}{4} \sum_{\langle ij \rangle} (1 - \cos \theta_i)(1 - \cos \theta_j) \cos \phi_i \cos \phi_j$$

$$- \frac{t}{8} \sum_{\langle ij \rangle} (1 - \cos \theta_i)(1 - \cos \theta_j) \sin \phi_i \sin \phi_j \cos (\alpha_i - \alpha_j).$$

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 $\beta$, so the $\beta$ remains undetermined. Below we denote $\delta = \Delta/t$ and $\nu = V/t$. 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 $\langle S_{A,B}^2 \rangle \neq 0$ and three charge ordered phases with $\langle S_{A,B}^2 \rangle = 0$ but different types of the sublattice occupation (pseudospin $S_z$ components):

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

**Supersolid (SS) phase:** $\langle S_{A,B}^2 \rangle = 1$,

$$\langle S_{A,B}^2 \rangle = n \mp \sqrt{1 + n^2 - \frac{4n}{\nu^2 + 1}}, \quad \langle S_{A,B}^2 \rangle = \frac{1}{2} \sqrt{1 + n^2 - \frac{4n}{\nu^2 + 1}}.$$ 

**Charge ordered COI phase:** $\langle S_{A,B} \rangle = 0$, $\langle S_{A,B}^2 \rangle = 0$,

$\langle S_{Bz} \rangle = 2n$, $\langle S_{Bz}^2 \rangle = 2|n|$, $\{ |n| \leq 0.5 \}$.

**Charge ordered COII phase:** $\langle S_{A,B} \rangle = 2n - \text{sgn} n$, $\langle S_{A,B}^2 \rangle = 2n - \text{sgn} n$,

$\langle S_{Bz} \rangle = 1 - 2|n|$, $\langle S_{Bz}^2 \rangle = 2n - \text{sgn} n$, $\langle S_{Bz}^2 \rangle = 1$, $\{ |n| \leq 0.5 \}$.

**Charge ordered COIII phase:** $\langle S_{A,B} \rangle = \text{sgn} n$,

$\langle S_{A,B}^2 \rangle = 1$, $\langle S_{Bz} \rangle = 2n - \text{sgn} n$, $\langle S_{Bz}^2 \rangle = 2|n| - 1$, $\{ |n| \geq 0.5 \}$.

Interestingly, all the local order parameters do not depend on the correlation parameter $\Delta$, 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-
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 $\delta$ stabilize a limiting COI phase with $<S_{A,Bz}> - <S_{A,Bz}^0> = 0$, or a “parent Cu$^{2+}$ phase” for a model cuprate, while positive values of $v$ stabilize a limiting COII phase with $<S_{A,Bz}> = \pm 1$; $<S_{A,Bz}^0> = 1$, 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 $\delta \leq 2v$. 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 COII-COIII 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 $\delta$. In Fig. 2 (top panel, solid lines) we present the $n$-dependence of the correlation functions $S_{zz}^2(\pi, \pi) = \langle S_z^2, S_z^2 \rangle$ (static structure factor) and $S_{zz}(0,0) = \langle S_z^2, S_z^2 \rangle$ at $\delta=1.5$, $v=0.75$, 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 $8 \times 8$ 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 $S_{zz}(0,0)$. 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