The MFA ground states for the extended Bose-Hubbard model with a three-body constraint

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\textbf{Abstract}

We address the intensively studied extended bosonic Hubbard model (EBHM) with truncation of the on-site Hilbert space to the three lowest occupation states \( n = 0, 1, 2 \) in frames of the \( S = 1 \) pseudospin formalism. Similar model 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 \( \text{Cu}^{1+;2+;3+} \). 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 with a two-particle transport to find the ground state phase with its evolution under deviation from half-filling.

\textit{Keywords:} cuprates, pseudospin formalism, mean-field

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\textbf{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 \( M = -1, 0, 1 \), respectively (see \cite{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 \([\text{CuO}_4]^{7-;6-;5-} \) (nominally \( \text{Cu}^{1+;2+;3+} \)) \cite{2,3,4,5}.

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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 \( Q_{ij} = \frac{1}{2} \{ S_i, S_j \} - \frac{4}{3} \delta_{ij} \) 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 \( \pm 1 \), while \( S_\pm^2 \) 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:

\[
\hat{H} = \sum_i (\Delta S_{iz}^2 - \mu S_{iz}) + V \sum_{\langle ij \rangle} S_{iz} S_{jz} - t \sum_{\langle ij \rangle} (S_{iz}^2 S_{jz}^2 + S_{iz} S_{jz}^2),
\]

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 \( \parallel Z \) which acts as analog of chemical potential \( \mu \) for doped charge with a charge constraint:

\[
\sum_i \langle S_{iz} \rangle = nN,
\]

where fixed \( n \) is the doped charge density. 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 \( \hat{H} \) 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 parameter \( \Delta = U/2 \) 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.

3. Mean-field approximation

To analyze 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 $|c\rangle = c_{-1}|-1\rangle + c_0|0\rangle + c_{+1}|+1\rangle$, (3) where the $c_M$ coefficients can be represented as follows
\[
c_{-1} = \sin \frac{\theta}{2} \cos \frac{\phi}{2} e^{-i \frac{\beta}{2}}, \quad c_0 = \cos \frac{\theta}{2} e^{i \frac{\beta}{2}}, \quad c_{+1} = \sin \frac{\theta}{2} \sin \frac{\phi}{2} e^{i \frac{\beta}{2}}
\] (4)
with $\theta$, $\phi$, $\alpha$, $\beta$ to be parameters defined by the minimization of the energy. The MFA energy can be written as follows
\[
E = \frac{\Delta}{2} \sum_i \left(1 - \cos \theta_i\right) + \frac{V}{4} \sum_{(ij)} \left(1 - \cos \theta_i\right) \left(1 - \cos \theta_j\right) \cos \phi_i \cos \phi_j -
\frac{t}{8} \sum_{(ij)} \left(1 - \cos \theta_i\right) \left(1 - \cos \theta_j\right) \sin \phi_i \sin \phi_j \cos(\alpha_i - \alpha_j) -
- \frac{\mu}{2} \sum_i \left(1 - \cos \theta_i\right) \cos \phi_i.
\] (5)

Here, the term with the chemical potential $\mu$ takes into account the constraint \[2\]. 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.

In a two-sublattice A-B model, we arrive at the five MFA uniform phases for the ground state (GS). The energies and parameters of solutions are listed in Table 1. We use the notations: $\varepsilon = E/(tN)$, $\delta = \Delta/t$, $\nu = V/t$, $\sigma = \text{sgn} \, n$, $a = \sqrt{\frac{2\nu+1}{2\nu-1} - |n|}$, $b = \sqrt{\frac{2\nu-1}{2\nu+1} - |n|}$. In all phases, the value of chemical potential $\mu$ satisfies the regular expression $\mu = t \partial \varepsilon / \partial n$. The solutions for SF and SS phases imply that $\alpha_A - \alpha_B = 0$ or $\pi$, in other phases this difference remains undefined.

| $\varepsilon$ | $\cos \theta_j$ | $\cos \phi_j$ |
|--------------|----------------|----------------|
| SF $\delta - 1 + n^2(2\nu + 1)$ | $-1$ | $n$ |
| SS $\delta - 2\nu + 2|n|\sqrt{4\nu^2 - 1}$ | $-1$ | $n + (-1)^j ab$ |
| CO1 $|n| \delta$ | $1 - 2|n| + 2(-1)^j n$ | $\sigma$ |
| CO2 $(1 - |n|) \delta + 4 \left(|n| - \frac{1}{2}\right) \nu$ | $-1 + 2|n| + 2(-1)^j n$ | $(-1)^{j+1}$ |
| CO3 $|n| \delta + 4 \left(|n| - \frac{1}{2}\right) \nu$ | $1 - 2|n| + 2(-1)^j \sigma (1 - |n|)$ | $\sigma$ |

Table 1: The energies and parameters of MFA GS phases. The index $j$ is 0(1) for A(B) sublattice. The details of notations see in the text.
The GS MFA phases differ by local charge density $\langle S_z\rangle$ and local density of $M = 0$ (Cu$^{2+}$) states $\langle P_0\rangle = 1 - \langle S_2^z\rangle$:

$$\langle S_z\rangle = \frac{1}{2} (1 - \cos \theta) \cos \phi, \quad \langle P_0\rangle = \frac{1}{2} (1 + \cos \theta),$$

and by local superfluid order parameter, or pseudospin nematic order $\langle S_2^\pm\rangle$:

$$\langle S_2^\pm\rangle = \frac{1}{4} (1 - \cos \theta) \sin \phi \ e^{\pm i \alpha}.$$  

The density of superfluid component is related to helicity modulus [8]. This allow us to find an expression of the superfluid density $\rho$ in terms of local superfluid order parameters in the two-sublattice MFA:

$$\rho = \text{Re} \left( \langle S_{2A}^\pm\rangle \langle S_{2B}^\pm\rangle \right).$$

The local order parameters for the GS MFA phases are listed in Table 2. Bose superfluid (SF) and supersolid (SS) phases are completely analogous to phases of charged hard-core bosons [6, 9] as these phases have no the $M = 0$ states. The superfluid density in SF phase, $\rho = (1 - n^2)/4$, has maximum value at $n = 0$ and does not depend on inter-site density-density interactions parameter $\nu$. In SS phase, the superfluid density $\rho = |n|/(2\sqrt{4\nu^2 - 1})$ decreases with rising of $\nu$. The charge density differs on sublattices in SS phase and this phase becomes the pure charge-ordered one at $n = 0$.

Stability conditions for SF phase

$$\delta < 2, \quad n^2 > \frac{2\nu - 1}{2\nu + 1},$$

and for SS phase

$$\delta < 2, \quad \nu > \frac{1}{2}, \quad \sqrt{\frac{2\nu - 1}{2\nu + 1} - \frac{(1 - \frac{\delta}{4\nu^2 - 1})^2}{\delta\sqrt{4\nu^2 - 1}}} < |n| < \sqrt{\frac{2\nu - 1}{2\nu + 1}}.$$
define the boundary expression for SF and SS phases: 
\[ n^2 = \frac{(2
\nu - 1)}{(2\nu + 1)} \].
As the energies of SF and SS phases have the same dependence on the correlation parameter \( \delta \) (see Table [1]), the line of the SF-SS transition does not change with \( \delta \).

Three charge ordered MFA phases with \( \langle S_{A,B,\pm}^2 \rangle = 0 \) but different types of the sublattice occupation emerge if \( \delta > 0 \) and completely displace the superfluid phases at \( \delta > 2 \).

Stability conditions for the charge ordered 1 (CO1) are given by inequality

\[ |n| < \min \left\{ \frac{1}{2}, \frac{\delta}{4
\nu} \right\}. \]  

(11)

Given \( n = 0 \) the CO1 phase consists of \( M = 0 \) centers. The striking feature of the CO1 phase is the independence of energy on inter-site interaction parameter \( \nu \). According to the two sublattices mean field approach, upon doping only one of the sublattices begins to be filled by \( M = \pm 1 \) centers depending on the sign of \( n \). Numerical simulations with classical Monte-Carlo show that there is no difference in the sublattices occupations while \( |n| \ll 1/2 \), but this difference arises at \( |n| \to 1/2 \) according to the MFA expressions for \( \langle S_z \rangle \) and \( \langle P_0 \rangle \).

Charge ordered 2 (CO2) phase has the stability conditions given by the expression

\[ |n| < \min \left\{ \frac{1}{2}, 1 - \frac{\delta}{4
\nu}, \frac{8\delta\nu - \delta^2 - 2}{8|1 - \delta\nu|} \right\}. \]  

(12)

At \( n = 0 \), the CO2 phase is fully polarized, and with a deviation from \( n = 0 \) one of the sublattices is filled by \( M = \pm 1 \) centers depending on the sign of \( n \).

The line of the CO1-CO2 transition for all \( |n| < 1/2 \) is defined by the equality of energies of these phases.

Given \( |n| = 1/2 \) the parameters of CO1 and CO2 phases become equal to that of the charge ordered 3 (CO3) phase. Stability conditions of the CO3 phase are given by

\[ \frac{1}{2} \leq |n| < \min \left\{ 1, \frac{8\delta\nu + \delta^2 + 4}{8(1 + \delta\nu)} \right\}. \]  

(13)

For the CO3 phase at \( n = 1/2 \), one of the sublattices is completely filled with \( M = 1 \) or \( M = -1 \) centers depending on the sign of \( n \), while the second is completely filled by \( M = 0 \) centers. With the \( |n| \) rising, the second sublattice is also filled by \( |M| = 1 \) centers.

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 and the stability conditions \([9,13]\) we arrive at very rich and intricate phase diagrams for the model system as compared with relatively simple phase diagrams for hard-core bosons \([4,9]\). The kind of transition between the GS phases is determined by the limiting values of the order parameters (see Table [2]) on the transition lines. The SF-SS transition does not lead to discontinuities of the order parameters (the transition of the second kind) except the jump of the local superfluid order parameter.
Figure 1: (Color online) The MFA GS phase diagrams for the inter-site interaction parameter $\nu$ variation (upper panels) and for the on-site correlation parameter $\delta$ variation (lower panels).

$\langle S^2 \rangle$ at $n = 0$ (the point of the first kind transition). The CO1-CO3 and CO2-CO3 transitions at $n = 1/2$ are also continuous (of the second kind). All other transitions are discontinuous (of the first kind).

In Fig. 1 (upper panels) we show the MFA GS phase diagrams for the inter-site interaction parameter $\nu$ variation and for the on-site correlation parameter $\delta$ variation (lower panels). For $\delta = 0$, the phase diagram is the same as for hc-bosons [6]. With increasing $\delta$, superfluid phases are rapidly replaced with the charge ordered phases. The replacement of the SS phase begins at $\delta > 0$ in the region of large values of the parameter $\nu$. SS phase disappears completely when $\delta \approx 1.15$. For $\delta > 1$, in the region of small values of the parameter $\nu$, the CO1 phase appears, which begins to displace the SF phase. This process begins at $n = 0$, where the value of the density of the superfluid component is maximal. For $\delta \geq 2$, the SF phase is completely replaced with the charge ordered phases.

Evolution with a change in the parameter $\nu$ also shows a rapid decrease in the fraction of superfluid phases on the phase diagram in comparison with the charge ordered phases. The most complicated phase diagram is observed for $\delta \approx 1.1$, $\nu \approx 0.65$ where the competition of the on-site and inter-site interactions manifests itself most strongly. At half-filling $n = 0$ the positive values of the correlation parameter $\delta$ stabilize a limiting CO1 phase with $\langle S_{A,Bz} \rangle = \langle S_{A,Bz}^2 \rangle = 0$, or a "parent Cu$^{2+}$" phase for a model cuprate, while positive values of $\nu$ stabilize a limiting CO2 phase with $\langle S_{A,Bz} \rangle = \pm 1$, $\langle S_{A,Bz}^2 \rangle = 1$, 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" CO1 phase for $\delta > 2\nu$ or CO2 phase for $\delta \leq 2\nu$. At $n = 0.5$ we see a transformation of the CO1
Figure 2: (Color online) The $n$-$\delta$ GS phase diagrams for the model system given $\nu = 0.75$. Left panel shows the MFA results, right panel shows the QMC results.

Figure 3: (Color online) Left panel: Correlation functions for the model $S = 1$ pseudospin system given $\delta = 1.5$, $\nu = 0.75$, solid lines are the MFA results, dotted lines are the QMC results. Right panel: QMC data for the sublattice $S_z$-components as functions of the deviation from the half-filling. Filling points to a CO3-SF coexistence phase typical for the first kind phase transition.

and CO2 phases into the CO3 phase. The line of the first order phase transition CO3-SF in Fig. 2 corresponds to the equality of the respective energies. It is worth to note that the critical concentration $n$ for the SS-SF, CO1-CO3 and CO2-CO3 transitions does not depend on the correlation parameter $\delta$.

In Fig. 3 (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 $S_{z-}(0,0) = \langle S_z^2, S_z^2 \rangle$ at $\delta = 1.5$, $\nu = 0.75$, determining the long-range CO and SF orders, respectively, given $\delta = 1.5$, that is in an immediate closeness to CO2-CO1 phase transition for small $n$.

4. Quantum Monte-Carlo calculations

We have performed Quantum Monte-Carlo (QMC) calculations for our model Hamiltonian $H$. In Fig. 2 we compare the ground state $\delta$-$n$ phase dia-
gram of our model 2D system calculated on square lattice $12 \times 12$ given $\nu = 0.75$ with that of calculated within MFA approach. As for a simple hard-core counterpart [6, 9], despite some qualitative agreement, we see rather large quantitative difference between two diagrams in Fig. 2. 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. The SF-SS transition line does not depend on the correlation parameter $\delta$ in MFA calculations as well as in QMC ones since both these phases consist of only the $M = \pm 1$ states having the same dependence of the energy on $\delta$. The location of the CO1-CO3 and CO2-CO3 transition lines at $|n| = 0.5$, both for MFA and QMC, has a trivial structural reason. The filling of the lattice by $M = \pm 1$ centers for CO1 phase or by $M = 0$ centers for CO2 phase during the doping leads on the lines $n = \pm 0.5$ to identical result that minimizes the energy of the inter-site density-density interactions. Namely, this is the initial state of CO3 phase, when the first sublattice is completely filled by $M = 0$ centers and the second one is completely filled by $M = \pm 1$ centers. In contrast to MFA, the CO1-CO2 transition line in QMC calculations shows evident dependence on $n$ that implies a more complicated structure of the CO1 and CO2 phases as compared with MFA. This leads, in particular, to the fact that the triple point of the CO1-CO2-CO3 phases shifts from the MFA values $n = 0.5, \delta = 1.5$ to $n = 0.5, \delta = 2.0$.

In Fig. 3 (left 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. Right panel in Fig. 3 shows the $n$-dependence of the mean sublattice $S_z$ values, $S_{A_z}$ and $S_{B_z}$, that clearly demonstrates the pseudospin quantum reduction effect within CO2 phase and specific features of the sublattice occupation, or "pseudomagnetization" under CO2-CO3-SF transformation. Also, note that these QMC data points to the CO3-SF phase coexistence typical for the first kind phase transition, but obviously absent in MFA.

It should be noted that the results of QMC calculations for the system $12 \times 12$ presented here vary slightly compared to the system $8 \times 8$, that supports their validity. Calculations for larger lattices are in progress.

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. We have obtained the ground-state phase diagrams and correlation functions given different values of the coupling parameters with a focus on the role of the on-site correlation effect (single-ion anisotropy). The comparison of the two methods allows us to uncover fundamental shortcomings of the MFA technique and clearly demonstrate the role of quantum effects.
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