Critical Temperatures of Hard-Core Boson Model on Square Lattice within Bethe Approximation

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Abstract—Neighboring correlations are considered for a two-dimensional hard-core boson model on square lattice within Bethe approximation for the clusters consisting of two and four nodes. Explicit equations are derived for the determination of critical temperatures of charge and superfluid ordering and their solutions are considered for various ratios of the parameter of between-centers charge correlations to the transfer integral. It is demonstrated that assumption of neighboring correlations for the temperatures of charge ordering results in the appearance of the critical concentration of bosons, which restricts the existence domain of the solutions of charge ordering type. In the case of superfluid ordering with the assumption of neighboring correlations, the critical temperature is reduced up to zero values at half filling. A phase diagram of the hard-core boson model is constructed with the assumption of phase separation within Maxwell construction and it is shown that consideration of neighboring correlations within Bethe approximation quantitatively approximates the form of phase diagram to the results of Monte Carlo quantum method.

Keywords: hard-core bosons, phase diagram, Bogolyubov inequality, Bethe approximation

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1. INTRODUCTION

Lattice boson models are extensively employed for the description of the systems demonstrating nontrivial phase diagram with competing or mixed states. The hard-core boson model was initially suggested for rationalization of the features of phase diagram of superfluid 4He [1, 2] and various variants of this model are currently used for the description of the characteristics of a large number of physical systems including high-temperature superconductors [3, 4], ultracold atoms in optical lattices [5], excitons in nanotubes [6], and magnetic insulators in external field [7]. An interest in these models has grown in recent years after discovery of the coexistence of charge ordering and superconductivity in cuprates [8–10].

Hamiltonian of hard-core charged bosons is following [1, 3]:

\[ \mathcal{H} = -t \sum_{\langle i,j \rangle} (b_i^+ b_j + b_j^+ b_i) + V \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_i n_i, \]

where \( b^+ (b) \) corresponds to the creation (annihilation) operators of hard-core bosons with Bose-type commutation relations for different nodes \( [b_i, b_j^+] = 0, i \neq j \), and Fermi-type relations on one node: \( [b_i, b_j^+] = 1 \), \( n_i = b_i^+ b_i \) is the operator of the number of hard-core bosons on a node, \( t \) and \( V \) correspond to the transfer integral and parameter of charge correlations between closest neighbors, and \( \mu \) is chemical potential, which is necessary for the assumption of the conditions of constant concentration of bosons: \( nN = \sum_i \langle n_i \rangle \), where \( N \) is the total number of nodes. We further consider hard-core bosons on a planar square lattice.

Diagram of the main state of the system of hard-core bosons within mean-field approximation (MFA) is well known [3, 11] and is given in Fig. 1a in \( (n, V/t) \) variables. Superfluid (SF) represents the main state at all \( n \) values on the left from the Heisenberg point \( V/t = 2 \); charge ordering (CO) is realized on the right at \( n = 1/2 \); SF phase is realized at \( |n - 1/2| > \eta^* \); and the main state is represented by supersolid (SS) at \( 0 < |n - 1/2| < \eta^* \), the phase, in which the charge and superfluid ordering parameters are different from zero. The conditions for the existence of the SS phase and its stability against phase separation (PS) into macroscopic domains of SF and CO phases remain the subject of discussion and detailed studies. Numerical calculations using quantum Monte Carlo method show the stability of the SS phase in the models with frustrating interactions on triangular lattice [12–15] or on square lattice with the assumption of interaction with secondary neighbors [16–19]. A stable SS phase was also identified in various variants of the Bose—Hubbard model.
[5]. PS and SS phases coincide in the case of model (1) within MFA in the main energy state and the existence domain, while the SS phase is metastable at final temperature [20, 21]: its energy is always larger than that of the PS state. Phase (n, T) diagram of model (1) within MFA [11] is given in Fig. 1b for V/t = 3. Its interesting feature is the presence of the CO phase at n ≠ 1/2, which transforms into PS state with a decrease in temperature. The PS domain starts from a tricritical point M. Phase diagram of model (1) for V/t = 3 (Fig. 1c) obtained by quantum Monte Carlo method at V/t = 3 (according to the data from [22]).

A large number of studies of the lattice boson models is devoted to the calculations using quantum Monte Carlo method. Analytically different characteristics of the hard-core boson system were studied using spin wave method [3, 23–27] and different variants of Green function method [3, 8, 29], in addition to the mean-field method. In this work, influence of the assumption of neighboring correlations within Bethe approximation was considered. In the case of the clusters consisting of two and four nodes, critical temperatures of model (1) were determined and evolution of phase diagrams in (n, T) variables depending on these approximations was considered.

The paper is organized as follows. Main relationships for Bethe approximation in the hard-core boson model on a two-dimensional square lattice were written in section 2. Section 3 is devoted to the study of the behavior of critical temperatures for various V/t ratios and phase (n, T) diagrams were constructed with the assumption of phase separation. We compare these results with MFA and Monte Carlo quantum method. The last chapter is devoted to conclusions.

2. BETHE APPROXIMATION FOR CLUSTERS CONSISTING OF TWO AND FOUR NODES

The hard-core boson system is equivalent to quantum magnetic with a constant magnetization, the system of pseudospins s = 1/2 in external field directed along the z axis [1], which is described by following Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} (s_i^+ s_j^- + s_i^- s_j^+) + V \sum_{\langle i,j \rangle} s_i^z s_j^z - h \sum_i s_i^z + E_0,$$

where $s_i^+ = b_i^*, \ s_i^- = b_i$, $s_i^z = 1/2 - n_i$, $h = 2V - \mu$, and $E_0 = N\epsilon_0 = N(V - \mu)/2$.

In order to evaluate large potential $\Omega(\mathcal{H})$, we employ Bogolyubov inequality: $\Omega(\mathcal{H}) \leq \Omega = \Omega(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0 \rangle$, where zero-order Hamiltonian $\mathcal{H}_0$ appears as the sum of Hamiltonians $\mathcal{H}_c$ for noninteracting Bethe clusters from c nodes covering the entire lattice: $\mathcal{H}_0 = \Sigma \mathcal{H}_c$. Variants of the clusters employed by us are given in Fig. 2. Let us define two sublattices $\alpha = A, B$ on a square lattice and write equation for $\mathcal{H}_c$ as follows:

$$\mathcal{H}_c = -t \sum_{\langle i,j \rangle} (s_i^+ s_j^- + s_i^- s_j^+) + V \sum_{\langle i,j \rangle} s_i^z s_j^z - g_a \sum_{i=1}^{c} s_i - g_a \sum_{i=1}^{c} (-1)^\alpha s_i,$$

Here, summation is performed by cluster nodes, $(-1)^A = 1$ and $(-1)^B = -1$, and $g_{\alpha, \sigma}$ are molecular...
fields, which represent variational parameters and consider interaction of Bethe cluster with environment. MFA formally corresponds to Hamiltonian (3) containing only the components with molecular fields.

Isotropic character of transfer in \((x, y)\) plane allows one to restrict only to \(x\) and \(z\) components of molecular fields. After calculating the statistical sum for the cluster \(Z_c = \text{Tr}_\text{exp}(-\beta \mathcal{H}_c), \) where \(\beta = 1/(k_B T)\) (we further consider that \(k_B = 1\)), let us write equations through molecular fields for the deviation of the concentration of bosons from half filling, \(\eta = 1/2 - n\), and various ordering parameters (OPs):

\[
\eta = \frac{1}{c\beta} \frac{\partial \ln Z_c}{\partial g_f^z}, \quad \xi = \frac{1}{c\beta} \frac{\partial \ln Z_c}{\partial g_a^z}, \\
\rho = \frac{1}{c\beta} \frac{\partial \ln Z_c}{\partial g_f^x}, \quad \chi = \frac{1}{c\beta} \frac{\partial \ln Z_c}{\partial g_a^x}.
\]

(4)

Here, \(\xi\) and \(\rho\) correspond to charge and superfluid OPs and \(\chi\) is the asymmetry of superfluid OP.

Estimate of the large potential calculated on one lattice node, \(\omega = \Omega/N\), is following:

\[
\omega = -\frac{1}{c\beta} \ln Z_c + aV(\eta^2 - \xi^2) - 2at(\rho^2 - \chi^2) + \eta g_f^z + \xi g_a^z + \rho g_f^x + \chi g_a^x - h\eta + \epsilon_0,
\]

(5)

where \(a = 2\) for MFA, \(a = 3/2\) for the cluster made from two nodes, and \(a = 1\) for the cluster made from four nodes. Minimizing \(\omega\) by molecular fields, we have the equations for OP:

\[
2aV\eta = -g_f^z + h, \quad 2aV\xi = g_a^z, \quad 4at\rho = g_f^x, \quad 4at\chi = -g_a^x.
\]

(6)

Let us determine critical temperatures from the condition of loss of stability of minimum \(\omega\) for the NO phase relative to the variation by corresponding molecular field. Following equation is derived for the temperature of charge ordering, \(T_{\text{CO}}\):

\[
2aV \left( \frac{\partial \xi}{\partial g_a^z} \right)_0 = 1,
\]

(7)

whereas the equation is written as follows for the temperature of superfluid transition, \(T_{\text{SF}}\):

\[
4at \left( \frac{\partial \rho}{\partial g_f^x} \right)_b = 1.
\]

(8)

In Eqs. (7) and (8), derivative is calculated at \(g_a^z = 0\), \(g_f^z = 0\), and \(g_a^x = 0\). In order to obtain the dependence on the concentration of bosons, these equations need to be solved along with Eq. (4) for \(\eta\). It should also be noted that analogous equation for critical temperature of disorder–order transition related to variation of \(g_a^z\) does not have solution.

The PS domain on the phase diagram in \((n, T)\) variables can be determined using Maxwell construction [30–32]. Solving Eq. (6) individually for the CO phase and for the SF phase, we determine the parameter \(\eta^*\), at which the values of large potential are identical in these phases, \(\omega_{\text{CO}}(\eta^*) = \omega_{\text{SF}}(\eta^*)\), and we determine boundary concentrations of the PS domain for \(\eta\) from Eq. (4), \(\eta_{\text{CO}}(\eta^*)\) and \(\eta_{\text{SF}}(\eta^*)\).

3. RESULTS

Equations (7) and (8) within MFA result in well-known equations [11] for critical temperatures:

\[
\frac{T_{\text{CO}}}{V} = 1 - 4\eta^2, \quad \frac{T_{\text{SF}}}{2t} = 4\eta \left( \ln \frac{1 + 2\eta}{1 - 2\eta} \right)^{-1}.
\]

In the case of the Bethe cluster made from two nodes, Eq. (7) is following for \(T_{\text{CO}}\):

\[
\cosh(\beta t) + 2g = \frac{3V}{4t}(1 - 4\eta^2),
\]

(9)

where

\[
g = \frac{1}{2} \sqrt{(1 - 4\eta^2)e^{-\beta V} + 4\eta^2 \cosh^2(\beta t)}.
\]

Equation (8) for \(T_{\text{SF}}\) with the assumption of Eq. (4) for the Bethe cluster made from two nodes can be reduced to following form:

\[
x^2 - \left( \frac{V}{2} + t \right)^2 = 6t \left( \frac{V}{2} + t \right) \frac{2\eta^2 \sinh(\beta t) - 2e^{\beta t} \left( \frac{1}{4} - \eta^2 \right) + g}{\cosh(\beta t) + 2g} + \eta x
\]

(10)

\[
= 6t \left( \frac{V}{2} + t \right) \frac{2\eta^2 \sinh(\beta t) - 2e^{\beta t} \left( \frac{1}{4} - \eta^2 \right) + g}{\cosh(\beta t) + 2g} + \eta x
\]

(11)
where
\[ x = \beta^{-1} \ln((2\eta \cosh(2\beta t) + 2g)/(1 - 2\eta)) + V/2. \]

In the case of the Bethe cluster made from four nodes, explicit form of equations for critical temperatures becomes more labor-consuming. Equation (7) for TCO can be written as follows:
\[ Z_0^{-1}[2\beta V + \frac{V}{t} \sinh(2\beta t)] \cosh(\beta y) + e^{\beta V} \frac{V^2}{2r} \left( \frac{\cosh(\beta d) + \frac{V^2}{2} + 8r}{Vd} \sinh(\beta d) - e^{\beta y} \right) = 1, \]

where \( d = \sqrt{V^2/4 + 8r^2} \) and
\[ Z_0 = 3 + e^{\beta V} + 2e^{2\beta V} \cosh(\beta d) + 2e^{-\beta V} \cosh(2\beta y) + 4(1 + \cosh(2\beta t)) \cosh(\beta y). \]

Here, \( Z_0 \) means a statistical sum of Bethe cluster in the NO phase. Equation (12) needs to be solved along with Eq. (4) for \( \eta \), which can be written as follows in this case:
\[ Z_0^{-1} \sinh(\beta y)(1 + \cosh(2\beta t) + 2e^{-\beta V} \cosh(\beta y)) = \eta. \]

Finally, Eq. (8) for the determination of \( T_{SF} \) can be written in explicit form as follows:
\[ 2tZ_0^{-1} \left[ \frac{2}{y} \sinh(\beta y) - \alpha e^{\beta y} (b_1 \cosh(\beta d) + b_2 \sinh(\beta d)) \right] \]

+ \[ ce^{\beta y} - 2e^{-\beta V} (c \cosh(2\beta y) + s \sinh(2\beta y)) \]

+ \[ e^{\beta y} (b_1 c \cosh(\beta y) + b_2 s \sinh(\beta y)) \]

− \[ e^{-2\beta V} (c \cosh(\beta y) + s \sinh(\beta y)) \]

\[ = 1. \]

Here, the parameters \( a = 2t + V, c = a/(a^2 - y^2), \) and \( s = y/(a^2 - y^2) \), and
\[ b_0 = y^4 - y^2 \left( 24t^2 - 4tV + V^2 \right) + 4a^2 t^2, \]
\[ b_1 = (y^2 + 4t(V - 7t))/b_0, \]
\[ b_2 = (y^2(8t + V) - 4t(40t^2 - 5tV + V^2))/b_0, \]
\[ b_3 = (y^4 - 4a^2 t(5t - V) - y^2(V - 4t^2))/b_0, \]
\[ b_4 = (y^2(32t^2 + 4tV + 3V^2) - 2a^2 (30t^2 - 8tV + V^2) - y^4)/(2db_0), \]

were introduced.

Equation (15) should also be solved along with Eq. (14).

Figure 3 shows solutions of Eqs. (10) and (12) for various \( V/t \) ratios. In the case of MFA, the reduced critical temperature of charge ordering, \( T_{CO}/V \), is described by a universal parabolic dependence on the concentration of bosons at all values of \( t \) parameter according to Eq. (9). Assumption of neighboring correlations within the Bethe approximation results in a quantitative decrease in the \( T_{CO}/V \) value and a fundamental change of the form of dependences of critical
temperature of charge ordering on the concentration of bosons. In the case of the final value of the \(V/t\) ratio, a critical concentration of bosons arises, \(|n_c - 1/2| = \eta_c\), which restricts the existence domain of critical temperature of charge ordering. In the case of two-node Bethe approximation, analysis of Eq. (10) gives the value of \(\eta_c = 1/2 - t/3V\), which could provide the critical value of \(V/t = 2/3\), below which there is no solution of Eq. (10) for \(T_{CO}\). It should also be noted that solutions of Eq. (10) are related to metastable states (for local minima of large potential) at the \(V/t\) values below the Heisenberg point, \(V/t < 2\); whereas at \(V/t > 2\), solutions of Eq. (10) correspond to the NO–CO transition only up to the tricritical point. Numerical analysis of Eq. (12) shows that there are no solutions at \(V/t < 1\) in the case of a four-node Bethe approximation. As follows from Fig. 3, the limiting dependence for \(T_{CO}\) at \(V/t \to \infty\) exists in the entire concentration range; however, the maximum value of reduced temperature at half filling is less than the MFA value by 5.5% in the case of two-node and by 12.5% in the case of four-node Bethe approximation.

The reduced critical temperatures of superfluid ordering, \(T_{SF}/(2t)\), which represent solutions of Eqs. (11) and (15) at different \(V/t\) ratios, are given in Fig. 4. A universal dependence for MFA (9) corresponds to the dotted line. Assumption of neighboring correlations within two- and four-node Bethe approximation results in the reduction of \(T_{SF}/(2t)\) value with an increase in the \(V/t\) ratio. This effect is always more pronounced in the case of four-node approximation.

Fundamental change involves a decrease in \(T_{SF}\) up to zero values at half filling with an increase in the \(V/t\) ratio. The limiting dependence of the reduced critical temperature at \(V/t \to 0\) possesses the maximum temperature at half filling as in the case of MFA; however, the magnitude is less than the MFA value by 7.5% in the case of two-node and by 16.5% in the case of four-node Bethe approximation. In contrast to charge ordering, solutions of Eqs. (11) and (15) for \(T_{SF}\) exist in the entire concentration range \(0 < |n| < 1/2\); however, a NO–SF transition corresponds only to the concentrations on the right from tricritical point at \(V/t > 2\).

Figure 5 shows the phase diagram of the hard-core boson model obtained within two- and four-node Bethe approximation at \(V/t = 3\). Dotted lines indicate the results of MFA for comparison [11]. Assumption of neighboring correlations leads to the narrowing of the domains for CO and PS phases; both maximum temperature and the concentration range decrease. The maximum of the temperature of charge ordering at half filling decreases by nearly 7% for two-node approximation and by 16% for four-node approximation relative to MFA. In the case of quantum Monte Carlo method, such decrease corresponds to 50%. The maximum temperature of ordering in the case of the SF phase also decreases after assumption of neighboring correlations and the concentration range increases. Tricritical point shifts towards half filling along the CO–PS line. On the whole, assumption of neighboring correlations within two- and four-node Bethe approximation approaches the form of phase diagram to the results obtained through quantum
Monte Carlo method [22]; however, fundamental feature related to the NO–PS transition is not reproduced within Bethe approximation; tricritical point represents the boundary point of the PS range within Bethe approximation.

4. CONCLUSIONS

We have considered the effect of the assumption of neighboring correlations for a two-dimensional hard-core boson model on a square lattice within Bethe approximation using the clusters made from two and four nodes. Explicit equations for critical temperatures of charge and superfluid ordering within mentioned approximations have been derived. Analysis of the obtained solutions for various ratios of the parameter of between-centers charge correlations and transfer integral \( V/t \) has shown fundamental differences of the concentration dependences of critical temperatures as compared to MFA. A critical concentration of bosons, which restricts the existence domain of solutions of CO type, arises at the temperatures of charge ordering. In the case of superfluid ordering, there is a reduction of critical temperature up to zero values at half filling. Phase diagram of the hard-core boson model has been constructed, which is obtained within two- and four-node Bethe approximation at \( V/t = 3 \) with the assumption of phase separation within Maxwell construction. It has been shown that assumption of neighboring correlations within Bethe approximation approaches the form of phase diagram to the results obtained by quantum Monte Carlo method [22].

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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