Cluster mean-field approach with density matrix renormalization group: Application to the hard-core bosonic Hubbard model on a triangular lattice

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We introduce a new numerical method for the solution of self-consistent equations in the cluster mean-field theory. The method uses the density matrix renormalization group method to solve the associated cluster problem. We obtain an accurate critical value of the supersolid-superfluid transition in the hard-core bosonic Hubbard model on a triangular lattice, which is comparable with the recent quantum Monte Carlo results. This algorithm is applicable to more general classes of models with a larger number of degrees of freedom.

KEYWORDS: cluster mean-field approach, density matrix renormalization group

1. Introduction

Ultracold bosonic gases have attracted current interest since the successful observation of the Bose-Einstein condensation in $^{87}$Rb atoms [1]. One of the interesting systems is a bosonic gas in the optical lattice, where local particle correlations suppress an itinerancy of atoms and yield the competition between the superfluid and solid states. In fact, the phase transitions between them have been observed in the bosonic systems on the cubic [2] and triangular lattices [3]. On the other hand, it has theoretically been suggested that a coexistence between the superfluid and solid states, a so-called supersolid state, is realizable in some models [4–6]. In the hard-core bosonic model, it has been clarified that the lattice geometry as well as intersite correlations play an important role to stabilize the supersolid state [7–9].

In the hard-core bosonic system on the triangular lattice, the existence of the supersolid state has been clarified in terms of the quantum Monte Carlo (QMC) method [7, 8]. However, around the half filling, some quantum states compete with each other and the nature of the phase transitions was not so clear. Recently, it has been clarified that on the symmetric case, a quantum phase transition is of second order, while it is of first order away from half filling by means of various methods [10–12]. Among them, the cluster mean-field (CMF) theory [13] is one of the simple and efficient methods to study the nature of the phase transitions. However, it is not so clear how the phase boundary depends on the cluster size treated in the CMF method, which may be crucial to determine the second-order critical point.

In this paper, we introduce the density matrix renormalization group (DMRG) technique [14–17] as a cluster solver. We then deal with different clusters systematically in the CMF+DMRG method to discuss the quantum phase transitions in the hard-core bosonic Hubbard model on the triangular lattice quantitatively.

The paper is organized as follows. In §2, we introduce the model Hamiltonian for the bosonic
system on the triangular lattice and summarize the CMF method with the DMRG technique. In §3, we discuss the quantum phase transition between the supersolid and superfluid states, and find that the obtained critical point is comparable with the recent results obtained by the QMC method [11]. A summary is given in the final section.

2. Model and Method

We consider zero-temperature properties in interacting bosons on the triangular lattice. Here, we assume sufficiently large onsite interactions. In the case, the system should be described by the following hard-core bosonic Hubbard model as,

\[ H = -t \sum_{\langle i, j \rangle} (\hat{a}_i \hat{a}_j^\dagger + \text{h.c.}) + V \sum_{\langle i, j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i, \tag{1} \]

where \( \langle i, j \rangle \) denotes the summation over nearest neighbor sites, \( \hat{a}_i \) is the creation (annihilation) operator at site \( i \) and \( \hat{n}_i = \hat{a}_i \hat{a}_i^\dagger \) is the number operator. \( t \) is the hopping integral, \( V \) is the intersite repulsion, and \( \mu \) is the chemical potential.

It is known that three kinds of ground states appears in the system depending on the ratio \( t/V \) and the filling \( \rho(= \sum_i \langle \hat{n}_i \rangle / N) \), where \( N \) is the total number of sites. When the interaction strength is small enough, the superfluid state with the order parameter, \( \Psi(= \sum_i \langle \hat{a}_i \rangle / N) \), is realized. On the other hand, in the strong coupling region, the solid states with \( \rho = 1/3 \) and \( 2/3 \) are realized, where the spatial distribution of bosons is schematically shown in Fig. 1. These solid phases are characterized by the structure factor \( S_Q[= \sum_i \langle \hat{n}_i \rangle \exp(-iQ \cdot r)/N] \), where \( Q = (4\pi/3, 0) \). Between these superfluid and solid states, two kinds of supersolid states appear with distinct fillings, where both order parameters (\( \Psi \) and \( S_Q \)) are finite [8].

To discuss the quantum phase transitions in the hard-core bosonic Hubbard model on the triangular lattice quantitatively, we make use of the CMF method. In the CMF method, the original lattice model is mapped to an effective cluster model, where particle correlations in the cluster can be taken into account properly. The expectation values of the inter-cluster Hamiltonian are obtained via a self-consistency condition imposed on the effective cluster problem. This method has an advantage in discussing quantum phase transitions correctly since not only stable and metastable states but also unstable states can be treated. Therefore, the CMF method has successfully been applied to the quantum spin systems [13, 18] and bosonic systems [10, 19]. As for the hard-core bosonic Hubbard model on the triangular lattice, the reasonable phase diagram has been obtained by means of the CMF method with the exact diagonalization (ED) [10, 19]. However, around the second-order critical point, the correlation length should diverge and the CMF+ED method with small clusters may not describe the critical phenomena.
To deal with larger clusters, we make use of the DMRG technique as an effective cluster solver. It is known that this method is powerful for the one-dimensional systems [14–17]. Furthermore, by combining the DMRG method with a mean-field theory, the phase transitions in the higher dimensions has been discussed in the Heisenberg models [20] and fermionic Hubbard models [21, 22]. Here, using the DMRG technique, we solve the effective cluster model with a ladder structure \((n_{\text{legs}} \times L)\), where \(n_{\text{legs}}\) is the number of legs and \(L\) is the length of the ladder, as shown in Fig. 2. The effective Hamiltonian is explicitly given as,

\[
H = H_{\text{intra}} + H_{\text{inter}},
\]

\[
H_{\text{intra}} = -t \sum_{(i,j)} (\hat{a}_i^\dagger \hat{a}_j + \text{h.c.}) + V \sum_{(i,j)} \hat{n}_i \hat{n}_j,
\]

\[
H_{\text{inter}} = -t \sum_{(i,k)'} (\hat{a}_i^\dagger \langle \hat{a}_k \rangle + \text{h.c.}) + V \sum_{(i,k)'} \hat{n}_i \langle \hat{n}_k \rangle,
\]

where the symbol \((i, j)\) \([(i, k)']\) denote the summation over nearest neighbor sites in the ladder (between ladders). \(\langle \hat{n}_k \rangle\) and \(\langle \hat{a}_k \rangle\) are the expectation values of the number and annihilation operators at site \(k\) in the nearest neighbor cluster. In the paper, we introduce \([4(L + n_{\text{legs}} - 1)]\) mean-fields \(\{\langle \hat{n}_k \rangle, \langle \hat{a}_k \rangle\}\). By solving the cluster model and calculating the expectation values by means of the DMRG method, we newly obtain mean-fields. In the CMF method, this iteration process is performed until these mean-fields are converged. Note that in the DMRG calculations, the quantum states \(M\) kept in each step are limited since the particle number does not conserve in the effective cluster model [eq. (2)]. However, the large number of the quantum states \(M\) is not needed in the framework of the CMF method. In fact, we did not find a visible difference of the results with \(M = 32\) and \(M = 64\). Therefore, we fix the number of quantum states as \(M = 32\) in our CMF+DMRG calculations.

3. Results

We discuss the quantum phase transition between the supersolid and superfluid states on the symmetric line \((\mu/V = 3)\). Here, we focus on the order parameter characteristic of this phase transition \(\Delta(= \rho_+ - \rho_-)\) [10], where \(\rho_{\pm}\) is the filling for the system with \(\mu/V = 3 \pm \delta\), where \(\delta\) is infinitesimal. In the superfluid state, the system is half-filled and \(\Delta = 0\). On the other hand, in the strong coupling region, two degenerate supersolid states are realized with distinct fillings and thereby \(\Delta\) is
finite. In the following, we calculate this quantity to discuss the quantum phase transition between the supersolid and superfluid states.

In the CMF method, the scaling analysis for the data obtained from finite clusters is important to discuss critical phenomena. First, we consider the length dependence of the data. By solving the self-consistency equations of the CMF theory for two-leg ladders with \( L = 12, 24, 36, 72, 120, \) and 240, we obtain the results for \( t/V = 0.108 \), as shown in Fig. 3 (a). It is found that the order parameter \( \Delta \) as a function of the inverse of the length \( L \) in the two-leg ladders with \( t/V = 0.108 \). Solid circles (triangles) represent the results for the effective ladders with the BAB (ABB and BBA) structure (see Fig. 2). (b) the quantity \( \Delta \) as a function of the inverse of the number of legs \( n_{\text{legs}} \) when \( t/V = 0.100 \) (circles) and 0.108 (triangles).

![Fig. 3.](image)

Fig. 3. (Color online) The system size dependence of the order parameter in the model with \( \mu/V = 3 \). (a) the quantity \( \Delta \) as a function of the inverse of the length \( L \) in the two-leg ladders with \( t/V = 0.108 \). Solid circles (triangles) represent the results for the effective ladders with the BAB (ABB and BBA) structure (see Fig. 2). (b) the quantity \( \Delta \) as a function of the inverse of the number of legs \( n_{\text{legs}} \) when \( t/V = 0.100 \) (circles) and 0.108 (triangles).

By performing similar calculations, we obtain the order parameter \( \Delta \) in the thermodynamic limit, as shown in Fig. 4. When \( t/V \) is small, the order parameter is finite, implying that the system is on the phase boundary between two supersolid states. The increase in the hopping integrals between sites decreases the order parameter \( \Delta \). Finally, it vanishes and the second-order transition occurs to the superfluid state. The critical point is obtained as \( (t/V)_c = 0.1125(15) \), which is in good agreement with the recent results obtained by the QMC method [11]. On the other hand, this value is slightly larger than \( (t/V)_c = 0.108 \) obtained by the CMF + ED method with small clusters [10]. This implies that the CMF+DMRG method with large clusters is more appropriate to discuss quantum phase transitions in the hard-core bosonic system.

This algorithm is applicable to more general classes of models with a larger number of degrees of freedom. One of the examples is a bosonic system on layered triangular lattices, which may be realized experimentally. It is an interesting problem how the interlayer coupling affects the stability of the supersolid states in the bosonic system, which is now under consideration [23].
4. Summary

We have studied quantum phase transitions in the hard-core bosonic Hubbard model on the triangular lattice, combining the cluster mean-field theory with the density matrix renormalization group. Solving the effective Hubbard ladder model with two, three, four, and five legs systematically, we have extrapolated the order parameter for the supersolid-superfluid transition in the thermodynamic limit. We have obtained the critical point at half filling \((t/V)_c = 0.1125(15)\), which is comparable with the recent results obtained by the QMC method [11].

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