Cluster mean field plus density matrix renormalization theory for the Bose Hubbard models

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Abstract

The cluster mean-field with density matrix renormalization (CMFT + DMRG) method which combines the simplicity of the mean-field theory and the numerical power of the density-matrix renormalization group method is applied to understand the quantum phases of the one-dimensional Bose–Hubbard models. We show that the CMFT + DMRG method is an effective numerical technique with moderate computational resources to determine relevant order parameters and correlation functions of large one-dimensional systems. We apply the CMFT + DMRG for the Bose Hubbard and extended Bose Hubbard models to account for the superfluid, Mott insulator, and density wave phases in these models. Our results are in good agreement with the known phase diagram of these models, demonstrating the efficacy of this method.

Keywords: density matrix renormalization group, mean-field theory, Bose Hubbard models, superfluid, Mott insulator, density wave phases

(Some figures may appear in colour only in the online journal)

1. Introduction

Experimental advances in ultra-cold atoms in optical lattices have considerable thrust in the study of a many-body quantum system [1, 2]. The prominent example of quantum phase
The transition is the superfluid (SF) to Mott insulator (MI), and it has been experimentally realized in one-dimension [3–6], two-dimensions [7–10], and 3D [5, 11, 12] optical lattices. The Bose–Hubbard model, which describes interacting bosons on optical lattices, has been widely used to study the SF to MI phase transition even before the experiments on cold atoms and still holds a significant role in the current studies [13–16].

Cold bosonic atoms in an optical lattice in the tight-binding regime are described by the Bose Hubbell model (BH) [16],

\[
\hat{H} = -t \sum_j \left( \hat{a}^\dagger_{j+1} \hat{a}_j + \hat{a}^\dagger_j \hat{a}_{j+1} \right) + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1) - \mu \sum_j \hat{n}_j, \tag{1}
\]

where bosons hop between nearest neighboring pairs of site with amplitude \(t > 0\), \(\hat{a}^\dagger_j (\hat{a}_j)\) is the boson creation (annihilation) operator for the site \(j\). The second term is the on-site interaction with strength \(U > 0\). The last term controls the boson number for a given chemical potential \(\mu\). The ratio between \(U/\nu t\), where \(\nu\) is the filling factor (the number of bosons per site), controls the ground state of the BH model. When \(U/\nu t \lesssim 1\) SF phase is favored at any filling. Increasing \(U/\nu t\) for integer filling quantum fluctuations drive the system into the MI phase.

Bose–Hubbell model is not exactly solvable even in one dimension. Hence, this model has been studied by several approximate and numerical techniques. Mean-field theories [13–15], numerical techniques such as quantum Monte Carlo simulation [17, 18] and strong-coupling-expansion techniques [19, 20] for 2D and 3D system and density matrix renormalization group (DMRG) [21–24] and time-evolving block decimation [25, 26] for one dimension system have been applied to determine the phases and the critical SF to MI transition point \(U/\nu t\). As such, these methods have certain advantages as well as limitations. Focusing on one-dimensional systems, for example, the simplest of all numerical methods is the mean-field theory, which is exact in the limit of infinite dimension [14, 15]. In the mean-field theory, the BH model (1) is decoupled from the surrounding lattice, into a single site Hamiltonian which is easily diagonalized. The fluctuations are described by a mean-field SF parameter \(\psi = \langle \hat{a} \rangle\). The ground state energy is minimized with respect to \(\psi\). The phases are characterized based on SF order parameter which is finite in the SF phases and vanishes in the MI phases. The mean-field theories for model (1) predict the SF and the MI phases correctly. However, mean-field theories are known to overestimate the SF phase boundaries [27]. The DMRG, on the other hand, is an effective numerical technique with moderate computational resources to determine the ground state energy and the correlation functions of a large one-dimensional systems [28]. It has been observed that the DMRG method works well when the ground state has a gap in the energy spectrum [28, 29]. When DMRG is applied to the Bose–Hubbell model, the quantum phases are determined by analyzing the behavior of the gap in the energy spectrum and the correlation functions such as single-particle density matrix \(\langle \hat{a}^\dagger_{j+1} \hat{a}_j \rangle\) and density-density correlation \(\langle \hat{n}_j \hat{n}_{j+1} \rangle\) [21–24]. The DMRG method generally works in the canonical ensemble. Hence the SF order parameter \(\psi = \langle \hat{a} \rangle = 0\) in all phases.

Several extensions of the Bose–Hubbell model, notably the extended Bose–Hubbell model, spin-1 Bose–Hubbell model, show exotic gapless phases like supersolid, polar/ferro SF, and pair SFs. It is desirable to determine the SF order parameter to characterize these exotic phases. Unlike the mean-field theories, the DMRG method cannot resolve these phases directly due to its limitation in determining SF order parameters.

The cluster mean-field theory (CMFT), which is an extension of the single-site mean-field theory considers a cluster of sites in the build-up of mean-field Hamiltonian [27]. It has been reported that CMFT improves the phase boundary compared to simple single site mean-field theory [27, 30]. However, there are limitations in forming more extensive cluster sizes as the
Hilbert space of the cluster increases exponentially with the number of sites. There has been recent reports of overcoming this limitation to build larger cluster sizes using the cluster mean-field method with DMRG [31–36].

In this paper, we extended this approach, which utilizes the DMRG capability to handle larger system sizes and the simplicity of the CMFT method. In this way, this approach captures the success of both the DMRG and the CMFT methods. The primary aim of this work is to demonstrate this approach, which we call CMFT + DMRG for the Bose Hubbard model, and test and compare with the DMRG method.

This paper is organized as follows: section 2 describes the CMFT + DMRG formalism. The results and the comparisons are given in section 3. Finally, we conclude our work in section 4.

2. CMFT + DMRG method

First, we set up to solve the model (1) in the cluster mean-field framework [27, 30]. The whole lattice is partitioned into $N_C$ clusters with each cluster having $L$ number of sites. The Hamiltonian (1) is then written as

$$\hat{H} = \sum_p \hat{H}_{p}^{\text{loc}} + \sum_p \hat{H}_{p}^{\text{hop}}, \quad (2)$$

where $p$ represents the cluster index and

$$\hat{H}_{p}^{\text{loc}} = -t \sum_j \left( \hat{a}_{p,j}^{\dagger} \hat{a}_{p,j+1}^{\dagger} \hat{a}_{p,j} \hat{a}_{p,j+1} + \frac{U}{2} \hat{n}_{p,j}(\hat{n}_{p,j} - 1) - \sum_j \mu \hat{n}_{p,j} \right). \quad (3)$$

Here $\hat{a}_{p,j}$ (and $\hat{a}_{p,j}^{\dagger}$) is theboson creation (annihilation) operator for the site $j$ in the cluster $p$ and $\hat{n}_{p,j} = \hat{a}_{p,j}^{\dagger} \hat{a}_{p,j}$ is the number operator. The second term in the Hamiltonian equation (2) represents the hopping of bosons between the clusters and is given by

$$\hat{H}_{p}^{\text{hop}} = -t \left( \hat{a}_{p,1}^{\dagger} \hat{a}_{p-1,L} + \hat{a}_{p-1,L}^{\dagger} \hat{a}_{p,1} \right). \quad (4)$$

We now decouple each cluster from its neighbor clusters by using standard mean-field decoupling i.e., $\alpha_{p,j} = \langle a_{p,j} \rangle + \delta \alpha_{p,j}$ where $\alpha_{p,j} = \psi_{p,j}$ is the SF order parameter. Considering the fluctuation $\delta \alpha_{p,j}$ to be small and thus neglecting second-order fluctuations, we approximate

$$\hat{a}_{p,j}^{\dagger} \hat{a}_{p-1,L} + \hat{a}_{p-1,L}^{\dagger} \hat{a}_{p,1} \approx \hat{a}_{p,j}^{\dagger} \psi_{p-1,L} \psi_{p,1} + \hat{a}_{p,1} \psi_{p-1,L}^{\dagger} \psi_{p,1}$$

$$+ \psi_{p-1,L} \psi_{p,1}^{\dagger} + \hat{a}_{p,L} \psi_{p+1,1} \hat{a}_{p,1} + \hat{a}_{p,1} \psi_{p+1,1}^{\dagger} \psi_{p,L}$$

$$- \frac{1}{2} \left( \psi_{p+1,1} \psi_{p,L} + \psi_{p+1,1} \psi_{p,L}^{\dagger} \right). \quad (5)$$

Assuming, without loss of generality, the SF order parameter $\psi_{p,j}$ to be real and homogeneous, equation (4) is written as

$$\hat{H}_{p}^{\text{hop}} = -t \left( \langle \hat{a}_{p,1}^{\dagger} + \hat{a}_{p,1} \rangle \psi - |\psi|^2 \right) - t \left( \langle \hat{a}_{p,L}^{\dagger} + \hat{a}_{p,L} \rangle \psi - |\psi|^2 \right). \quad (6)$$

Using equations (3) and (6) in equation (2), we get

$$\hat{H} = \sum_p \hat{H}_{p}^{\text{loc}}, \quad (7)$$
where $\hat{H}_p^C$ is the Hamiltonian for a cluster of $L$ sites. Dropping the cluster index $p$

$$\hat{H}_p^C = -t \sum_{j=1}^{L-1} \left( \hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1} \right) + \frac{U}{2} \sum_{j=1}^{L} \hat{n}_j(\hat{n}_j - 1) - \sum_{j=1}^{L} \mu \hat{n}_j - t \left( (\hat{a}_1^\dagger + \hat{a}_1) \psi - |\psi|^2 \right) - t \left( (\hat{a}_L^\dagger + \hat{a}_L) \psi - |\psi|^2 \right). \quad (8)$$

This cluster Hamiltonian has been studied in different limits. For example, in the limit, $L = 1$ equation (8) is nothing but the single site mean-field theory Hamiltonian $[14, 15]$. McIntosh et al have considered this Hamiltonian with cluster size up to $L = 8$ [27]. DMRG method exploits the Bose–Hubbard Hamiltonian in the canonical ensemble with a fixed number of particles. If we neglect the last three terms in the Hamiltonian (8), we get the Bose–Hubbard model in the canonical ensemble and has been studied using DMRG to obtain an accurate phase diagram [21–23].

Because the DMRG method works in the canonical ensemble the number of particles is fixed, hence the SF order parameter $\psi = \langle a \rangle = 0$ in all phases. However, the cluster Hamiltonian works in the grand-canonical ensemble and commutation $[\hat{H}_p^C, N] \neq 0$. The SF parameter $\psi = \langle a \rangle$ can be finite, and such phase can be identified as the SF phase. In the MI phase, $\psi = 0$ and the Hamiltonian $\hat{H}_p^C$ commutes with the $N$, which implies that our study can reproduce earlier DMRG results. Thus, the CMFT + DMRG method interplay between single-site mean-field theory to the DMRG in the one-dimension Bose Hubbard model.

The task now is to obtain the ground state energy and the wave function of the Hamiltonian (8) for any given length $L$ using the CMFT + DMRG method with open boundary condition. We describe these steps below.

Step 1 Consider a lattice of small size $l$, say $l = 1$ forming the system block $S$. The Hilbert space of $S$ has dimension $M^l$ and is represented by states $\{ \{ \mu \} \}$. For example, if $l = 1$, $\{ \{ \mu \} \}$ can be Fock states $\{ |0\rangle, |1\rangle, |2\rangle, \ldots, |n_{\text{max}}\rangle \}$ $n_{\text{max}}$ being the maximum number of bosons allowed per site and $M^l = n_{\text{max}} + 1$. It may be noted that $n_{\text{max}} = \infty$ for bosons, however, for numerical calculation, we will truncate Fock states to $M^l$ states. The value of $n_{\text{max}}$ depends on the parameters of the model (1) such as $U/t$ and $\mu$.) Obtain the Hamiltonian $\hat{H}_p^C$ and operators acting on the block. Similarly, form an environment block $E$.

Step 2 Form a new system block $S'$ from $S$ and one added site as shown in figure 1. Hilbert space of the new system block $S'$ has dimension $M^l \times N_s$ and is represented by states $\{ \{ \mu \} \}$. Here $N_s = n_{\text{max}} + 1$ is the number of states per site. Similarly, form an environment block $E'$.

Step 3 Now build a superblock of length $L = 2l + 2$ as shown in figure 2. Construct the Hamiltonian matrix $\hat{H}_{2l+2}$ for a given initial guess for $\psi$ and find the ground state energy $E_L(\psi)$ and the wave function by large sparse-matrix diagonalization. This is the most time-consuming step in this algorithm. Minimize the ground state energy $E_L(\psi)$ with respect to $\psi$ to obtain global ground state energy $E_{GS}$, the wave function $\Psi_{GS}$ and the SF order parameter $\psi_J = \langle \Psi_{GS}|\hat{a}_j|\Psi_{GS}\rangle$.

The ground state wave function is given by

$$|\Psi_{GS}\rangle = \sum_{S'E'} C_{S'E'} |S'E\rangle = \sum_{\rho_2^\dagger \rho_1^\dagger \rho_1 \rho_2} C_{\rho_2^\dagger \rho_1^\dagger \rho_1 \rho_2} |\rho_2^\dagger \rho_1^\dagger \rho_1 \rho_2\rangle. \quad (9)$$
Figure 1. New system block $S'$ is formed from system block $S$ and one added site represented by open circle.

Figure 2. Super block of length $L = 2l + 2$. The continuous lines represent hopping term $(-t(a_j^\dagger a_{j+1} + \text{h.c.}))$ in the equation (8) and dashed lines represent $-t((a_{1L}^\dagger + a_{1L})\psi - |\psi|^2)$.

Step 4 Construct a reduced density-matrix $\hat{\rho}_S'$ for the block system $S'$.

$$\hat{\rho}_S' = Tr_E |\Psi_{GS}\rangle \langle \Psi_{GS}|.$$  

That is

$$\langle \mu_i^S \sigma^S | \hat{\rho}_S' | \nu_j^S \sigma^S \rangle = \sum_{\sigma^S} C_{\mu_i^S \sigma^S \nu_j^S \sigma^S} C_{\nu_j^S \sigma^S \mu_i^S \sigma^S}.$$  

(11)

Diagonalize $\hat{\rho}_S'$ to obtain its eigenvectors

$$|\alpha\rangle = \sum_{\mu_i^S \sigma^S} O^\dagger_{\alpha \mu_i^S \sigma^S} |\mu_i^S \sigma^S\rangle,$$

(12)

and the eigenvalues $\omega_\alpha$, $\omega_\alpha$ measures the weight of the state $|\alpha\rangle$ in the $|\Psi_{GS}\rangle$ and satisfy $\sum_\alpha \omega_\alpha = 1$. Form a new (reduced) basis for $S'$ by taking the $M^S$ eigenstates with the largest weights $\omega_\alpha$. The new basis is represented by $M^S$ eigenstates of the reduced density matrix. This way we have truncated the Hilbert basis of the system block $S'$ from $M^S \times N^S$ to $M^S$. This is the most important step of the DMRG method. Transform $H^S_{l+1}$ and operators to the new basis. i.e.,

$$\hat{H}^S_{\text{new}} = O^\dagger \hat{H}^S O,$$

(13)

where $O$ is $M^S \times N^S$ rectangular transformation matrix from equation (12). Proceed likewise for the environment.

Step 5 Repeat step I to IV with block size $l + 1$ and continue the iteration until the desired length $L$. The system size is increased by 2 in each iteration. Calculate the ground state properties (energies, order parameters, and correlators for all $L$).

3. Results

3.1. Bose–Hubbard model

We now discuss the results of the Bose–Hubbard model. The CMFT + DMRG calculations are performed by retaining $M^S = 50$ eigenstates in the left/right block reduced density matrix
and taking $n_{\text{max}} = 3$, which is found to be sufficient if we restrict the density of bosons $\rho < 2$ as done in the present report. The neglected truncated weight $\epsilon = 1 - \sum_{\alpha=1}^{M} \omega_{\alpha}$ is of the order of $10^{-8}$. We set the energy scale by $t = 1$.

We begin our discussion by analyzing the behavior of the SF order parameters $\psi(j)$, and density of bosons $\rho(j)$. For $U = 5$, and $\mu = 0.6$, we plot $\psi(j)$ and $\rho(j)$ as a function of lattice position $j$ for a system length with $L = 50$ in figure 3. This depicts a typical behavior of $\psi(j)$ and $\rho(j)$. The edge sites have higher SF order parameter values compared to the center. $\psi(j)$ decreases as the lattice position $j$ moves away from the edges and has the least value when $j = L/2$. Similarly, density $\rho(j)$ increases from the edges to the center. This behavior of $\psi(j)$ is not difficult to understand. The mean-field approximation affects the edge sites and as the lattice position moves away from the edges, the effect of the approximation tampers off. The mean-field approximation is known to overestimate the SF phase, hence, the values of the SF order parameter are larger at the edges compared to the center. In order to understand the converges of the SF order parameters with system length $L$, we plot $\psi(j)$ (where $j = 1$ to $L/2$) for different lengths; $L = 100, 300, 700$, and, $1000$ in figure 4. We observe that the SF order
parameters start converging from the edges as the system length $L$ increases. For example, for $L = 100$, $\psi(j)$ have been converged for all $j$ except near the center of the lattice $j \sim 50$. As length increases, $\psi(j)$ converges for more range of values of $j$ and eventually, for larger $L$, $\psi(j)$ converges for the entire system. To demonstrate this behavior further, we plot $\psi(1)$, $\psi(L/2)$, $\rho(1)$ and $\rho(L/2)$ in figures 5 and 6, respectively, for $\mu = 0.6$ and 1.4 keeping $U = 5$.

The densities, $\rho(1)$ and $\rho(L/2)$, and the SF parameter for the edge site $\psi(1)$ converge faster with $L$ compare to $\psi(L/2)$. $\psi(L/2)$ converges eventually as length increases further. For $\mu = 0.6$, $\psi(L/2)$ converged to a finite value which implies a SF phase. However, for $\mu = 1.4$, $\psi(L/2)$ converge to zero yielding a MI phase. It may be noted that $\psi(1)$ is finite for both cases. We conclude from the above behavior of convergence of SF order parameters and densities that $\psi(L/2)$ and $\rho(L/2)$ can be taken as the SF fluid order parameter and density of system with length $L$. We denote these by $\psi_L$ and $\rho_L$, respectively.

We now compare the CMFT + DMRG result with the standard DMRG. In DMRG, the ground state energy $E_L(N)$ of the system of length $L$ having $N$ bosons is obtained using finite-size DMRG procedure [37]. The density of the system $\rho_L = N/L$ and chemical potential
corresponding to this density is determined using the relation

\[ \mu = \frac{(\mu^+ + \mu^-)}{2}, \]

where \( \mu^+ = E_L(N + 1) - E_L(N) \) and \( \mu^- = E_L(N) - E_L(N - 1) \). We plot the density calculated using the DMRG method (for \( L = 300 \)) and the CMFT + DMRG method (for \( L = 200 \)) for different chemical potentials in figure 7 for \( U = 5 \). We observe that the density obtained from both methods agree with each other. Density increases with chemical potential and remains pinned at \( \rho = 1 \) for a range of \( \mu \) values. This region corresponding to the MI phase has finite gap \( \Delta = \mu^+ - \mu^- \) and vanishing compressibility \( \kappa = \left( \frac{d\rho}{d\mu} \right) \). The region outside \( \rho = 1 \) has finite compressibility. This region is considered a SF phase. The DMRG method, unlike the CMFT + DMRG method, however, does not have access to SF order parameters to identify SF and MI phases directly. We plot the SF order parameter obtained from the CMFT + DMRG method (for \( L = 200 \) and 500) in the same figure. We observe that \( \psi \) vanishes in the MI phase as it should be and is finite in the SF phase. Thus the CMFT + DMRG method gives direct access to different phases in the model.

We now address the question of convergence of the SF order parameter \( \psi \) and density \( \rho \) to the system length \( L \). The convergence of \( \psi \) and \( \rho \) depend on (i) the value of the on-site interaction \( U \) compared to \( U_C \) and (ii) the value of chemical potential \( \mu \) compared to \( \mu^+/\mu^- \). Here \( U_C \) is the critical on-site interaction for SF-MI transition for \( \rho = 1 \) and \( \mu^+(U) \) and \( \mu^-(U) \) are the lower and upper edge of the Mott lobe for a given \( U \). If \( U \gg U_C \) and \( |\mu - \mu^+(U)| \gg 0 \), the SF order parameter and density converge rapidly with \( L \). However, in the opposite limit i.e., \( U \sim U_C \) and \( |\mu - \mu^+(U)| \sim 0 \) the convergence is very slow. In these limits, the correlation length \( \xi \) is large, and the convergence of the SF order parameter is guaranteed if and only if \( L \gg \xi \). To demonstrate this behavior, we plot \( \psi_L \) and \( \rho_L \) obtained from CMFT + DMRG for \( U = 5 \) and \( U = 4 \) in figures 8 and 9, respectively. It may note that the best estimate of \( U_C \approx 3.28 \) [23, 24]. For \( U = 5 \), length \( L = 500 \) is sufficient for the convergence of the SF order parameter. However, as we decrease the on-site interaction, say \( U = 4 \), the convergence is slow and requires a larger length.
The CMFT + DMRG method also allows us to calculate the phase coherence correlation function

$$\Gamma(|(j-j')|) = \frac{1}{2}\langle [a_j^\dagger a_{j'} + \text{h.c.}] \rangle. \tag{15}$$

Here the brackets $\langle \ldots \rangle$ denote the mean value of an observable in the system $|\Psi_{GS}\rangle$. We plot $\Gamma(r = |(j-j')|)$ for the SF and the MI phases in figure 10. We consider on-site interaction $U = 5$, length $L = 1000$ and restrict $350 \leq j, j' \leq 650$ so that the $j, j'$ are far from the system edges and the SF order parameters are converged in this region. In figure 10(a), it is observed that $\Gamma(r) \to \psi^2$ as $r \to \infty$. $\Gamma(r)$ decay as a power-law with $r$ in the SF phase and exponential
in the MI phase. The Fourier transform of the phase coherence correlation function

\[ n(k) = \frac{1}{L^2} \sum_{j,j'} \Gamma(|j-j'|) e^{-ı k |j-j'|} \]  

(16)
gives the number of particles of the system with a wave vector \( k \). \( n(0) \) is the condensate fraction giving the fraction of bosons occupying the SF ground state. We plot \( n(0) \) and the SF density \( \rho_S \) as a function of \( \mu \) across SF-MI phase transition for \( U = 5 \) in figure 10(b). The condensate fraction increases sharply in the SF phase. Finally we compare the phase diagram obtained using DMRG [37] and CMFT + DMRG in figure 11. The phase diagram agrees with each other except near \( U_C \) where the Mott gap is extremely small and scales with logarithmic correction [24]. Hence we could not resolve the Mott phase from the SF order parameter for \( U < 3.8 \). The SF-MI transition at fixed integer density belongs to Berezinskii–Kosterlitz–Thouless transition (BKT transition) [38]. The order parameter shows a discontinuity at the BKT transition. It is interesting to apply the CMFT + DMRG method to observe the discontinuity at the SF-MI transition. However, we were not successful in observing this discontinuity due to (i) the lack of known accurate relation between \( \mu \) and \( U \) to fix density \( \rho = 1 \) and (ii) the need to keep a larger number of states in the DMRG procedure when \( U \) is close to \( U_C \). We could, however, observe such discontinuity across the SF to density wave transition in the extended Bose–Hubbard model.

3.2. Hard-core extended Bose–Hubbard model

The extended Bose–Hubbard model is given by

\[ \hat{H} = -t \sum_j \left( \hat{a}_j^\dagger \hat{a}_{j+1} + \hat{a}_{j+1}^\dagger \hat{a}_j \right) + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1) + V \sum_j \hat{n}_j \hat{n}_{j+1} - \mu \sum_j \hat{n}_j, \]  

(17)

where the third term is the nearest neighbor interaction with strength \( V > 0 \). The other terms have the same meaning as in the equation (1). In the hard-core limit (\( U = \infty \)) and for \( \mu = V \), the model (17) maps into spin-1/2 XXZ model, which has a BKT transition from the SF phase.
Figure 11. Phase diagram of Bose Hubbard model close to density $\rho = 1$.

(equivalent to XY order) to the density wave phase (Ising order) at $V = 2$. The density of bosons alternate between $\rho_A$ and $\rho_B \neq \rho_A$ in the density wave phase. Here $\rho_{A,B}$ represents density of bosons at $A(B)$ sub-lattices.

Applying the CMFT + DMRG method to the extended Bose–Hubbard model, we find working with the system having an odd number of sites is preferred over systems with an even number of lattice sites. Since the lattice has left–right symmetry, the density of bosons at the left edge site ($\rho_1$) and the right edge site ($\rho_L$) are equal. This symmetry forces $\rho_L = \rho_1$ if $L$ is even in all possible phases, including the density wave phase. Since the density of bosons alternate between the nearest neighboring sites in the density wave phase, this symmetry forces density variation to have a node at the center. However, if $L$ is an odd integer, the left–right symmetry is preserved with no such restrictions.

To set up the cluster Hamiltonian for the extended Bose–Hubbard model, we decouple both the hopping and the nearest neighbor interaction terms following the procedure discussed in the earlier section. The resultant cluster Hamiltonian is given by

$$\hat{H}_C = -t \sum_{j=1}^{L-1} \left( \hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1} \right) + \frac{U}{2} \sum_{j=1}^{L} \hat{n}_j (\hat{n}_j - 1) + \frac{V}{2} \sum_{j=1}^{L-1} \hat{n}_j \hat{n}_{j+1}$$

$$- \sum_{j=1}^{L} \mu \hat{n}_j - t \left( \hat{a}_1^\dagger \hat{a}_1 \psi_B - \psi_A \psi_B \right) - t \left( \hat{a}_L^\dagger \hat{a}_L \psi_B - \psi_A \psi_B \right) + V (\hat{n}_1 + \hat{n}_L) \rho_B - \frac{V}{2} \rho_A \rho_B,$$  

where $\psi_A (\psi_B)$ and $\rho_A (\rho_B)$ are the SF order parameter and the density of bosons of $A$-($B$-)sub-lattices, respectively. The minimization of the ground state energy is done with respect to $\psi_{A(B)}$ and $\rho_{A(B)}$. The SF phase has non-zero $\psi_A$ and $\psi_B$. The density wave phase has $\psi_A = \psi_B = 0$ and $\rho_A \neq \rho_B$.

The CMFT + DMRG calculations are performed by retaining $M^S = 50$ eigenstates in the left/right block reduced density matrix and taking $n_{\text{max}} = 1$ ($U = \infty$). The neglected truncated weight $\epsilon = 1 - \sum_{\omega}^M \omega \alpha$ is of the order of $10^{-8}$ or less. We set the energy scale by $t = 1$. We summarize our results in figure 12. We have built the lattice starting with $L = 3$ to $L = 2001$ and calculate the SF order parameters $\psi_{A(B)}$, density wave order parameter $\Delta = |\rho_A - \rho_B|$, the...
condensate fraction $n(0)$ and structure factor $S(\pi)$ where

$$S(\pi) = \frac{1}{L^2} \sum_{j,j'} (-1)^{j-j'} \langle \hat{n}_j \hat{n}_{j'} \rangle.$$  

We find the SF order parameter $\psi_A = \psi_B = \psi$ is finite in the SF phase and vanishes in the density wave phase with a universal discontinuity at the transition $V = 2$. Similarly, the density wave order parameter is finite in the density wave phase and vanishes in the SF phase with a discontinuity at $V = 2$. The condensate fraction and $S(\pi)$ also show similar discontinuity at $V = 2$. These results are consistent with the BKT transition between SF to DW phase.

4. Conclusions

We have developed CMFT + DMRG method integrating the key features of the mean-field theory and the DMRG methods to understand quantum phases in the one-dimensional Bose Hubbard models. The CMFT + DMRG method overcomes many limitations of the mean-field theory and the DMRG technique. Notably, the small system size in the former and direct calculation of SF order parameters in the latter. We apply the CMFT + DMRG method to the Bose–Hubbard model and the extended Bose–Hubbard model to test its usefulness. The Bose–Hubbard model has two phases; SF and MI. We identify these phases with the SF order parameters and the condensate fraction. Our results agree with the earlier studies done using the DMRG method. The extended Bose–Hubbard model in the hard-core limit at the density of bosons equal to half shows the SF and the density wave phases. We identify these phases using the SF and the density wave order parameters, condensate fraction, and structure factor. The discontinuous jump in these physical quantities at the SF to density wave phase boundary
confirms the BKT nature of the phase transition. This method can be extended to other models such as the soft-core extended Bose–Hubbard model, spin-1 Bose–Hubbard model, etc, to understand the exotic SF phases such as supersolids, polar/ferro SFs, and pair SFs. The DMRG and the CMFT + DMRG methods work complementary with each other to understand the entire phase diagram of Bose–Hubbard models. The former method works in the canonical ensemble and is most suitable for characterizing the gaped phases. The CMFT + DMRG, however, works in the grand-canonical ensemble and is very useful to understand the gapless quantum phases.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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