Study of 1-D Bose-Hubbard model with Complex Order Parameter

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DECLARATION

I hereby declare that the data presented in this Dissertation report entitled, "Study of 1-D Bose-Hubbard model with complex order parameter" is based on the results of investigations carried out by me in the Physics Discipline at the School of Physical and Applied Sciences, Goa University under the Supervision of Dr. Ramesh V. Pai and the same has not been submitted elsewhere for the award of a degree or diploma by me. Further, I understand that Goa University or its authorities will be not be responsible for the correctness of observations/experimental or other findings given in the dissertation.
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COMPLETION CERTIFICATE

This is to certify that the dissertation report "Study of 1-D Bose-Hubbard model with complex order parameter" is a bonafide work carried out by Mr. Darshan Tavanappa Hosamani under my supervision in partial fulfilment of the requirements for the award of the degree of Masters in the Discipline Physics at the School of Physical and Applied Sciences, Goa University.

Date: 8 May 2024

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Date: 8/5/24.

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PREFACE

The dissertation on the topic "The study of 1-D Bose-Hubbard Model with Complex order parameter" was conducted under the guidance of Dr. Ramesh V. Pai. The project focused on understanding the significance of phase of the order parameter. Also, to understand the phase separation in the lattice when a harmonic trap potential is introduced.

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Abbreviations

Entity	**Abbreviation**
Bose-Hubbard Model	BHM
Bose-Einstein Condensate	BEC
Super-fluid	SF
Mott Insulator	MI
Mean Field Theory	MFT
Cluster Mean Field Theory	CMFT
Self Consistent Method	SCM
Quantum Monte Carlo	QCM
Density Matrix Renormalisation Group	DMRG
One Dimensional	1-D

ABSTRACT

The one dimensional Bose-Hubbard Model was studied with complex order parameter by using the CMFT-DMRG method. The aim was check how the phase of the order parameter varies in the lattice and whether it gives a quasi-long range ordering in the superfuild phase. However, it was found that the phase of the SF order parameter remains constant through out the lattice and CMFT-DMRG does not yield quasi long range order. The same system was studied with a harmonic trap potential which showed a smooth transition from SF to MI phase where the SF order parameter decayed exponentially into the MI phase. Also, it was found that was some correlation between the particles in two different SF regions separated by a MI region.

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Chapter 1

Introduction

1.1 Introduction

In quantum mechanics, the identical and indistinguishable particles are classified into two types - Fermions and Bosons. Fermions have anti-symmetric wavefunction under exchange and they obey the Pauli exclusion principle, which means that two fermions cannot occupy the same quantum state. Examples of fermions are electrons, neutrinos, quarks, protons, neutrons, and helium-3 nuclei. On the other hand, bosons have a symmetric wavefunction under exchange and they can occupy same quantum states. Examples of bosons are photons, gluons, phonons, helium-4 nuclei and all mesons.

The symmetric nature of the bosons lead to the discovery of Bose-Einstein Condensate (BEC) which occurs at very low temperature. Satyendranath Bose and Albert Einstein predicted that at certain low temperature bosons have the ability to occupy the lowest quantum state and form a condensate having a wavefunction at macroscopic level [1, 16]. Bosons also show super-fluid nature at low temperature, where the bosons flow without any resistance.

To observe BEC several experiments were carried out to trap and cool down atoms to very low temperature. In 1995, first experimental observation of pure BEC was done at

JILA using Rubidium-87 atoms [5] and at MIT using Sodium-27 atoms [6] by using laser cooling [10] and further cooling by evaporation [7]. This was possible with low density of atoms which made them weakly interacting. But in 1998 D. Jaksch and his group [9] tried loading BEC in laser induced periodic potentials called optical lattice [21] and observed a strongly interacting quantum phase called Mott Insulator (MI). Optical lattice is formed by the superimposition of laser beams, forming standing waves with periodic potential wells [13]. When the atoms are loaded in the optical lattice they are trapped and cooled in these potential wells leading to BEC. Depending on the potential depths the atoms tunnel through the potential wells and spread through the lattice. During BEC, there is phase coherence between the atoms and they show superfuildity. The tunnelling process can be controlled by tuning the potential wells and the transition from SF to MI can be observed when there is no tunnelling allowed. The optical lattice can be constructed in 1D, 2D and 3D which helps to study the system in all dimensions.

Theoretically, the system of bosons in optical lattices is characterised by the Bose-Hubbard Hamiltonian. For one dimensional optical lattice with homogeneous potential and considering a grand canonical ensemble of bosons, the Hamiltonian is:

$$H = -t \sum_i \hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \ + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \ - \mu \sum_i \hat{n}_i \tag{1.1}$$

This Hamiltonian allows nearest-neighbour tunnelling and on-site interactions only. Here, i denotes the site index of the lattice, $\hat{a}_i(\hat{a}_i^\dagger)$ is the annihilation(creation) operator of a boson at site i, $\hat{n}_i$ is the particle number operator at site i, which gives the number of bosons at site i. The tunneling of bosons is represented by $\hat{a}_i^\dagger \hat{a}_{i+1}$ or $\hat{a}_{i+1}^\dagger \hat{a}_i$ and t is the tunnelling amplitude and tells how much energy is released when a boson hops from a site to the nearest-neighbouring site. U is the on-site interaction amplitude and it tells about the repulsive energy between multiple bosons at a site. In the third term, μ is the chemical potential needed to add or remove a particle in/from the system at a given instance.

The SF and MI phase are seen according the ratio of $\frac{U}{J}$ which can be controlled by tuning the lasers as

$$\frac{U}{J} = \frac{\sqrt{8}\pi a_s}{4a} exp\left(2\sqrt{\frac{V_0}{E_r}}\right)$$

where a_s is the s-wave scattering amplitude of atoms, $a = \frac{\lambda}{2}$ is the lattice constant with λ as the laser wavelength [19].

1.2 Literature Review

The Bose Hubbard model is not solvable exactly in any dimension. Therefore, different approximations are used to solve the hamiltonian given in equation 1.1 at temperature $T = 0K$. Such methods are Mean-field Theory (MFT)[18], Cluster Mean-field Theory (CMFT), Random Phase Approximation, Quantum Monte Carlo Simulation (QMC) [3] and Density Matrix Renormalisation Group Theory (DMRG) [12, 14, 17]. Mean-field Theory decouples each site from its surroundings and converts the hamiltonian into a single effective hamiltonian which can be easily diagonalised. The expectation value of the annihilation operator $\langle \hat{a} \rangle$ is set as the SF order parameter ψ and $|\psi|^2$ gives the superfuild density. When $|\psi| > 0$, the system is in superfuild phase (SF) and when $|\psi| = 0$ with integer density, it is in mott insulator phase (MI). The MFT is simple and predicts the quantum phase transitions but it overestimates the superfuildity and the critical values are not accurate. CMFT is an extended version of MFT. Whereas QMC and DMRG are complex methods but give more accurate results. However, the DMRG and QMC methods work in canonical ensemble which makes $\langle \hat{a} \rangle = 0$. Hence, the SF phase cannot be analysed directly.

Recently, a new method was developed called CMFT-DMRG method which combines the ideas of CMFT and DMRG [22]. This method is found to be efficient and more accurate in analysing the SF and MI phase transitions. It overcomes the limitations of CMFT to find accurate critical values by using the DMRG method, where the SF to MI phase transition for density 1 is found to be at $U_c = 3.3$. The DMRG method also shows the

same result.

1.3 Motivation

Though a lot of work has been done on the Bose-Hubbard model, we could not find any work done which considers the SF order parameter as complex. The order parameter is believed to be a complex quantity of the form $\psi = |\psi|e^{i\theta}$, where $|\psi|$ is the magnitude and θ is the phase angle. It may be interesting to know how the phase angle varies in the lattice. Also, the 1-D Bose Hubbard system is believed to have quasi long-range ordering in superfuild phase [8, 15], which was not seen in the previous CMFT-DMRG method. Therefore, the same can be checked by including the phase angle in the SF order parameter.

It will also be interesting to use the CMFT-DMRG method to solve 1-D Bose-Hubbard model with a harmonic trap potential. This system is studied using QMC and DMRG [20] in the canonical ensemble. Therefore, the superfuildity is not analysed.

1.4 Objectives

The objective of this dissertation are as follow

- To develop a code for CMFT-DMRG method with complex order parameter and apply it on the one-dimensional Bose Hubbard Model in a homogeneous potential (without the trap potential) at temperature $T = 0K$
- To study the same system in presence of a harmonic trap potential by modifying the CMFT-DMRG method.
- Understand how the phase angle varies in the lattice and how the properties differ from the case of the real order parameter.

Chapter 2

Methodology

2.1 Introduction

The Hamiltonian of the 1-D Bose-Hubbard model for bosons in optical lattice with homogeneous potential is:

$$H = -t \sum_i \hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \ + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \ - \mu \sum_i \hat{n}_i \tag{2.1}$$

Here, t is the hopping amplitude and tells how much energy is released when a boson hops from a site to the nearest-neighbouring site, U is the on-site interaction strength and it tells about the repulsive energy between multiple bosons at a site. In the third term, μ is the chemical potential needed to add or remove a particle in/from the system at a given instance.

However, it is not possible to solve the above model exactly for large lattice size. Hence, different approximations like Mean-Field Theory, Cluster-Mean-field Theory, Density Matrix Renormalisation Group Theory and Quantum Monte Carlo Method are used.

In this study, a combination of CMFT and DMRG methods, which was recently introduced with successful results [22]. The reason CMFT was chosen along with DMRG

method was simply because we need to analyse the superfuild order parameter for a large lattice, which can neither be achieved with CMFT nor DMRG solely. By using mean-field approach one can analyse superfuildity present in the system but it is not computationally possible to use it on a large cluster size. On the other hand, DMRG makes it is possible to study a large cluster size, but is used with fixed number of bosons due to which the superfuild order parameter is always zero. The details of each of these methods is discussed in the next section.

2.2 Mean Field Theory and Cluster Mean Field Theory

The Bose Hubbard (2.1) is not exactly solvable for very large lattice because of the hopping term which couples the nearest-neighbouring sites. Therefore, to break the coupling between the nearest neighbouring sites a mean value with a first order fluctuation is considered for the annihilation operator at every site[18]. That is $\hat{a}_i = \psi_i + \delta\hat{a}_i$, where i denotes the site number in the lattice and ψ is the expectation value of the annihilation operator, i.e $\psi = \langle\hat{a}\rangle$. Since the system is analysed at zero temperature, the expectation value is with respect to the ground state. Here, ψ is set as the order parameter for superfuildity in the system which helps in determining superfuild phase.

By neglecting the second order fluctuations in the system, the first term of equation 2.1 is approximated as,

$$-t\sum_i \hat{a}_i^\dagger\hat{a}_{i+1} + \hat{a}_{i+1}^\dagger\hat{a}_i \;\approx\; 2t\sum_i(|\psi_i|^2 - \psi_i\hat{a}_i^\dagger - \psi_i^*\hat{a}_i)$$

Further, the homogeneity of the system makes all ψ_i equal, which allows us to write $\psi_i = \psi$. And the lattice hamiltonian can be written as a sum of single site hamiltonians

as shown below.

$$\begin{aligned} H &= \sum_i H_i \\ H_i &= 2t|\psi|^2 - 2t\psi\hat{a}_i^\dagger - 2t\psi^*\hat{a}_i + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i \end{aligned} \tag{2.2}$$

Since all the single site hamiltonians are independent and identical, the properties and energies of all will be the same. Therefore, we just have to analyse one single site hamiltonian. Also, as seen in equation 2.2 the hamiltonian is a function of ψ for a given set of the hamiltonian parameters (U, μ, t). Therefore, for those parameters the system will set the value of ψ such that the energy is minimum. At zero temperature, it will be the ground state energy. This means we have to minimise the ground state energy with respect to ψ. This is achieved using the self-consistency method (SCM).

The self consistency method is an iterative process beginning with an initial guess for ψ. Using this value the hamiltonian is diagonalised and its ground state energy and ground state eigenvector are obtained. Then, using this eigenvector, the expectation value of $\hat{a}$ is calculated. If the guessed value of ψ is the correct value for the actual ground state, then $\langle\hat{a}\rangle = \psi$. So, it is checked whether ψ is equal to $\langle\hat{a}\rangle$ within a certain margin of error. If this condition is not satisfied, then the current value of $\langle\hat{a}\rangle$ is considered as the new guess for ψ for the next iteration. It is seen that $\langle\hat{a}\rangle$ begins to converge to a certain value with increasing iterations and the iterations are continued until the required convergence is achieved. At the end of the SCM we obtain the actual ground state of the system for the given parameters.

Since there can be any number of bosons present at a single site, the basis states for forming the single site hamiltonian are $|0\rangle, |1\rangle, |2\rangle, |3\rangle \ldots$. Though this makes the basis states infinitely many, the repulsive nature of the bosons do not allow too many bosons at a site. The maximum number of bosons can be restricted to a value (say n_{max}) depending on the value of the on-site interaction amplitude U. Then, the hamiltonian is constructed with the basis states $|0\rangle, |1\rangle, |2\rangle, |3\rangle \ldots |n_{max}\rangle$ and its dimension is $n_{max} + 1$. Also, the

hamiltonian elements are constructed with respect to t. Hence, t is consider as unity and the energy is with respect to t.

Equation 2.2 is easily solvable and gives satisfying results. However, the results are not accurate. The accuracy is increased when we apply mean-field approximation across clusters of sites instead of applying it at every site. This is called the cluster mean field theory. In this, the lattice is divided into several clusters of equal size (say L) and the mean field approximation is applied to the edge sites of these clusters. This way, each cluster is decoupled from each other and the net Hamiltonian can be written as a sum of the hamiltonian of each cluster.

$$\begin{aligned} H &= \sum_k H_k \\ H_k &= -t\sum_{i=1}^{L-1}(\hat{a}^\dagger_{k,i}\hat{a}_{k,i+1} + \hat{a}^\dagger_{k,i+1}\hat{a}_{k,i}) \ + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_{k,i}(\hat{n}_{k,i}-1) \ - \mu\sum_{i=1}^{L}\hat{n}_{k,i} \\ &\quad + 2t|\psi|^2 - t\psi(\hat{a}^\dagger_{k,1} + \hat{a}^\dagger_{k,L}) - t\psi^*(\hat{a}_{k,1} + \hat{a}_{k,L}) \end{aligned} \tag{2.3}$$

In equation 2.3, each cluster consists of L sites. k denotes the cluster index and i denotes the site index in a given cluster. The order parameters at the edge sites of a cluster may not be considered to be equal. However, in this case they will be equal due to the homogeneous potential. Even in this case, the maximum number of bosons per site can be restricted depending upon U. The dimension of the hamiltonian varies according to number of sites considered in a cluster. For a cluster size L and maximum number of bosons n_{max}, the dimension is $(n_{max}+1)^L$. The hamiltonian for the cluster is constructed by using equation 2.3. The ground state energy and the wavefunction is obtained by SCM.

The phases of the system are further understood by calculating other associated quantities like average density and compressibility. It is seen that the accuracy increases with increasing cluster size. However, the size of the Fock space increases exponentially with

the number of sites and thus the dimension of the hamiltonian increases exponentially. Therefore, it is computationally not possible to work with large cluster size. This is where the DMRG method can be used to build up a large cluster and incorporate mean field into it.

2.3 Density Matrix Renormalisation Group Theory

The density matrix Renormalisation group (DMRG) is another well known approximation method used to approximate the ground state wavefunction of a large sized system. It is an iterative procedure and as the name suggests, it involves renormalising the ground state wavefunction in each iteration. We already know that the dimension of Hamiltonian matrix (Hilbert space) for a system increases exponentially with increasing size of the system. For 1-D system, the dimension of the Hamiltonian matrix varies as n^L, where n is the number of basis states for each site and L is the length of the system (total number of sites). This means that for $n = 4$ and $L = 100$, dimension is 4^{100}, which is quite a large number. Computationally, it becomes very difficult to store and operate this large matrices. This is where the renormalisation group theory helps.

The idea of renormalisation group theory is to build an effective hamiltonian for a large system by beginning with a smaller sized system called the superblock. The process is to reduce/truncate the number of basis associated with this superblock and calculate an effective hamiltonian whose dimension is less than that of the original. This is done such that the ground state wavefunction does not change much and it still contains almost all the information of the system. Also, the effective hamiltonian is close to the original hamiltonian. Then, the system is increased by adding new sites (usually one or two) to the current superblock. This increased system is considered as the new superblock. Now, obtaining the ground state wavefunction is easier than the original system because the dimension of the Hamiltonian has reduced. After this, the process of truncating the basis of the current superblock to use it in the construction of the new increased superblock is continued until the system grows to the desired length.

The most important and effective step in the renormalisation procedure is choosing the right basis for truncation. This is where the density matrix is used (hence the name DMRG). It is found that if a block and its environment are considered as a system, then the eigenvectors of the reduced density matrix of the block serve as the effective basis for forming the truncated wavefunction [12, 14, 17]. The eigenvalues of the density matrix are the probabilities of these eigenvectors. Therefore, only those which are highly probable can be considered for truncation. In other words, we can divide our superblock into two subsystems, say blocks A and B and treat one as the system and the other as an environment at a time. Then, the truncated eigenvectors of the reduced density matrices of block A and block B will be the new basis of these blocks, respectively.

The above DMRG is carried till any length of interest and for that reason, it is called Infinite-Sized Density Matrix Renormalization Group Method (IS-DMRG). The step wise procedure for IS-DMRG is as given below.

1. Begin with a small cluster for which exact diagonalisation is possible. Construct the hamiltonian for this cluster and diagonalise to obtain the ground state energy and its eigenvector $|\Psi\rangle$.

2. Divide the cluster into two blocks, say left block A and right block B. Usually, A and B are chosen to be symmetric. With this the ground state can be written as $|\Psi\rangle = \sum_{i=1,j=1}^{N_A,N_B} C_{ij}|i\rangle|j\rangle$, where $|i\rangle$,$|j\rangle$ are the basis states of block A and block B, respectively. N_A and N_B are the number of basis associated with the left and the right blocks.

3. Compute the reduced density matrix of A.

$$\hat{\rho}_A = \sum_{i,i'} \sum_{j} C_{ij} C^*_{i'j} |i\rangle\langle i'|$$

4. Diagonalise $\hat{\rho_A}$. Use the eigenvalues to obtain the M ($M < N_A$) highest probable eigenvectors, such that the sum of the their probabilities is very close to 1. This

eigenvector space of dimension M is used as the new truncated basis for block A. In matrix form it is written as $O = [v_1, v_2, ..., v_M]$, where $v_1, v_2, ..., v_M$ are the M chosen eigenvectors.

5. Using the new basis O, transform all the operators corresponding to block A. For example, the transformation of an operator $\hat{A}$ will be $\hat{A}' = O^\dagger \hat{A} O$.

6. Perform similar steps from 3 to 5 for block B.

7. Then, add two new sites in between block A and block B, which will together make a new superblock. Construct the hamiltonian of the superblock ($\hat{H}_{SB}$) by using the transformed operators of A, B and the basis of the two added sites. Diagonalise ($\hat{H}_{SB}$) to obtain the ground state energy and its eigenvector.

8. Repeat the process from step 2 and continue until the desired length of cluster is reached. At the end, the ground state energy and its wavefunction for that length is obtained.

The IS-DMRG method is performed in canonical ensemble where the number of particles is fixed for a given length. Usually, it is used near average density of bosons equal to 1, to study the gap in the energy, where the gap corresponds to a Mott Insulator [11]. In gap-less phases, the system maybe a superfuild or in some other phase. This can be determined by calculating some other quantities. However, with DMRG it is only understood whether the system is in superfuild or not. The measurement of the superfuildity (superfuild density) is not possible. This is because with fixed number of particles, the expectation value of $\hat{a}$ is always zero at every site.

This is where the combination of CMFT and DMRG methods helps. The details of this method is discussed in the next section, where it has been explained how it is used to study Bose Hubbard study model in one dimension with order parameter as a complex quantity.

2.4 CMFT-DMRG for homogeneous potential

In section 2.2, by using CMFT, the hamiltonian for 1-D BHM of cluster length L was found to be

$$\begin{aligned} H = -t\sum_{i=1}^{L-1}(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i) \; + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_i(\hat{n}_i - 1) \; - \mu\sum_{i=1}^{L}\hat{n}_i \\ + 2t|\psi|^2 - t\psi(\hat{a}_1^\dagger + \hat{a}_L^\dagger) - t\psi^*(\hat{a}_1 + \hat{a}_L) \end{aligned} \tag{2.4}$$

And we had said that it is possible to diagonalise the above hamiltonian upto a very small length (maybe up to $L = 4$). Therefore, the idea is to start with a cluster size of four and increase the size by using the DMRG method, along with minimising the ground state energy with respect to the order parameter at every length. The procedure for this method is as shown below.

1. Begin with a 2-site superblock. Divide this superblock into two subsystems, say left block L and right block R. Construct the single-site hamiltonians of these 2 sites.

2. Now add 2 more sites in between of these blocks and form a new superblock of length 4.

3. Construct the Hamiltonian matrix for the superblock by using equation 2.4.

4. Diagonalise the superblock Hamiltonian and minimise the ground state energy by using SCM. Since we are working with complex order parameter, ψ will have a form of $\psi = re^{i\theta}$, where $r = |\psi|$ is the magnitude and θ is the phase angle. Therefore, we have to minimise with respect to both, r and as well as θ. Once the minimisation is achieved, the ground state energy and its eigenvector for this particular length are obtained. The ground state wavefunction can be written as

$$|\Psi\rangle = \sum_{\alpha_L,\sigma_L,\sigma_R,\alpha_R} C_{\alpha_L\sigma_L\sigma_R\alpha_R}\, |\alpha_L\sigma_L\sigma_R\alpha_R\rangle$$

Here $|\alpha_L\rangle, |\sigma_L\rangle, |\sigma_R\rangle, |\alpha_R\rangle$ are the basis states of block L, the left site, the right site

and block R, respectively.

5. Again, divide this superblock into two subsystems, left block L' consisting of block L and its adjacent site and right block R' consisting of R and its adjacent site. Using the ground state eigenvector, construct the reduced density matrix for block L' by tracing out block R' from the overall density matrix. In this case, the reduced denisty matrix of L' is

$$\hat{\rho}_{L'} = \sum_{\alpha_L,\sigma_L,\alpha_L^{'},\sigma_L^{'}} \sum_{\sigma_R,\alpha_R} C_{\alpha_L\sigma_L\sigma_R\alpha_R} C^{*}_{\alpha_L^{'}\sigma_L^{'}\sigma_R\alpha_R} |\alpha_L\sigma_L\rangle\langle\alpha_L^{'}\sigma_L^{'}|$$

6. Diagonalise $\hat{\rho}_{L'}$ and choose M eigenvectors whose probabilities are the highest and their sum is close to 1.

7. Form the new basis matrix O (also called transformation matrix), which consists of these M eigenvectors.

8. Construct the hamiltonian of the left block L' and transform it using O, i.e. $H_L^{new} = O^{\dagger} H_L O$. Also, construct and transform the operators needed for the next length.

9. Perform the same steps from 5-8 for block R and the right site to obtain H_R^{new} and the other transformed operators of the new right block R'.

10. Set $L = L'$, $R = R'$, $H_L = H_L^{new}$ and $H_R = H_R^{new}$. Do the same the for other operators. These operators will be used in forming the hamitonian of the superblock in the next length.

11. Now, add 2 sites in between and increase the length of the superblock by 2. The hamiltonian of this superblock is

$$\hat{H}_{SB} = \hat{H}_L + \hat{H}_R + \hat{H}_{LS} + \hat{H}_{RS} + \hat{H}_{L,LS} + \hat{H}_{LS,RS} + \hat{H}_{RS,R}$$

Here, $\hat{H}_L$ and $\hat{H}_R$ are the hamiltonians of the left and the right blocks in the current basis, $\hat{H}_{LS}$, $\hat{H}_{RS}$ are the single site hamiltonians of the newly added left and right

sites and $\hat{H}_{LS,RS}$ is the hopping term between these two sites. $\hat{H}_{L,LS}$ and $\hat{H}_{RS,R}$ are the hopping terms between the left block - left site and the right block - right site, respectively.

12. Construct the superblock hamiltonian using the above equation.

13. Then, continue from step 4 until the desired length is achieved. In homogeneous potential, the process is continued until the energy per length converges.

After calculating the ground state wavefunction of the lattice, we can calculate the order parameters and the average density at the every site. For this, we have to calculate and transform the operators in the new basis at every length. Then, the expectation value of any operator $\hat{A}_i$ for site i can be calculated as

$$\langle \hat{A}_i \rangle = \sum_{\alpha_L,\sigma_L,\sigma_R,\alpha_R} \sum_{\alpha_L^{'},\sigma_L^{'},\sigma_R^{'},\alpha_R^{'}} C_{\alpha_L\sigma_L\sigma_R\alpha_R} C^{*}_{\alpha_L^{'}\sigma_L^{'}\sigma_R^{'}\alpha_R^{'}} \langle \alpha_L^{'}\sigma_L^{'}\sigma_R^{'}\alpha_R^{'}|\hat{A}_i|\alpha_L\sigma_L\sigma_R\alpha_R\rangle$$

2.5 CMFT-DMRG for Harmonic Trap Potential

In this section we will explain how CMFT-DMRG method is used to study the BHM in one dimension in the presence of a harmonic trap potential. Due to the harmonic potential, a new term is added to hamiltonian 2.1 and the hamiltonian changes to

$$H = -t\sum_i \hat{a}_i^{\dagger}\hat{a}_{i+1} + \hat{a}_{i+1}^{\dagger}\hat{a}_i \; + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \; - \mu\sum_i \hat{n}_i + V_T\sum_i n_i \left(\frac{L+1}{2} - i\right)^2 \quad (2.5)$$

Here, $V_T > 0$ which determines the shape of the parabola and L is odd.

The procedure for building the cluster in this case is similar to the homogeneous potential case. The only new thing here is how we include the trap potential for every site while building up the cluster size. A proper parabola can be shown with odd number of sites. However, we are working with even number of sites. So, to ensure that trap potential in

even number of sites is closer to a parabola, we slightly modified equation 2.5 to

$$H = -t\sum_i \hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i + V_T \sum_i n_i \left(\frac{L}{2} - i - 0.5\right)^2 \quad (2.6)$$

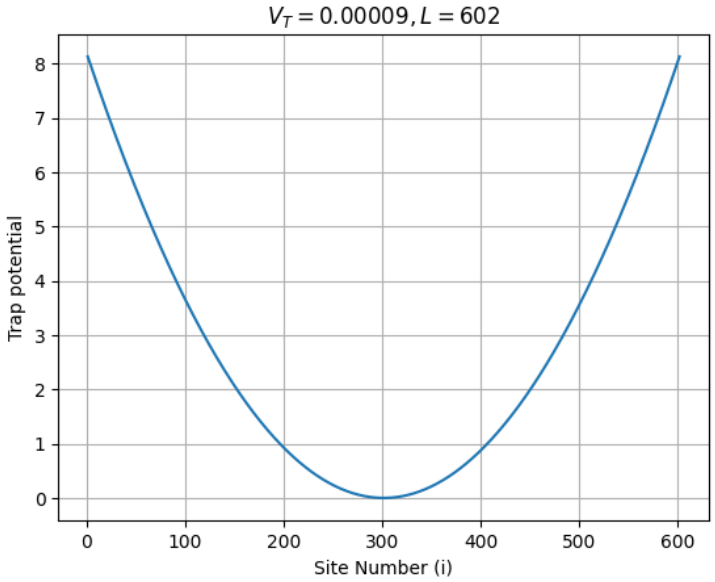

Figure 2.1: Plot of trap potential in the units of t as a function of lattice site

Applying CMFT on the above equation, we get

$$\begin{aligned} H &= \sum_k H_k \\ H_k &= -t\sum_{i=1}^{L-1}(\hat{a}_{k,i}^\dagger \hat{a}_{k,i+1} + \hat{a}_{k,i+1}^\dagger \hat{a}_{k,i}) + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_{k,i}(\hat{n}_{k,i} - 1) - \mu\sum_{i=1}^{L}\hat{n}_{k,i} \\ &\quad + 2t|\psi|^2 - t\psi(\hat{a}_{k,1}^\dagger + \hat{a}_{k,L}^\dagger) - t\psi^*(\hat{a}_{k,1} + \hat{a}_{k,L}) + V_T\sum_{i=1}^{L} n_i \left(\frac{L}{2} - i + 0.5\right)^2 \end{aligned} \quad (2.7)$$

Here, the aim is to start with a 4-site cluster and build it up to the desired length such that the final cluster contains a parabolic trap potential. For building a cluster with length L where potential at each site is $\left(\frac{L}{2} - i\right)^2$, we begin with the 4-site cluster and treat these sites as the edge sites of the final cluster, which are $1, 2, L-1, L$, respectively. Therefore, the potentials at these 4 sites are $\left(\frac{L}{2} - 0.5\right)^2$, $\left(\frac{L}{2} - 1.5\right)^2$, $\left(\frac{L}{2} - 1.5\right)^2$, $\left(\frac{L}{2} - 0.5\right)^2$ and $\left(\frac{L}{2} - 0.5\right)^2$, respectively. Then, the superblock hamiltonian is constructed using these potentials. Later, when the length is increased by 2, the newly added sites are numbered

as 3 and $L-3$ and the superblock hamiltonian is constructed accordingly. This way the harmonic potential is built from the edge to its centre. When the length of the cluster reaches L, the cluster will be having the harmonic trap as designed and we obtain the ground state energy and the wavefunction for this system. It is to be noted that the energy per length will not converge in this case because the potential is changing in each iteration. Once we achieve the final desired length, we calculate the order parameters and the average densities at every site in the cluster.

2.6 Davidson Algorithm

The most time consuming part in the CMFT-DMRG process is minimisation of the ground state energy, where we have to digonalise the hamiltonian several times. The dimension of the hamiltonian may go up to the order of 10^4 and diagnolising this large hamiltonian is time consuming. Since the Hamiltonians of BHM are highly sparse and we are concerned with obtaining only the ground state energy and its eigenvector, the Davidson Algorithm was used for diagnolisation. The Davidson algorithm is a well known algorithm which is used to approximate the few lowest or few highest eigenvalues and their corresponding eigenvectors of large, sparse and symmetric matrices [2, 4]. Since we are working with complex order parameter, the Hamiltonians are hermitian matrices. Therefore, using the Davidson algorithm a code was developed for obtaining the ground state and its eigenvector for our Hamiltonians.

The Davidson algorithm starts with an initial guess for the ground state eigenvector and finds a new ground state eigenvector closer to the actual one in each iteration. The new eigenvector is found by using a pre-conditioner. The procedure for the Davidson algorithm is as discussed below.

Suppose we want to obtain the ground state vector of a hermitian matrix A with dimension (n x n). Also, we have an orthonormal basis with dimension ($k << n$), which contains a good estimate to the ground state of A. To find a vector very close to the ground state eigenvector we,

1. Form a subspace of the original Hamiltonian by matrix multiplication, $H_k = V_k^\dagger A V_k$.
2. Diagonalise H_k and obtain its ground state energy (λ_k) and the corresponding eigenvector (y_k)
3. Now, the estimated eigenvector of the original Hamiltonian (A) is $x_k = V_k y_k$
4. Then, calculate the residual vector, $r_k = (x_k - \lambda_k I)\, A$.
5. For the best estimation of the ground state, r_k should be very close to null vector.
6. If r_k is a non-zero vector, calculate the new suitable vector, which will be added to the ortho-normal basis. Say $t_{k+1} = C_k r_k$, where C_k is some suitable transformation called the pre-conditioner.
7. Add t_{k+1} to V_k and orthonormalise the new basis.
8. Increment k by 1 and continue from step 1, until the desired convergence for the ground state is met.

The rate of convergence depends on the preconditioner used in the process. The preconditioner may depend on the form of the matrix. For diagonal dominant matrices, the preconditioner used is $C_k = (\lambda_k I - D)^{-1}$, where D is the digonal matrix of A. Usually, the hamiltonian of BHM is diagonally dominant and hence we use this preconditioner. We start the algorithm with $k = 1$. The initial guess for the energy is the lowest value of the diagonal elements (say i^{th} element) and the initial guess for the basis is a unit vector such that $V_1 = [x_m]_{n\times 1}$, where $x = 1$ if $m = i$, else $x = 0$. This algorithm gives the ground state energy and the eigenvector in lesser then the standard algorithm designed for general hermitian matrices. We have reduced the time for diagonalising even further by avoiding repetitive multiplications of the same rows and columns during the process and taking the advantage of the sparsity of the hamiltonian. It also has to be noted that we cannot use the same Davidson code for digonalising the density matrices as there we need to calculate several eigenvectors. We use the Lapack subroutine for this purpose.

Chapter 3

Results

3.1 In the absence of Trap Potential

In this section the results for the 1-D BHM without a trap potential are discussed. The system was analysed for two sets of parameters, $(U = 5, \mu = 0.6)$ and $(U = 5, \mu = 1.4)$. It is noticed that the average boson density (ρ) is less than or close to one in these two cases and there is no change seen in the values of the properties for $n_{max} \geq 3$. Therefore, the procedure was conducted with $n_{max} = 3$.

The first step was to determine the number of basis states (M) to be truncated after each length. To recall, M is the number of basis states to which the basis of the left and the right blocks is truncated after each length. If the number of basis states are less than M, then no truncation is considered. For this purpose the order parameter (ψ) and the average boson density (ρ) were analysed as functions of the lattice site (i) for a fixed length (L) and varying M. Here, the order parameter has two components, the magnitude $(|\psi|)$ and the phase angle (θ). $|\psi(i)|^2$ gives the superfuild density at a site. The plot for $U = 5, \mu = 0.6$ and $L = 602$ is shown in fig. 3.1. It is observed that the values of $\rho(i)$ and $\theta(i)$ do not change with respect to the number of truncated basis states. However, the values of $|\psi(i)|$ converge as the value of M is increased. Also, the energy per site at this length does not change much with respect to M.

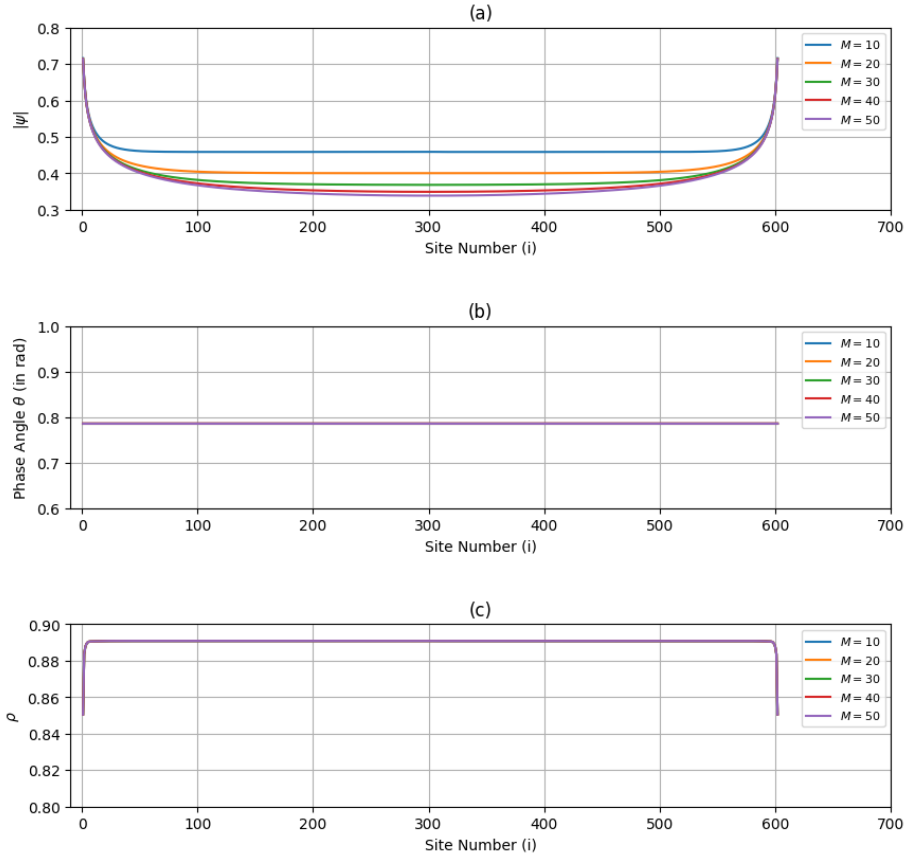

Figure 3.1: The above plot is for $U = 5$, $\mu = 0.6$ and $L = 602$. It shows variation of different parameters w.r.t lattice site, (a) Magnitude ($|\psi(i)|$) of order parameter, (b) The phase angle ($\theta(i)$) of order parameter (c) Average boson density ($\rho(i)$)

Also, it is observed that the superfuildity decreases and converges as we move from the edge to the centre of the lattice. The edge sites are expected to have higher superfuildity because of the mean-field calculation, which overestimates the superfuildity. The boson density is seen to be increasing from the edges initially and saturating to a constant value til the centre. Whereas, the phase angle of the order parameter is constant at all sites in the lattice. It is found that this value is equal to the initial value given in the SCM procedure.

From the above observations, it is understood that the values begin to converge at around $M = 50$. Therefore, it was decided to consider $M = 50$ for rest of the study.

The next step was to see how the energy, SF order parameter and average density vary with length of the lattice. It was found that the energy per site decreases with the length and converges to a finite value as seen in fig. 3.2.

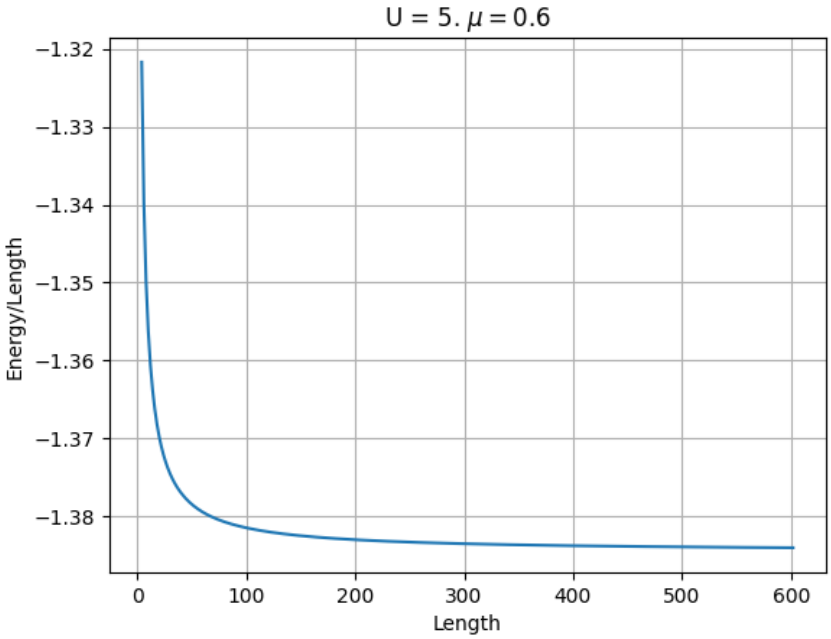

Figure 3.2: Plot of energy/length as a function of the lattice length for $U = 5$, $\mu = 0.6$ and $M = 50$

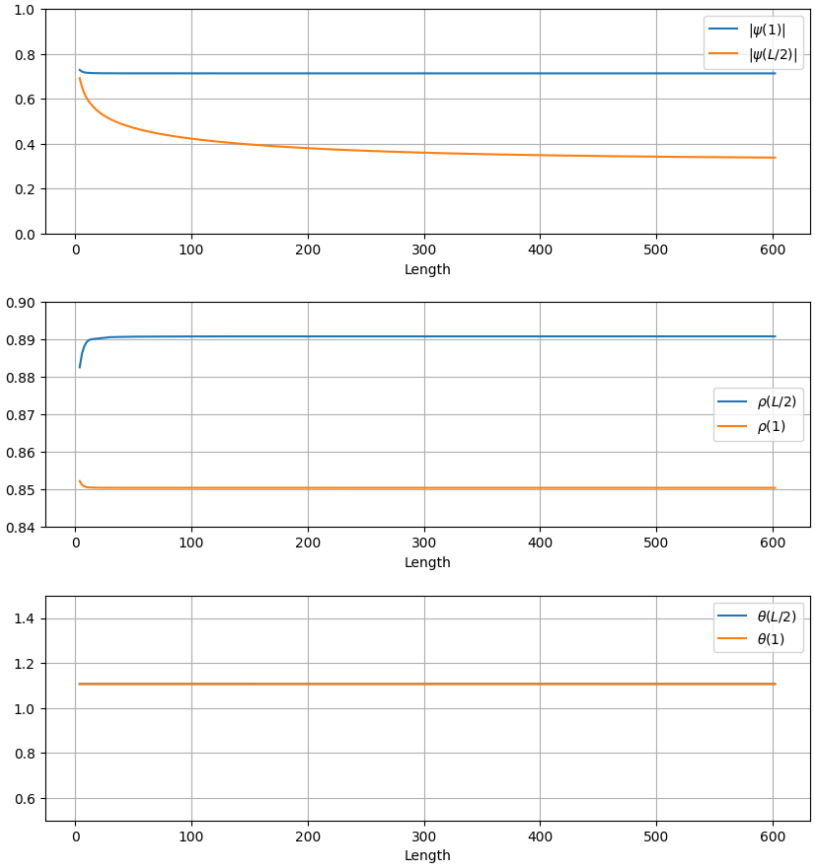

Figure 3.3: Plot of (a) magnitude of order parameters (b) phase angle of order parameters (c) average densities at the edge and the middle site, i.e. $i = 1, \frac{L}{2}$ as a function of length for $U = 5$, $\mu = 0.6$ and $M = 50$

Since in fig. 3.1 the values of SF order parameter components and the average density were continuous and converging with respect the site number, only the values at the first site and the middle site were calculated as function of lattice length. The values at the remaining sites will follow the same nature. In fig. 3.3 it is observed that $|\psi(1)|$ and $|\psi(\frac{L}{2})|$ converge with respect to the lattice length with $|\psi(1)| \geq |\psi(\frac{L}{2})|$. $|\psi(\frac{L}{2})|$ converging later than $|\psi(1)|$ shows the convergence of all $|\psi(i)|$ (for $i = 1, \frac{L}{2}$) as the lattice length is increased. The values of $\rho(1)$ and $\rho(\frac{L}{2})$ also converge to a finite value as the lattice length is increased. It is also seen that $|\psi(\frac{L}{2})|$ converges faster than $\rho(\frac{L}{2})$. This data matches with the data presented in the study of 1-D BHM with real order parameter [22]. The convergence of $|\psi(\frac{L}{2})|$ to a finite value indicates that at very large lattice length, the superfluidity is finite and constant at almost all the sites. This means that the system is in superfuild phase at $U = 5$, $\mu = 0.6$. However, it is seen that $\theta(\frac{L}{2})$ remains constant and equal to the initial guess at every length. This indicates that the energy is independent of the phase angle and will be constant through out the lattice.

The figures 3.4 and 3.5 show the cases of the system been in superfuild phase and mott insulator phase. It is seen that at $U = 5$, $\mu = 0.6$ the system is in superfuild phase with a finite superfuildity and a average density of about 0.9. It is seen that the phase angle is constant through out the lattice. At $U = 5$, $\mu = 1.4$, the system is found to have zero superfuildity at all sites expect the edge sites. The superfuildity at the edge sites is due to the mean-field approximation. Therefore, ignoring some of the edge sites, the system is seen to be in a mott insulating phase with a average density of 1. As seen previously, the phase angle is constant everywhere and equal to the initial guess.

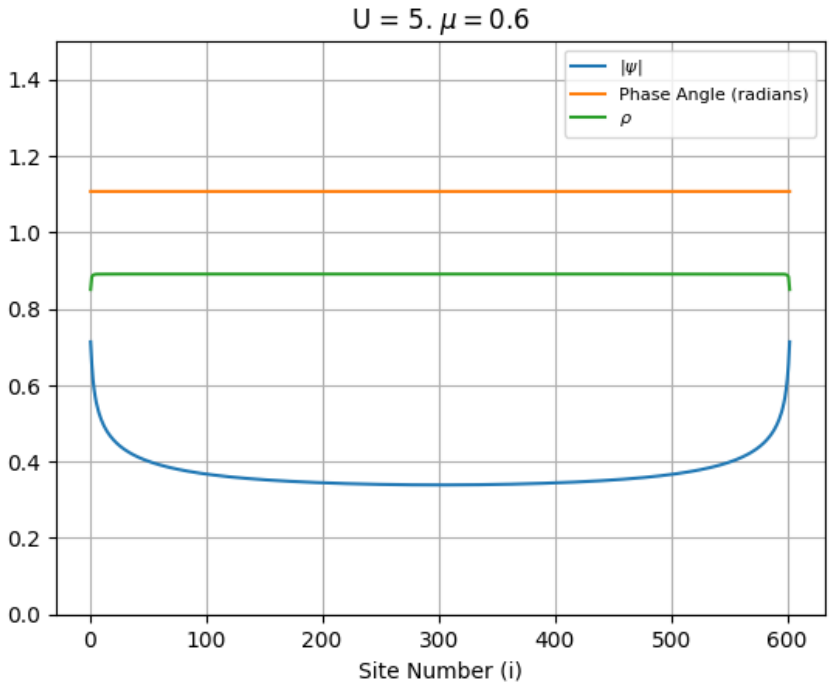

Figure 3.4: Plot of superfuild order parameter $(|\psi(i)|, \theta(i))$ and average density $(\rho(i))$ as a function of lattice site (i), for $U = 5$, $\mu = 0.6$ and $L = 602$.

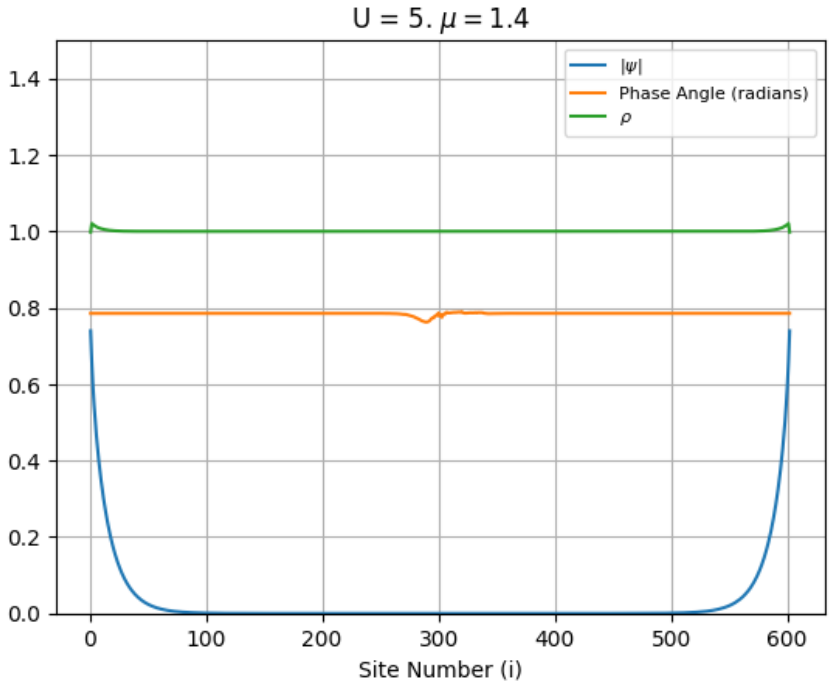

Figure 3.5: Plot of superfuild order parameter $(|\psi(i)|, \theta(i))$ and average density $(\rho(i))$ as a function of lattice site (i), for $U = 5$, $\mu = 1.4$ and $L = 602$.

This section can be concluded with the discussion of the phase coherence correlation

function, which is defined as

$$\Gamma(r) = 0.5\langle \hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \rangle \quad ; r = |i - j|$$

Here, $\langle \dots \rangle$ denotes the expectation value with respect to the ground state and i, j are any two sites in the lattice.

It was expected that the correlation function would show some interesting behavior if there was some variation of the phase angle in the lattice. Since the phase angle is same at all site, $\Gamma(r)$ is real for all r and behaves same as the case where the SF order parameter is considered to be real [22]. Fig. 3.6 shows the behaviour of the correlation function for $U = 5, \mu = 0.6$ and $U = 5, \mu = 1.4$. The data was taken for length $L = 600$ with fixing i at 300 and varying j from 301 to 500 such that i, j lie in the converged SF order parameter region.

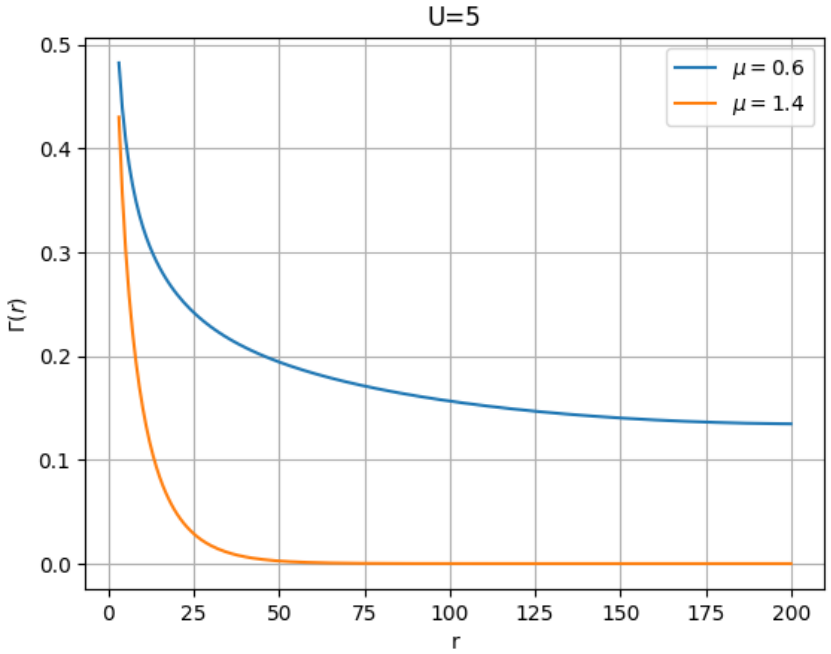

Figure 3.6: Plot of phase coherence correlation function $\Gamma(r)$

For $U = 5, \mu = 0.6$ the system is in SF phase and the correlation function decays as a power-law with r and $\Gamma \to |\psi(L/2)|^2$ as $r \to \infty$. In MI phase, for $U = 5, \mu = 1.4$ the correlation function decays to zero exponentially with r [22].

3.2 In the presence of Trap Potential

In this section, the results from the study of 1-D BHM in harmonic trap potential are presented. The harmonic trap potential was set up such that the boson density at the edges of the final lattice is zero. The value of M was chosen to be 50 which gave an error of the order 10^{-8} in the total probability of the new basis. The systems were built such that the maximum density went up to 1.5. It was found that $n_{max} = 4$ is sufficient for this purpose.

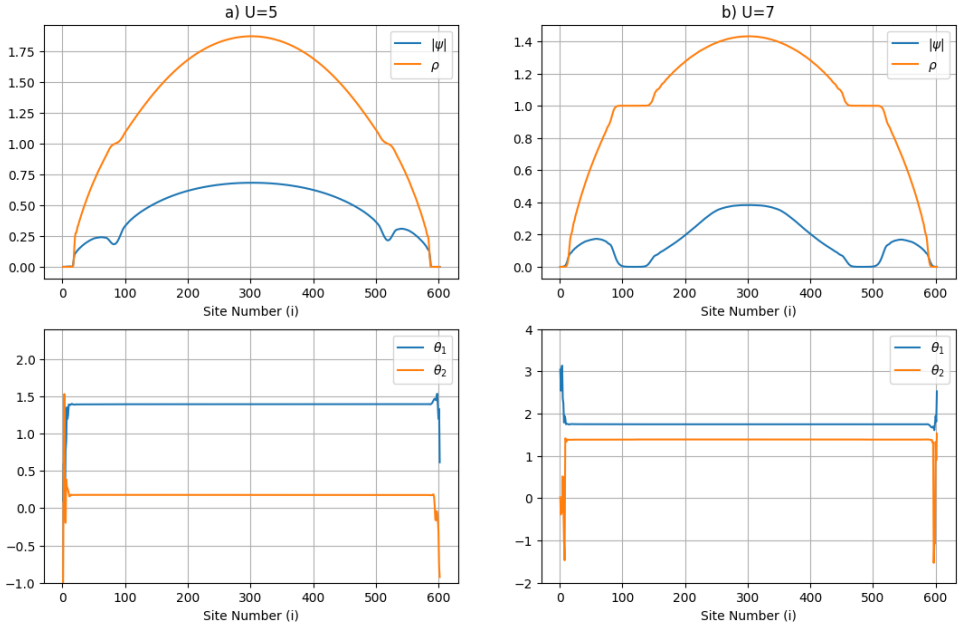

Figure 3.7: Plot of $|\psi|, \theta, \rho$ as a function of site i for $V_T = 9 \times 10^{-5}, \mu = 5.5$ and $U = 5, 7$

The CMFT-DMRG method was used for system with $V_T = 9 \times 10^{-5}, \mu = 5.5$ for length $L = 602$ such that the density at the edge is zero. The initial data was taken for two sets of U, $U = 5$ and $U = 7$. The components of the superfuild order parameter $|\psi|, \theta$ and the average density ρ were analysed as functions of lattice site (i) in both cases as shown in fig. 3.7. First it seen that the parameters are symmetric about the centre of the lattice. As set, the boson density is zero at the edges and increases smoothly along with the length, till the centre of the lattice. At the centre, it has a maxima. The superfuildity is seen to be zero near the edges but is finite in the remaining portion of the lattice. It is zero near the edge until the boson density is finite. Later, as the we go towards the centre, along with the density, the magnitude of the order parameter increases. As the

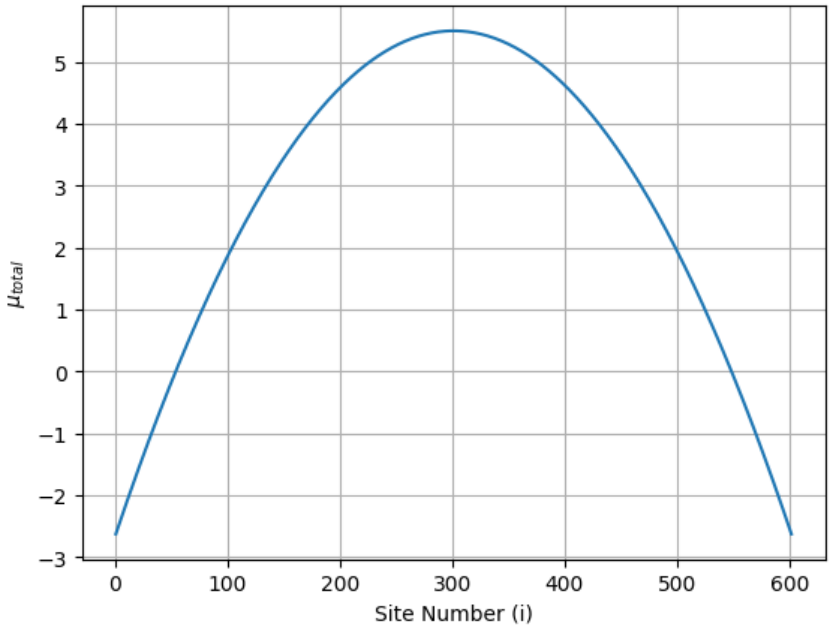

Figure 3.8: Plot of μ_{total} as a function of lattice site

density reaches towards one, the superfuildity decreases until density is equal to one and increases after that, till the centre. The behaviour of the density and the magnitude of superfuild order parameter can be understood by calculating the effective chemical potential at each site. Due to the harmonic potential, the total chemical potential is not uniform throughout the lattice. The total chemical potential at a site i can be written as $\mu_{total,i} = \mu - V_T \left(\frac{L}{2} - i + 0.5\right)^2$. It is minimum at the edges (negative in this case) and increases in a parabolic nature towards the centre, as shown in fig. 3.8. Due to the increase in net chemical potential, the density of the bosons increase towards the centre and the superfuildity also increase with it. This nature of superfuildity and density is already known in the literature [22]. As the density increase to more than one, the contribution of on-site interaction increases, which restricts the superfuild flow. Hence, there is a fall in the magnitude of superfuild order parameter at $\rho = 1$.

It is observed that the phase angle $\theta(i)$ of the order parameter is constant throughout the lattice and is equal to the initial guess (θ_1). To re-check this behaviour of the phase angle, the CMFT-DMRG method was carried out with a different initial guess (θ_2) for the phase angle. Again, it is constant at every site but equal to the new initial guess given. It can be said that the entire system is in superfuild phase with a uniform phase angle and it is

can be expected that the phase angle will vary if there is phase separation in the lattice, i.e. the formation of a MI phase in between of the SF phase. To analyse this, the data was collected for same system at $U = 7$, which is shown in part (b) of fig. 3.7. However, it is seen that the phase angle shows the same behaviour even with a phase separation in the lattice. With this it is understood that the phase angle of the order parameter in CMFT-DMRG does not show any significance in the system. Therefore, the system is further studied without including the phase and the magnitude of the order parameter is written as the order parameter.

Later, it was studied how the properties vary across the lattice for different values of on-site interaction strength U. The data was collected for systems of length $L = 602$ at $\mu = 5.5, V_T = 9 \times 10^{-5}$ and $U = 4, 5, 6, 7$.

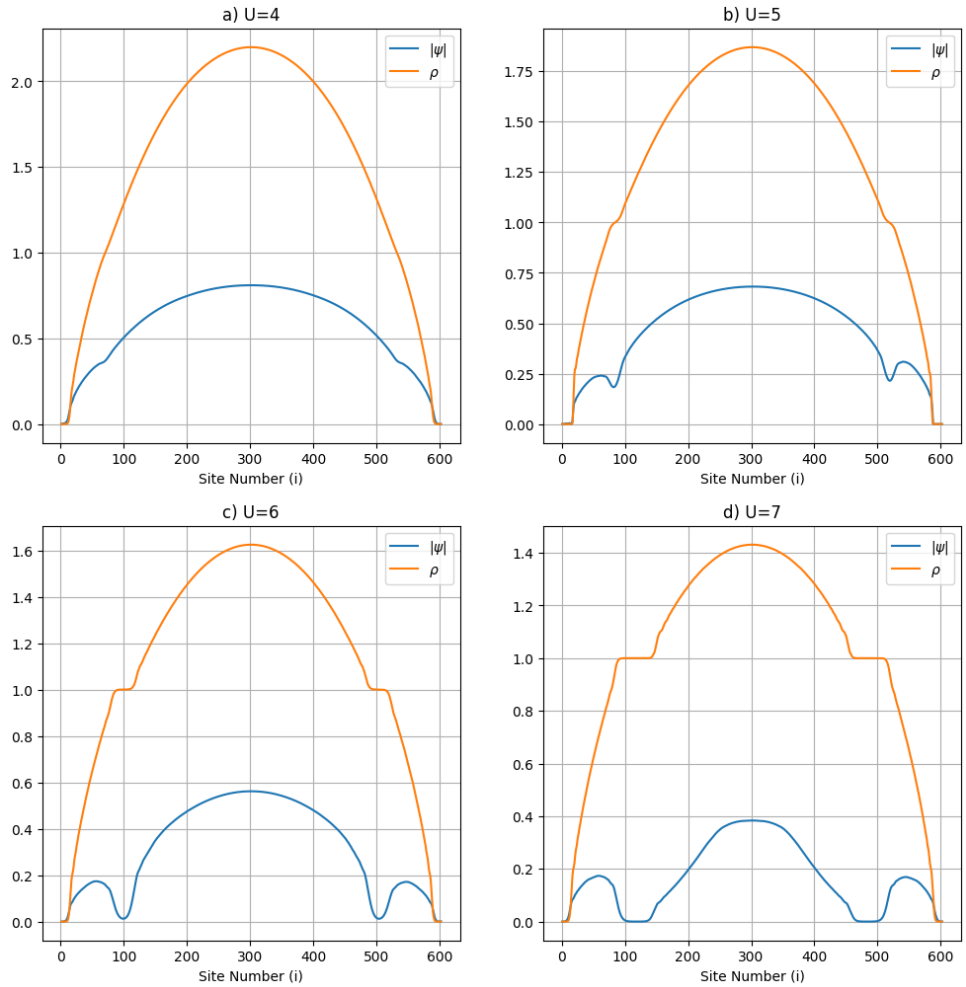

Figure 3.9: Plot of SF order parameter and average density as a function of lattice site for $\mu = 5.5, V_T = 9 \times 10^{-5}$ and $U = 4, 5, 6, 7$

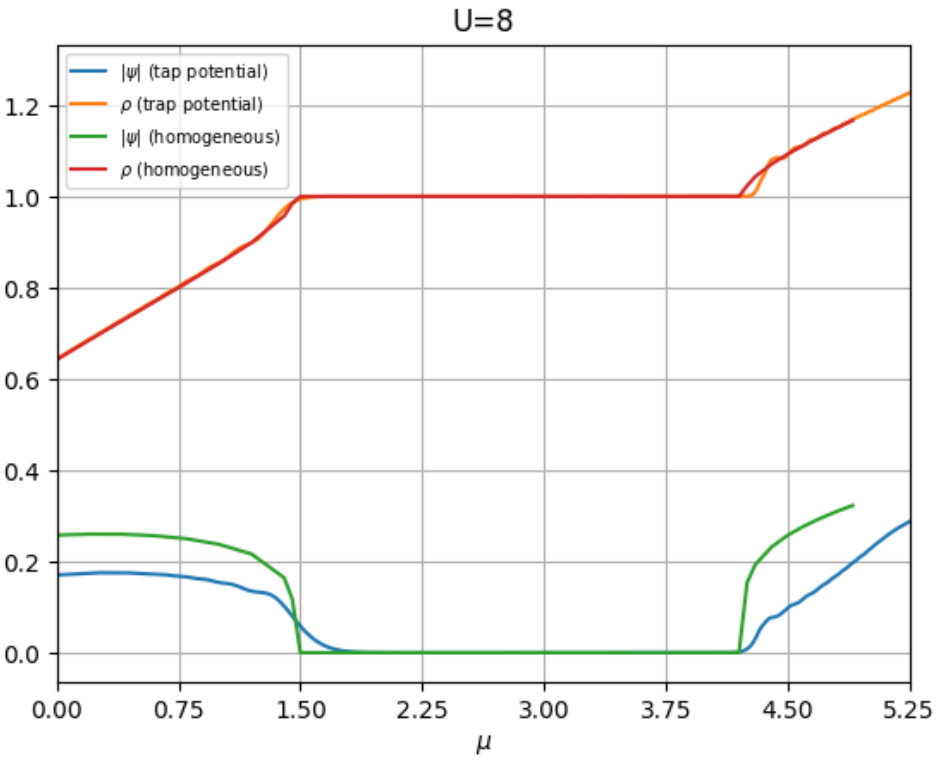

Figure 3.10: Comparison of $|\psi|, \rho$ as a function of μ between systems in homogeneous and in-homogeneous (trap potential)

It is seen that the superfuild order parameter $|\psi(i)|$ and the average density $\rho(i)$ behave as discussed earlier but the values at each site decrease as the on-site interaction strength (U) is increased. Further, the fall of the superfuildity at density 1 increases as U increases. At $U = 7$, it is seen that the superfuild order parameter goes to zero and the density is 1 in this region, which signifies that the region has undergone a phase transition from superfuild to mott insulator. Another noticeable point is that there is a smooth transition from superfuild to mott insulator unlike in the case of homogeneous potential where the transition is sharper. The comparison is shown in fig. 3.10. Here, the order parameter and average density is plotted as a function of μ for homogeneous system of length $L = 800$ at $U = 8$. Here, $|\psi(\frac{L}{2}|$ and $\rho(\frac{L}{2})$ are considered as the order parameter and the average density of the system [22]. Also, the order parameter and the average density for the trap potential case is plotted for a system with $L = 1200$, $U = 8$, $\mu = 5.5$ and $V_T = 9 \times 10^{-5}$. The values are plotted as a function of the total chemical potential at each site in the lattice. It can be seen that there is a sharp transition from SF phase to MI phase at $\mu = 1.5$ and from MI phase to SF phase at $\mu = 4.2$ in the case of homogeneous potential. In the

case of trap potential, the transition from SF to MI with increasing density is smooth and the SF order parameter decays exponentially, which does not make it possible to impose a boundary between superfuild and mott insulating phases. However, this nature is not seen when the transition happens from MI to SF with increasing density. The order parameter is seen to increase sharply at the transition. We predict that this may be because of the on-site interaction. As the average density increases from an integer value, the contribution of the on-site interaction increases which can restrict the superfuild flow until the chemical potential overcomes it.

The above points tell us that there is some penetration of the superfuildity into the mott insulating phase as compared to the homogeneous potential case. As a result, there can be small regions in the lattice which can have integer density with non-zero superfuildity. This is seen in graph (c) of fig. 3.9.

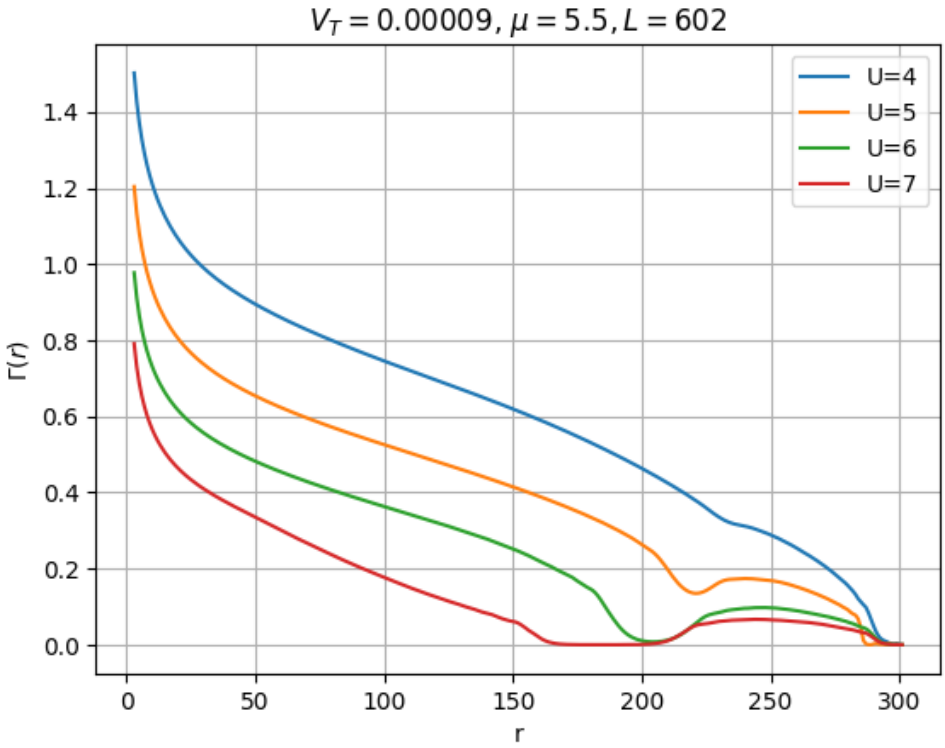

Figure 3.11: Phase coherence correlation function $\Gamma(r)$ in the case of the trap potential

In fig. 3.11 the phase coherence correlation function for the cases with $L = 602$, $\mu = 5.5$, $V_T = 9 \times 10^{-5}$ and $U = 4, 5, 6, 7$ is plotted as a function of $r = |i - j|$, where $i = 300$ and $303 \leq j \leq 602$. The aim was to check how the correlation function varies in the

presence of trap potential and how it behaves between particles across different phases. It is seen that for small values of U where there is no formation of MI regions, the correlation function is finite initially and decreases smoothly as j reaches to the edge of the lattice. It goes to zero at the edges as no particles can be present in that region. Also, the correlation decreases as U is increased. For large U where there is a formation of a MI region, the correlation function is seen to decay and become zero in the MI region. This was expected as no particle can be added in or removed from MI region. It interesting to see that it is non-zero (small) after j is outside the MI region. This implies that there is small correlation between the particles in two different SF phases separated by a MI phase. This correlation decreases as the MI region increases.

Chapter 4

Conclusion

The 1-D BHM was studied by using CMFT-DMRG method where the SF order parameter was considered as a complex quantity. It was found that the phase angle of the order parameter does not play any role in characterising the system. Hence, in mean-field approximation the system can be analysed with completely real order parameter. It is also seen this process does not show the quasi long-range ordering in the SF phase.

In the case of 1-D BHM in a harmonic trap, different regions of SF and MI phases can be found depending on the on-site interaction strength. When the density is increasing and the phase transition occurs from SF to MI phase, it is seen that SF order parameter penetrates into MI region and decays exponentially. The similar case is not seen when the phase transition occurs from a MI phase to a SF phase, when density is increasing. As a result, there can be small regions with density one but non-zero superfuildity. It is also found that the phase coherence correlation function decays to zero from a superfuild region to a mott insulating region but becomes finite again in the next superfluid region. This indicates that a particle from one SF region is correlated to a particle in another SF region.

Future Scope

One of the improvement that can be made in the project is by applying Finite-size Density Matrix Renormalisation Group (FS-DMRG) after every length in the IS-DMRG process. By using FS-DMRG at each length, the ground-state energy and its eigenvector for that length converge even more [12, 14, 17]. DMRG works fine in the case where the potential is homogeneous as the energy per site converges after certain length. However, the energy per site does not converge in the case of harmonic trap potential. Though IS-DMRG was sufficient to see the results but for better convergence of the order parameter FS-DMRG can be used.

The correlation function can be better understood by keeping U, μ, L constant and varying V_T as it will be possible to shrink and expand the MI region for the same on-site interaction strength and chemical potential. Unfortunately, the Davidson algorithm did not work for large values of V_T where the density is zero for many sites. Therefore, instead of the harmonic trap potential, a step potential can be introduced in the lattice. The step potential can be introduced for few sites at the centre of the large lattice where that the SF order parameter is converged for large number of sites. Then, a MI region can be introduced at the centre by manipulating the height of the step potential. The size of the MI region can be changed by changing the width of the step potential. With this it can be checked how the correlation function behaves across the MI region and how it varies with the size of MI region.

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