Cluster Mean Field Theory plus Density Matrix Renormalisation Group on Bose Hubbard Model with Ring Exchange

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DECLARATION

I hereby declare that the data presented in this Dissertation report entitled, "Bose Hubbard Model with Ring Exchange" is based on the results of investigations carried out by me in the Physics discipline at the School of Physical and Applied Science, Goa University under the Supervision of Ms.Pallavi Pandhari Gaude 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 or other findings given the dissertation.

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COMPLETION CERTIFICATE

This is to certify that the dissertation report,"CMFT+DMRG on Bose Hubbard Model with Ring Exchange"is a bonafide work carried out by Ms Pranjali Anant Shet Verenkar under my supervision in partial ulfilment of the requirements for the award of the degree of (M.sc Physics) in the Physics at the School of Physical and Applied Sciences, Goa University.

Pallavi P. Gaude

Signature and Name of Supervising Teacher

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ABSTRACT

We present the results of quasi 1-dimensional Bose Hubbard Model by accommodating Ring exchange hopping in a bi-ladder where the nearest neighbour hopping is allowed considering the Bosons to be spinless. Using the combination of Cluster Mean Field Theory and Density Matrix renormalization Group this model was studied in hard-core and soft-core limit. In the hardcore limit we observed decrease in the superfluidity, with increasing K strength, eventually transitioning into normal Bose liquid and $\rho = 0.5$ insulator. The phase separation which was predicted in this limit was not observed. In the soft-core limit, as the strength of K increases, the superfluid region shrinks and Mott Insulator phase region increases. In addition, insulating phases for $\rho = 1.5$ is also observed.

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Chapter 1

Introduction

Based on Bose's quantum statistics theories for photons, Einstein predicted Bose-Einstein condensation (BEC) in bosonic gases in 1925. The fundamental concept of BEC implies that a macroscopic number of particles occupy the lowest energy state below a critical temperature. The de-Broglie wavelength increases as the temperature, T, decreases and approaches the inter-particle mean separation at the critical point. It scales like $T^{-1/2}$. At this stage, particle wave functions are sufficiently overlapped, forming a Bose-Einstein condensate. The critical temperature T_c below which the condensate is formed is given by

$$T_c = \frac{2\pi\hbar^2}{mk_B}\left(\frac{n}{2.613}\right)^{\frac{2}{3}} \tag{1.1}$$

where $\hbar$ is the reduced Plank's constant, m is the mass of the boson, k_B is the Boltzman Constant and n is the number density of bosons. The extremely low temperature required was major hurdle in realizing the BEC. As the critical temperature T_c is proportional to m^{-1} and $n^{2/3}$, to increase T_c, high boson densities or lighter bosons were desired. But, with the very high densities as temperature decreases the transition to solid occurs before the formation of BEC. An example of this is ^4He, where transition to superfluid was observed where the boson flows without any resistance. Despite the strong interactions in this system, London

proposed that BEC may be the mechanism driving the phenomena of superfluidity in ^4He, even though Einstein's prediction pertained to a gas of non-interacting atoms. Further support for this perspective was provided by neutron scattering experiment.

One of the ways of studying quantum many body physics is through ultracold atoms and molecules. Ultracold atoms and molecules offer unparalleled freedom in designing, monitoring, and analysing the experiment. It has become possible because of advancements in theory and experimentation which permit the independent assessment of fundamental atomic and molecular properties, cooling and trapping methods that have been achieved since the 1980s, and advancements in optical control and imaging of atoms and molecules.

1.1 Optical lattices

Optical lattices are periodic potentials created by light-matter interactions. When an atom interacts with an electromagnetic field, the energy of its internal states depends on the light intensity. Therefore, a spatially dependent intensity induces a spatially dependent potential energy. Optical lattices have been widely used in atomic physics as a way to trap and cool atoms.

The additionally the control and ability to manipulate different system parameters such as dimensionality of the system, lattice constant, lattice geometry and, impurities and defects make them ideal simulators of the quantum many body systems

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1.2 Bose Hubbard Model

A theoretically straightforward model to represent cold atoms in an optical lattice at finite density is the combination of the kinetic energy in the lowest band with the on-site repulsion in the bounds of a sufficiently deep optical lattice is

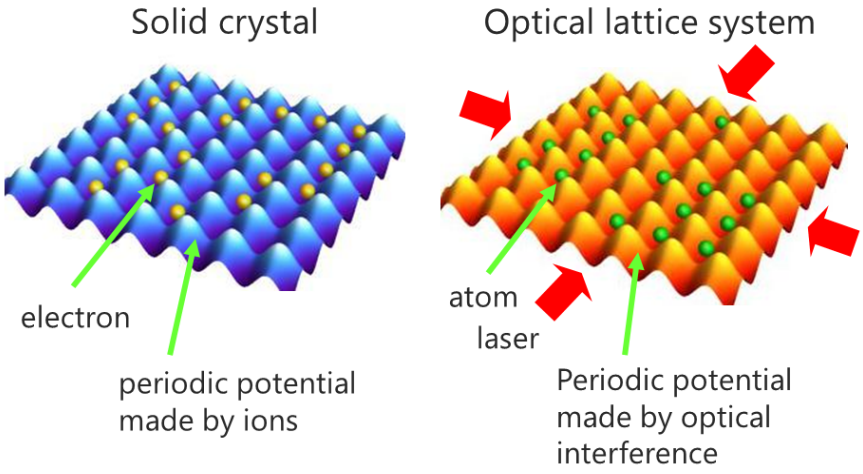

Figure 1.1: Representation of Optical Lattices

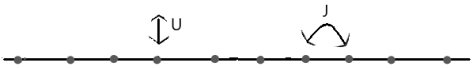

Figure 1.2: Bose Hubbard Model in 1D with nearest neighbour hopping

called Bose Hubbard Model. The following conditions are met in order to derive the Bose-Hubbard model from a generic many-body Hamiltonian with a pseudo-potential interaction.

- Both the thermal and mean interaction energies at a single site are much smaller than the separation to the first excited.
- The Wannier functions decay essentially within a single lattice constant.

Under these assumptions, only the lowest band needs to be taken into account in other words we need to work considering the ground state energy only.
We can represent the system through following figure.
Mathematically, we can describe the Bose Hubbard Model by giving it's Hamiltonian equation.

$$\hat{H} = -J \sum_{\langle ij \rangle} (\hat{a}_i \hat{a}_j^\dagger + \hat{a}_i^\dagger \hat{a}_j) + \frac{U}{2} \sum \hat{n}_i (\hat{n}_j - 1) - \mu \sum_i \hat{n}_i \tag{1.2}$$

Where $n^a = a_i^\dagger a_i$

J- Hopping amplitude along the leg

U-Amplitude of onsite interaction

μ - chemical potential

$a_i^\dagger$ -Creation operator

a_i -Annihilation operator

n_i^a -Number operator

1.3 Superfluid to Mott insulator transition

There are two distinct scenarios that the Bose-Hubbard Hamiltonian describes at zero temperature on the basis of interactions. One is when J is significantly less than U and the system is in the Mott insulator phase. The other is dominated by kinetic energy, in which the system displays superfluidity as the repulsion is overcomed by tunneling. The race between the kinetic energy, which seeks to delocalize the particles, and the interaction energy, which seeks to localize them and reduce the number fluctuations, leads to the rise of superfluidity.
When in the superfluid phase the Hamiltonian is ruled by the kinetic energy element . Since the many body state in this phase is practically a product over identical single particle wave functions, one may ignore quantum correlations and characterize the system using a macroscopic wave function. The system is a superfluid with a macroscopic well-defined phase. When the lattice is switched off, as would be expected from an array of phase coherent matter wave sources, atoms are delocalized over it with identical relative phases between neighboring sites, exhibiting an interference pattern. With the rise in interactions, atoms tend to get localised at specific lattice sites and number fluctuations decrease because the average kinetic energy needed for an atom to hop from one site to the next is no longer adequate to compensate for the potential energy cost. Instead, the

ground state of the system in the Mott insulator phase is made up of localized atomic wave functions with a set number of atoms per site. Particle-hole excitations, which involve both adding and withdrawing particles from the system, are the lowest lying excitations that retain particle number. There is an energy gap that exists throughout this time. The energy required to form a single particle-hole pair determines the gap.

1.4 Bose Hubbard Model with Ring Exchange

This dissertation aims at studying the Bose Hubbard Model by introducing a ring exchange term in a bi-ladder. We consider a system of two 1-dimensional lattices and connect them by allowing the particles to hop between the two legs. We are considering the particles to be spinless Bosons. Particles can hop between it's nearest neighbouring sites in both direction but not beyond that, in addition to this there is on-site repulsion that takes place. The below given figure tries to explain the system.

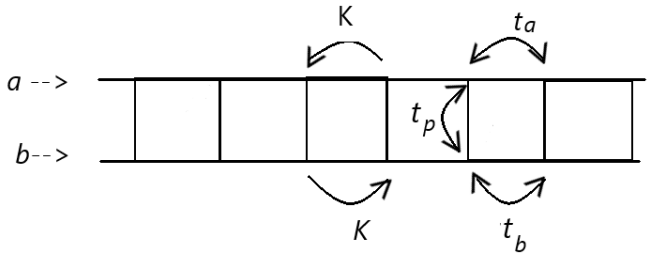

Figure 1.3: Bose Hubbard Model in bi-ladder with ring exchange

The Hamiltonian for the system can be described as below.

$$\begin{aligned}\hat{H} = & -t_a \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) - t_b \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) \\ & - t_p \sum_{\langle i \rangle} (\hat{a}_i^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{a}_i) \\ & + K \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_{i+1} \hat{b}_{i+1}^\dagger \hat{b}_i + \hat{a}_{i+1}^\dagger \hat{a}_i \hat{b}_i^\dagger \hat{b}_{i+1}) \\ & + U_a/2 \sum_{\langle i \rangle} (\hat{n}_i^a (\hat{n}_i^a - 1)) + U_b/2 \sum_{\langle i \rangle} (\hat{n}_i^b (\hat{n}_i^b - 1)) - \mu \sum_{\langle i \rangle} (\hat{n_i}^a + \hat{n_i}^b)\end{aligned} \tag{1.3}$$

(1.4)

Where $n^a = a_i^\dagger a_i$ and $n^b = b_i^\dagger b_i$

t_a, t_b - Hopping amplitudes along the legs a and b respectively

t_p -Hopping amplitude between the sites a_i and b_i

K-Ring exchange term

U_a, U_b-Amplitude of onsite interaction μ- chemical potential

$a_i^\dagger$ -Creation operator

a_i-Annihilation operator

n_i^a-Number operator

With addition of ring exchange term the phase involved in our model are not just limited to superfluidity and mott insulator.Since,we are working at zero temperature, we expect to observe Normal Bose Liquid and along with it phase separation.

Now let's move toward the methodology that we used in this dissertation.

Chapter 2

Methodology

2.1 CMFT+DMRG Method

For studying our model we make use of two methods namely cluster mean field theory and density matrix renormalization group . We use CMFT to simply our hamiltonian by considering a small cluster of sites out of the huge lattice and decouple all the coupled operators. Next we use DMRG to diagonalise the Hamiltonian and calculate the ground state energy (and wavefunction) which we get in the form of eigenvalues (and eigen vectors) of the diagonalised matrix . Let us first go through the Cluster mean field theory.

- Cluster Mean Field Theory

  We consider a small part of our bi-ladder lattice which we call cluster . We divide the whole lattice in number of identical cluster. We consider a cluster with 4 sites on both the legs and carry out mean field calculations on it . And then generalize it for the clusters thoughout our model.

  We consider sites with indices 1 to 4 within the cluster and connect it to the site index 5 on left and 0 on right . We treat all the terms of the hamiltonian which are within the cluster to be exact while the ones on the edges are treated with mean field approximations .

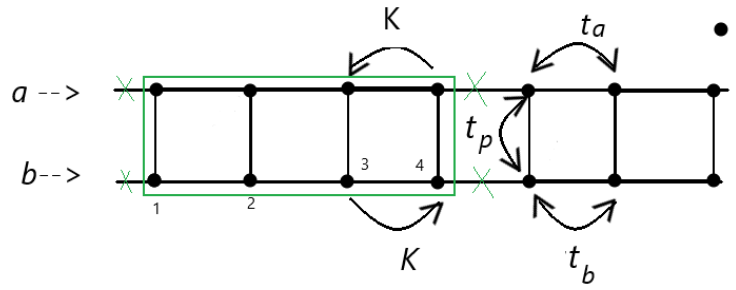

Figure 2.1: Cluster of 4 sites on both the legs of a bi-ladder

Our approximations are :

$$\hat{a_i} = \langle \hat{a_i} \rangle + \delta \hat{a_i} = \psi_a + \delta \hat{a_i} \tag{2.1}$$

$$\hat{a_i}^\dagger = \langle \hat{a_i}^\dagger \rangle + \delta \hat{a_i}^\dagger = \psi_a{}^\dagger + \delta \hat{a_i}^\dagger \tag{2.2}$$

i denotes site index.

Similarly for $\hat{b_i}$, $\hat{b_i}^\dagger$

$$\hat{b_i} = \langle \hat{b_i} \rangle + \delta \hat{b_i} = \psi_b + \delta \hat{b_i} \tag{2.3}$$

$$\hat{b_i}^\dagger = \langle \hat{b_i}^\dagger \rangle + \delta \hat{b_i}^\dagger = \psi_b{}^\dagger + \delta \hat{b_i}^\dagger \tag{2.4}$$

We have hamiltonian for our model as follows:

$$\begin{aligned}
\hat{H} = & -t_a \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) - t_b \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) \\
& - t_p \sum_{\langle i \rangle} (\hat{a}_i^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{a}_i) \\
& + K \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_{i+1} \hat{b}_{i+1}^\dagger \hat{b}_i + \hat{a}_{i+1}^\dagger \hat{a}_i \hat{b}_i^\dagger \hat{b}_{i+1}) \\
& + U_a/2 \sum_{\langle i \rangle} (\hat{n}_i^a (\hat{n}_i^a - 1)) + U_b/2 \sum_{\langle i \rangle} (\hat{n}_i^b (\hat{n}_i^b - 1)) - \mu \sum_{\langle i \rangle} (\hat{n_i}^a + \hat{n_i}^b)
\end{aligned} \tag{2.5}$$

By using the approximations (2.1), (2.2), (2.3), and (2.4) for the field operators we decouple the terms joining the two clusters. Remember that the

terms within the cluster are kept exact.Also we negelect the decouples terms from ring exchange.

Our hamiltonian gets modified using these approximations

$$\begin{aligned}\hat{H} = &-t_a \sum_{\langle i,j=1\rangle}^{n-1} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) - t_b \sum_{\langle i,j=1\rangle}^{n-1} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) \\ &- t_a(\hat{a}_1^\dagger + \hat{a}_1 + \hat{a}_n^\dagger + \hat{a}_n) - t_b(\hat{b}_1^\dagger + \hat{b}_1 + \hat{b}_n^\dagger + \hat{b}_n) \\ &- t_p \sum_{\langle i\rangle}^{n-1} (\hat{a}_i^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{a}_i) \\ &+ K \sum_{\langle ij\rangle} (\hat{a}_i^\dagger \hat{a}_{i+1} \hat{b}_{i+1}^\dagger \hat{b}_i + \hat{a}_{i+1}^\dagger \hat{a}_i \hat{b}_i^\dagger \hat{b}_{i+1}) \\ &+ U_a/2 \sum_{\langle i\rangle} (\hat{n}_i^a(\hat{n}_i^a - 1)) + U_b/2 \sum_{\langle i\rangle} (\hat{n}_i^b(\hat{n}_i^b - 1)) - \mu \sum_{\langle i\rangle} (\hat{n_i}^a + \hat{n_i}^b)\end{aligned} \tag{2.6}$$

Now that our Hailtonian decoupled , we move to on to understand the DMRG.

- Density Matrix Renormalisation Group

  The DMRG method works in the canonical ensemble, we keep the number of particles fixed , hence the superfluid order parameter $\psi = \langle a \rangle = 0$ in all phases. However, the cluster Hamiltonian works in the grand-canonical ensemble. The SF parameter $\psi = a$ can be finite, and such phase can be identified as the superfluid phase. In the MI phase,$\psi = 0$. So, this method produces can reproduce the results similar to those produced by the DMRG.

  Now we shall obtain the ground state energy and the wave function of the Hamiltonian for any given length L using the CMFT + DMRG method with open boundary condition.

  The steps involved are as below :

  - Consider a lattice of small size l, say l = 1 forming the system block S. The Hilbert space of S has dimension M^S and is represented by states

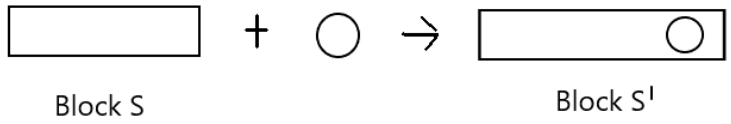

Figure 2.2: . New system block S^l is formed from system block S and one added site represented by open circle.

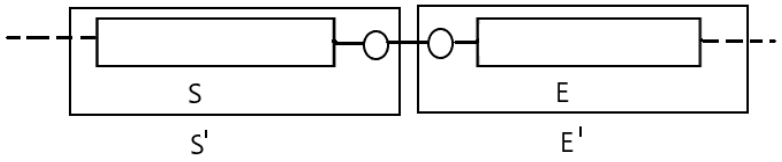

Figure 2.3: Super block of length $L = 2l + 2$

$\{|\mu_l^s\rangle\}$. Obtain the Hamiltonian $\hat{H}_l^s$ and operators acting on the block. Similarly, form an environment block E.

- Form a new system block S^l from S and one added site as shown in figure 2.2. Hilbert space of the new system S^l has dimension $M^S X N_S$ and is represented by states $\{|\mu_l^s|\sigma^S\rangle\}$. Here $N_S = nmax + 1$ is the number of states per site. Similarly, form an environment block $E^{'}$.
- Now build a superblock of length L = 2l + 2 as shown in figure 2.3. Construct the new Hamiltonian matrix for a given initial guess for ψ and find the ground state energy $E_L(\psi)$ and the wave function by sparse-matrix diagonalization. This is the most time-consuming step in this algorithm. Minimize the ground state energy $E_L(\psi)$ with respect to ψ to obtain global ground state energy $E_G S$, the wave function $|\psi_G S\rangle$ and the superfluid order parameter $\psi_j = \langle\psi_G S|a_j|\psi_G S\rangle$
- Construct a reduced density-matrix $\hat{\rho_{S^l}} = Tr_{E^l}|\psi_{GS}\rangle\langle\psi_{GS}|$ for the block system S^l. Diagonalize $\hat{\rho_{S^l}}$ to obtain its eigenvectors $|\alpha\rangle$. The eigen values measures the weights of the $|\alpha\rangle$ states and $|\psi_{GS}\rangle$ satisfies the con-

sidition that sum of the eigen values should be equal to 1 .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^l from $M^S X N_S$ to M^S. This is the most important step of the DMRG method.

Now we transform $\hat{H^{S^l}_{l+1}}$ and operators to the new basis. i.e.,

$\hat{H^{S^l}_{new}} = O^\dagger \hat{H_{S^l}} O$ where O is $M^S X N^S$ rectangular transformation matrix,likewise for the environment.

– Repeat step 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 for all lengths.

Chapter 3

Results

We considered two cases to test our model . First is hardcore while second is softcore.

3.1 Hardcore

The hardcore case follows the condition that the number of maximum Bosons allowed per site can be 1 and the on-site interaction is infinite . Since the number of Bosons is one here, we have only two possible states $|0\rangle$ and $|1\rangle$. So, with possibe combination of states the U part of the hamiltonian vanishes. We set t_a, t_b, t_p parameters as equal to 1. If keep them as reference and vary ring exchange amplitude K and chemical potential μ .

We plot graphs for ψ and ρ versus length of the lattice to check the convergence of order parameter and density and similarly for energy in Figure 3.1 .From this graphs we understand that The mean-field approximation is known to overestimate the superfluid phase, hence, the values of the superfluid order parameter are larger at the edges compared to the center.We see that the superfluid order parameters start converging from the edges as the system length increases.Similarly for energy.

Next, in Figure 3.2 we plot ψ_a, ψ_b, ρ_a, ρ_b along the length to compare if order

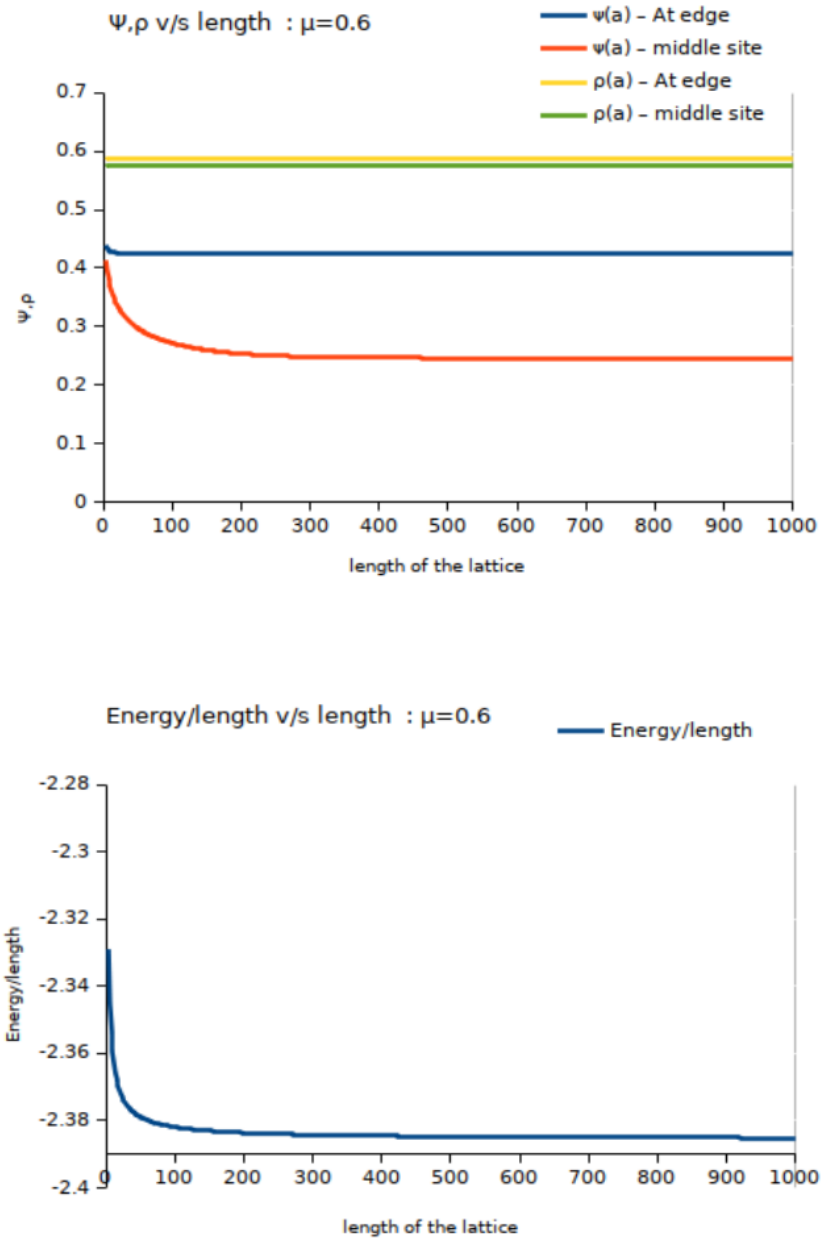

Figure 3.1: The convergence of ψ and ρ along the length is shown in the first graph while second graph shows the convergence of energy for hardcore model

parameter and densities remains the same along both the legs a and b for fixed value of chemical potential, μ.Chemical potential is the amount of energy required to insert or remove a Boson. We can see that as we have kept the hopping amplitude t_a and t_b equal and as expected order parameter and densities are

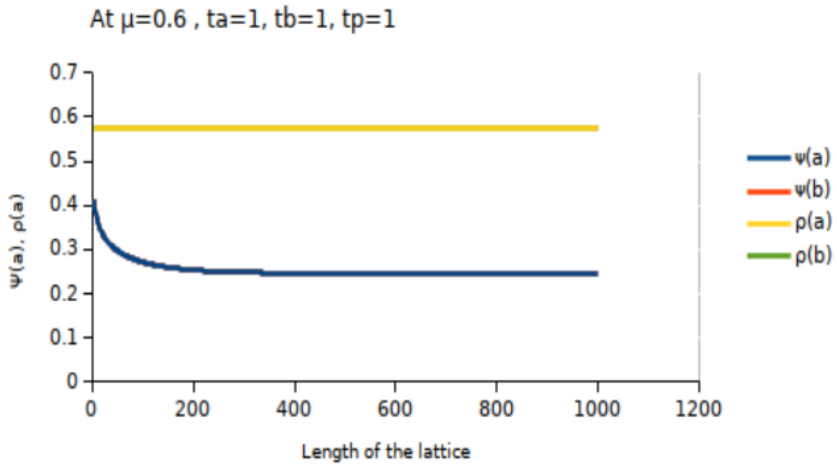

Figure 3.2: Comparison of the of ψ and ρ of leg a and b

observed to be the equal on both the legs.

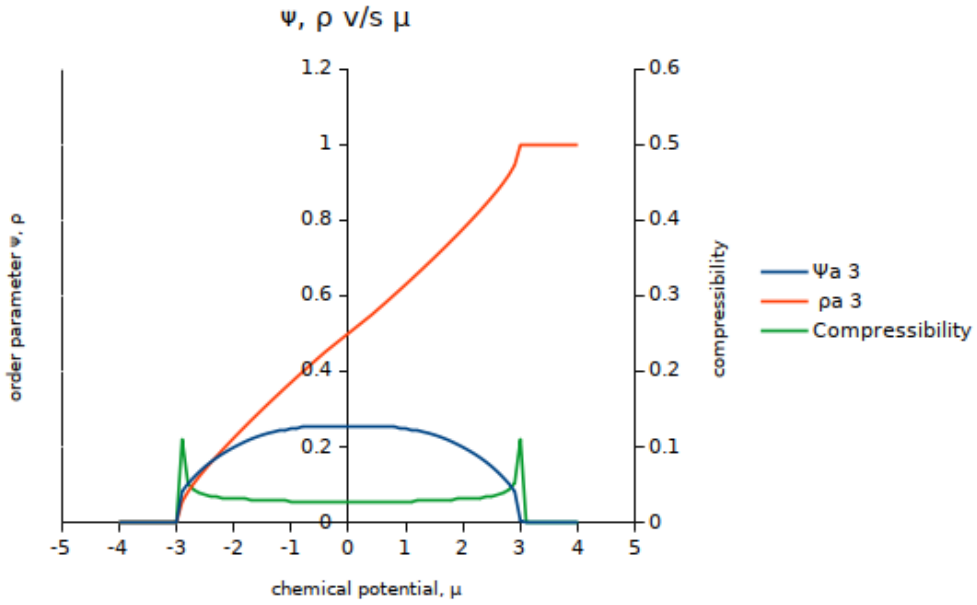

Figure 3.3: ψ ρ and compressibility versus the chemical potential μ

In Figure 3.3 , we plot the graph to observe different phases that can occur in the simple Bose Hubbard model in bi-ladder as we have kept hopping amplitude of ring exchange to be 0 .Compressibility is the rate of change of density with respect to chemical potential μ. We can see that ψ, ρ and compressibility all are

fixed to zero before $\mu = -3$ and again after $\mu = 3$ we see $\psi = 0$, $\rho = 1$ and compressibility=0 which means it is in Mott insulator in the μ range before -3 and after +3 but in between the order parameter ψ and ρ as well as compressibility all are finite which implies that it is in Superfluid phase.

This tables can helps us in identifying the phases.

Phases	Ψ	ρ	Compressibility
Superfluid	>0	>0	>0
Mott Insulator	=0	=1,2,... (Integers)	=0
Normal Bose Liquid	=0	>0	>0

Figure 3.4: Conditions for identifying the phases

Now, we proceed to introduce the ring exchange hopping in our model and observe the phases.

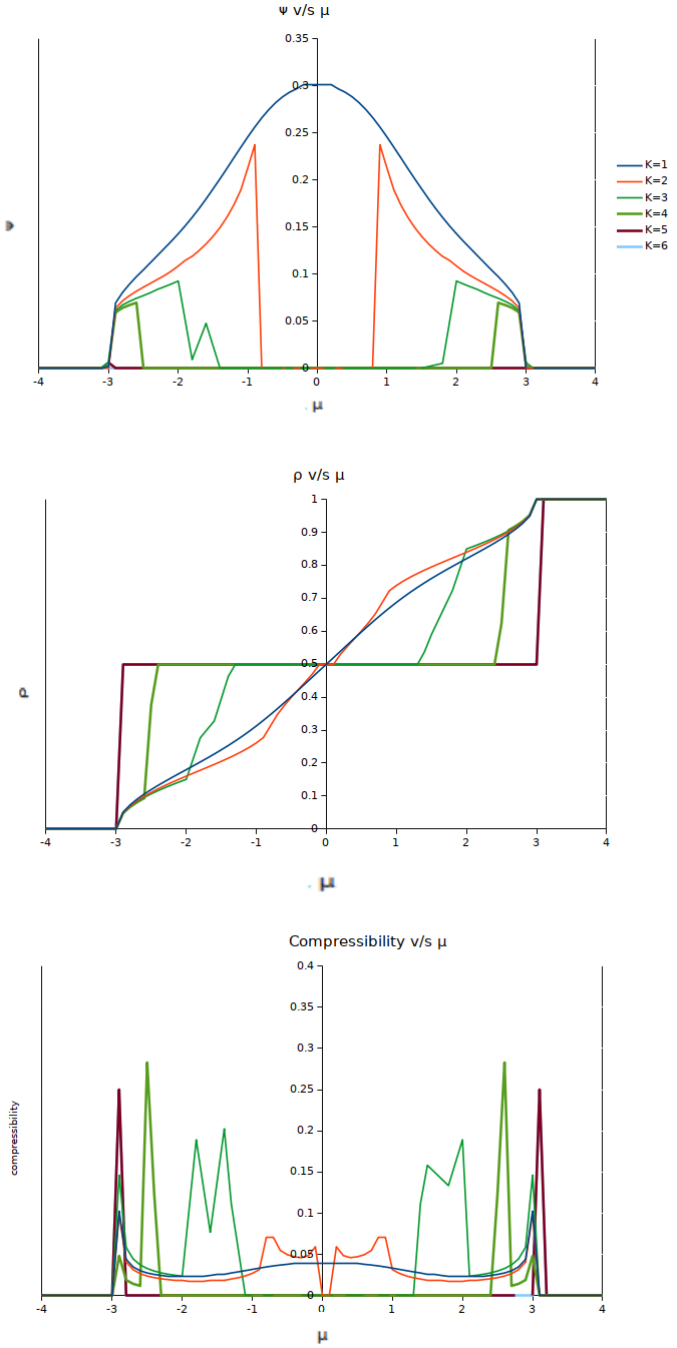

Figure 3.5: ψ, ρ, and compressibility varrying with chemical potential μ for different values of k. The values of K are specified in the legend along with colour coding

As we include k we can observe the variation in the strength of superfluidity.

With $k = 1$ we do not notice much difference in the phase but slight changes in the strength of order parameter. As k is increased to 2 we see that $\psi = 0$ for a range of μ which can be read from the graph, also in this region the compressibility as well as ρ are finite which tells us the occurance of another phase "Normal Bose Liquid" .This phase becomes a little more dominant as we increase the value of k gradually.

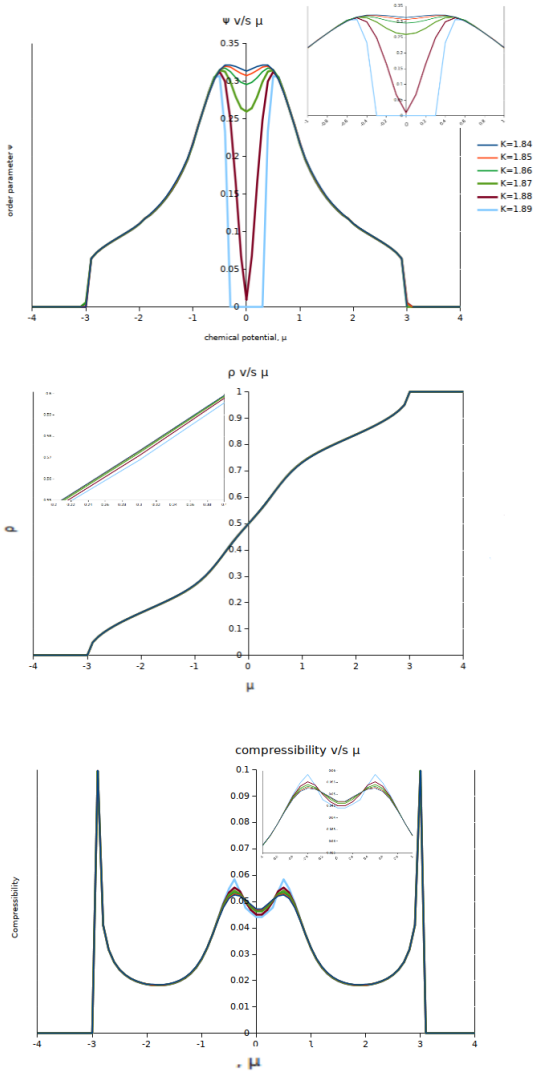

Figure 3.6: Critical value of k

With furher increase in the value of $k = 3, 4, 5$, it can be seen that the Normal Bose liquid disappears and a insulating phase with a non-integer density of 0.5 appears and it persists .

At $k = 6$ the system observes phase transitions only from a Mott insulator of integer density $\rho = 0$ to insulating phase of non-integer density $\rho = 0.5$ and finally to $\rho = 1$ .Which means at a sufficient value of k the superfluidity is completely destroyed.

From this observations we can make a statement that in the hardcore case Bosons hopping in the ring order works to supresses the superfluidity and this is opposite to how the chemical potential μ works . In the absence of onsite interaction U ,the μ tries to keep the system in Superfluid.The hardcore case in our model is the display of competition between ring hopping and chemical potential.

We make one more set of plots to find the critical value of k ,see Figure 3.5 . At this point the superfluid make transition to Normal Bose Liquid.

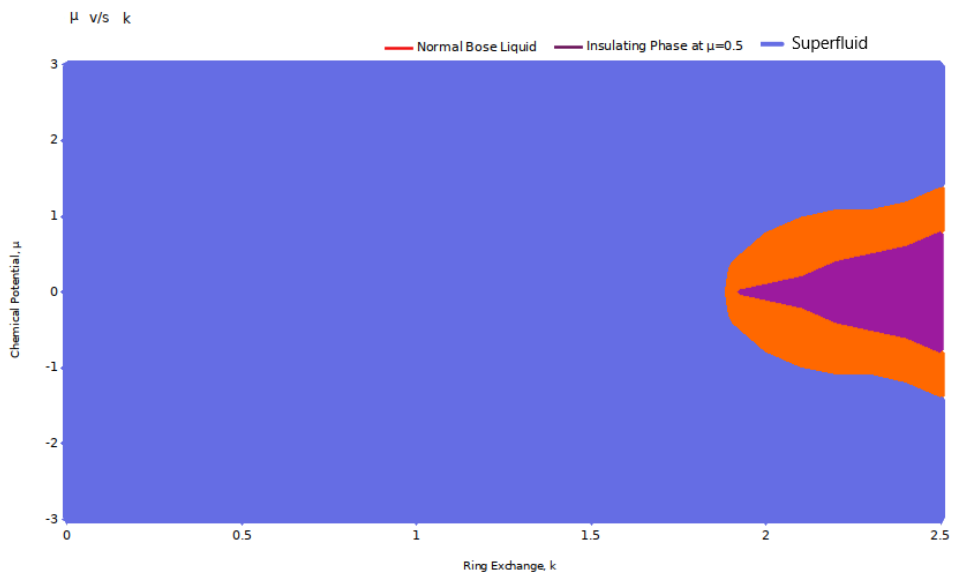

Figure 3.7: Phase Diagram - μ vs k

In this plot we can see the nature of k term which supresses the superfluidity. We found that $k = 1.88$ while $\mu = 0$ is the critical point where the Normal Bose Liquid starts appearing.

We plot the Phase diagram of Chemical Potential,μ versus Ring hopping amplitude ,k .

3.2 Softcore

The softcore case follows the condition that the number of maximum Bosons allowed per site is more 1 and the on-site interaction is finite.

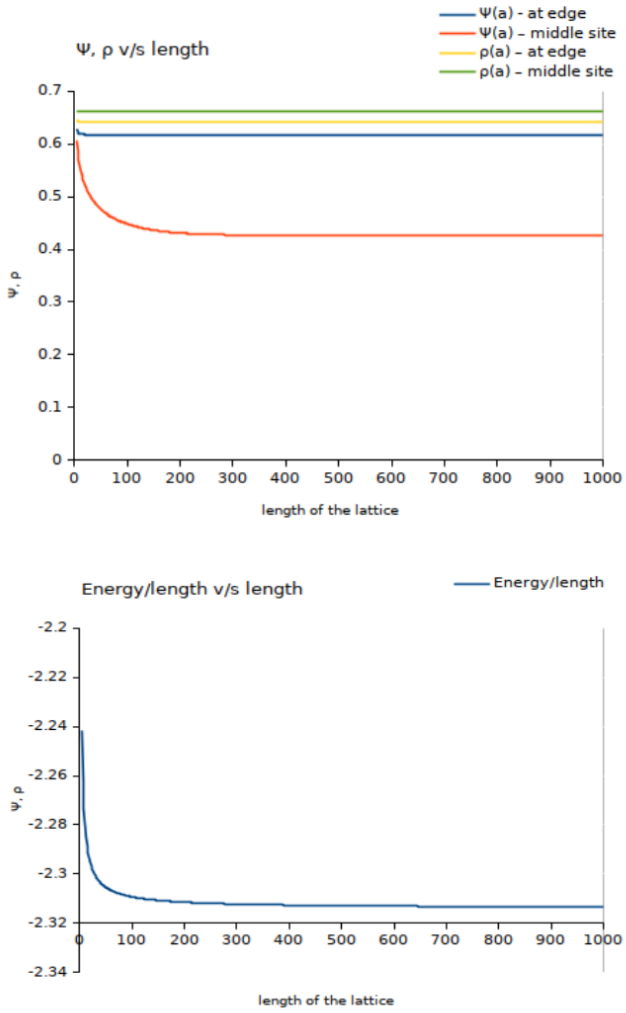

Figure 3.8: The convergence of ψ and ρ along the length is shown in the first graph while second graph shows the convergence of energy for softcore model

So, in this case it's not just a competition between Ring Hopping k and Chemical Potential μ as the On-site interaction U has a role to play.

In Figure 3.7 we plot similar graphs as hardcore case to observe the convergence of Order parameter ψ , density ρ and Energy along the lattice.

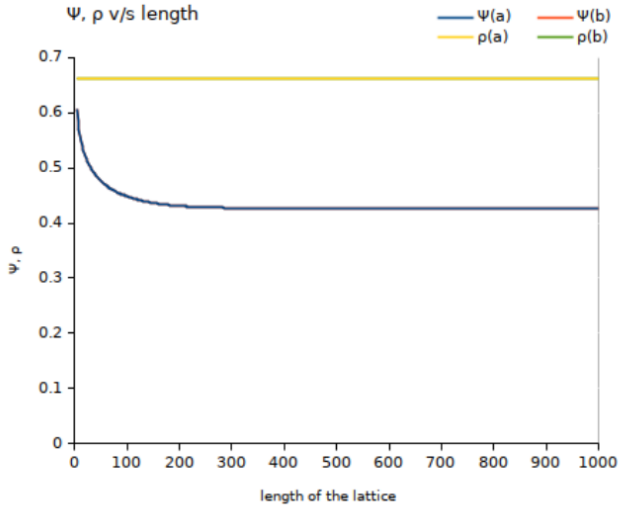

Figure 3.9: cmparing a and b

In figure 3.8 we plot the ψ_a, ψ_b, ρ_a, ρ_b along the length to compare if order parameter and densities remains the same along both the legs a and b.

In case of softcore case we can see that the system observes the Phase transitions similar to hardcore case. It displays the transition from intial Mott Insulator phase to Superfluid and then to Mott insulator. For higher values of k there is a occurance of non integer density at $\rho = 1.5$

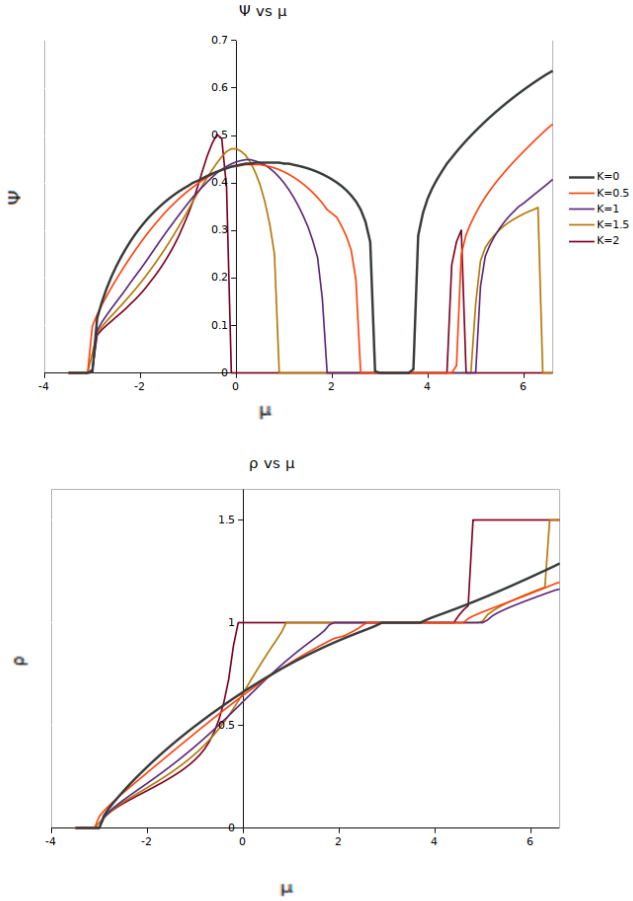

Figure 3.10: ψ,ρ versus μ

There is no appearance of Normal Bose Liquid is softcore case.This can be because of the onsite interaction term which dominates the hamiltonian.

Chapter 4

Summary

In this project we have been able successfully employed the Cluster Mean Field plus Density Matrix Renormalisation Group to our Model Hamiltonian which is Bose Hubbard Model with Ring Exchange hopping in bi-ladder and found out various phases.

We observe the usual Superfluid to Mott Insulator phase transition in the model initially. As we introduce our Ring hopping term we observed variation in the phases due to the competition between Ring exchange Hopping and the Chemical Potential which is favoured by the absence of onsite interaction in this case.

In case of hardcore , we notice the transition from superfluid to Normal Bose Liquid phase which is eventually conquered by an insulating phase a a non integer density of 0.5 as we keep in increasing the amplitude of ring hopping. The ring exchange term gradually suppresses and finally destroys the Superfluid. In case of softcore, we do see the insulating phases at non integer densities like 1.5 but there is no presence of Normal Bose Liquid . This can be because of the dominating presence of on-site interaction in this case.

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