Effect of Thermal Fluctuations on Anomalous Pair Superfluid

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DECLARATION BY STUDENT

I hereby declare that the data presented in this Dissertation / Internship report entitled, "Effect of Thermal Fluctuations on Anomalous Pair Superfluid" 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. Bhargav K. Alavani 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 the dissertation.

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This is to certify that the dissertation / internship report "Effect of Thermal Fluctuations on Anomalous Pair Superfluid" is a bonafide work carried out by Mr. Mayur Madhav Abhisheki under my supervision in partial fulfilment of the requirements for the award of the degree of M.Sc in Physics at the School of Physical and Applied Sciences, Goa University.

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Chapter 1

Introduction

The Bose-Einstein condensate (BEC) is a state of matter that arises from the pure quantum behavior of bosonic particles at ultra-low temperatures(10^{-9} Kelvin). This state was proposed by Satyendra Nath Bose and Albert Einstein in the 1920s [1]. After 75 years it was experimentally realized in the laboratory by Eric Cornell, Carl Wieman, and co-workers at JILA on 5 June 1995 using sophisticated techniques of laser cooling and trapping [2].

When non-interacting bosonic particles such as $He-4$, $Rb-87$, $Na-23$ atoms or $TlCuCl_3$ molecules are cooled below critical temperature T_C, they lose their individuality and merge into a single macroscopic quantum state, forming a BEC. The critical temperature 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 T_c is the Critical Temperature, $\hbar$ 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.

Below this temperature, a large number of particles occupy the same quantum state, and they behave coherently. Here the wave functions of the individual particles overlap with each other forming a giant matter wave. Due to this collective behavior and large wavefunction, particles flow with zero viscosity and this phase is called Superfluid (SF).

Optical lattices are periodic potentials formed by the interference of laser beams, which trap ultra-cold atoms in a periodic array of potential minima via AC-Stark shift. In the simplest form, the optical lattice is a standing wave formed by the interference of two or more monochromatic laser beams traveling in opposite directions. See Fig. 1.2. The potential felt by cold atoms in a 3D optical lattice is of the form

$$V(x,y,z) = V_0\left(\sin^2(kx) + \sin^2(ky) + \sin^2(kz)\right) \tag{1.2}$$

where V_0 is the maximum trapping potential, and it depends on laser intensity and frequency. $k = \frac{2\pi}{\lambda}$

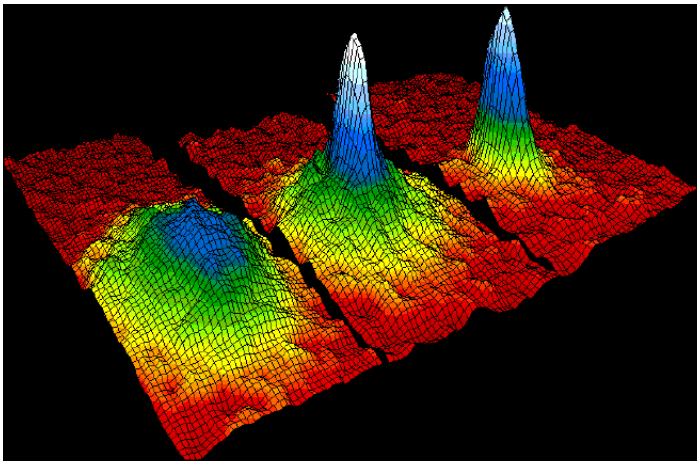

Figure 1.1: Velocity-distribution of a dilute gas of Rubidium atoms near BEC transition. Temperature T reduces from the left panel to the right. Left: just before the appearance of a Bose–Einstein condensate ($T > T_C$). Center: just after the appearance of the condensate($T \approx T_C$). Right: after further evaporation, leaving a sample of nearly pure condensate($T < T_C$). [2]

is the wave vector with λ as the wavelength of the laser beam. Here 6 counter-propagating laser beams will be required. Such lattice systems allow for precise control over the motion of the atoms, provide a disorder-free environment and lattice dimensionality can be changed easily. This creates a neat platform for studying interacting quantum many-body problems.

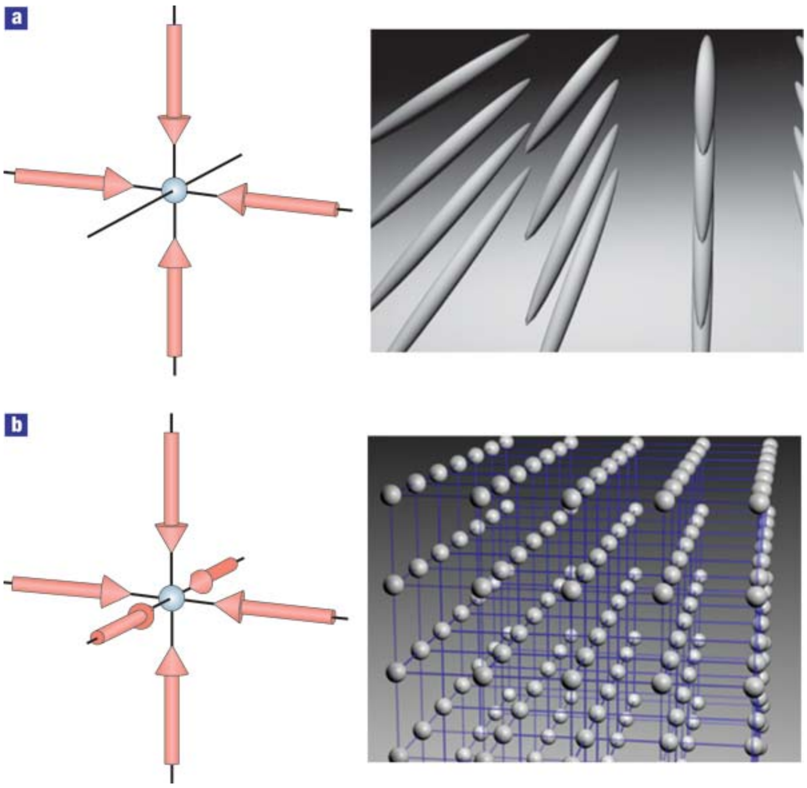

Figure 1.2: Schematic diagram of (a) 2d and (b) 3d optical lattices. Grey regions dipict the potential minimas felt by the ultracold atoms. It is made by interfering two and three pairs of counter propagating lasers. [3]

The model which best describes bosonic atoms loaded onto optical lattice is Bose Hubbard (BH) model. It is given by Hamiltonian

$$H = -J \sum_{<i,j>} (\hat{a_i}^\dagger \hat{a_j} + \hat{a_j}^\dagger \hat{a_i}) + \frac{U}{2} \sum_i \hat{n_i}(\hat{n_i} - 1) - \mu \sum_i \hat{n_i} \tag{1.3}$$

The first term represents hopping of bosons between nearest-neighbor pairs of sites $\langle i, j \rangle$ with amplitude J, $\hat{a}_i^\dagger$ ($\hat{a}_i$) is the boson creation (annihilation) operator at site i. U and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ are respectively on-site repulsive strength and number operator at site i. μ is the chemical potential. In optical lattices, U/J ratio can be changed as

$$\frac{U}{J} = \frac{\sqrt{8}\pi}{4} \frac{a_s}{a} \exp\left(2\sqrt{\frac{V_0}{E_r}}\right) \tag{1.4}$$

where a_s is the s-wave scattering amplitude of atoms. $a = \frac{\lambda}{2}$ denotes the lattice constant with λ as the laser wavelength. V_0 is the potential depth felt by bosons and E_r is the recol energy felt by the atoms. V_0 can be varied by changing the laser intensity.

When the potential is deep, and the interactions between the atoms are strong, resulting the system to be in a Mott insulator (MI) state. In this state, each lattice site is occupied by a fixed number of atoms. However, when the lattice potential is low, and the interactions between the atoms are weak, the system can undergo a transition to a superfluid (SF) state, where the atoms become delocalized over the lattice and exhibit quantum coherence.

Variety of analytical[4], semi-analytical[5] and numerical techniques[6, 7, 8, 9, 10] have been employed to study BH model and its variants like in-homogeneous BH model, Extended BH model, Spin-1 BH model etc. Cluster Mean Field Theory (CMFT) is a simple extension of traditional single site mean field theory[11, 12, 13]. It captures some of the fluctuations neglected in single site mean field theory at the cost of increased Hilbert state and computational power. This theory can be applied to do non-zero temperature calculations in straightforward manner.

1.1 Literature Review

In a seminal paper by D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller [5] titled **Cold Bosonic Atoms in Optical Lattices**they gave a proposal for converting weakly interacting BEC to MI, a strongly correlated quantum state was given. It was shown that the dynamics of the bosonic atoms on the optical lattices realizes a Bose-Hubbard model. The BHM predicts phase transition from a superfluid (SF) phase to a Mott insulator (MI) by increasing ratio of the on site interaction U (repulsion of atoms) to the tunneling matrix element J [14]. It optical lattices this ratio can be varied by changing the laser intensity. With increasing depth of the optical potential the atomic wave function becomes more and more localized and the on site interaction increases, while at the same time the tunneling matrix element is reduced. A signature of a MI phase is integer occupation number (density) $\rho =< \hat{n_i} >$. They used mean field theory (MFT) in the and found the critical values of the MI-SF transition, that are $U/zJ = 5.8$ with $z = 2d$ the number of nearest neighbors. This parameter regime is accessible by varying V_0 in the regime of a few tens of recoil energies E_R. An example of Sodium was taken where $E_R/\hbar = 2\pi \times 8.9$ kHz for a red detuned laser with $\lambda = 985$ nm, and the critical values for the first MI phase in 1D, 2D, and 3D are given by $V_{x0} = 10.8, V_{x,y0} = 14.4$ and $V_{x,y,z0} = 16.5E_R$.

Soon after this Group led by Griner and I.Bloch realized this phase transition in Optical Lattices[3] for the first time. The paper was tited as **Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms**. They put forward that for a system at a temperature of absolute zero, all thermal fluctuations are frozen out, while quantum fluctuations prevail. These microscopic quantum fluctuations can induce a macroscopic phase transition in the ground state of a many-body system when the relative strength of two competing energy terms is varied across a critical value. They observed a quantum phase transition in a Bose-Einstein condensate with repulsive interactions, held in a three-dimensional optical lattice potential. As the potential depth of the lattice is increased, a transition is observed from a superfluid to a Mott insulator phase. To illustrate this, atomic gas of bosonic at low enough temperatures is taken such that it forms BEC. The BEC is superfluid and is described by a wavefunction that has long range phase coherence [15]. This is then subjected to a lattice potential in which the bosons can move from one lattice site to the next only by tunnel coupling. It is then observed that if the lattice potential is turned on smoothly, the system remains in the superfluid phase as long as the atom-atom interactions are small compared to the tunnel coupling. In the opposite limit, when the repulsive atom-atom interactions are large compared to the tunnel coupling, the total energy is minimized when each lattice site is filled with the same number of atoms. The competition between two terms in the underlying hamiltonian (here between kinetic and interaction energy) is fundamental to quantum phase transitions and inherently different from normal phase transitions, which are usually driven by the competition between inner energy and entropy. The experimental setup consisted of spin polarized samples of laser-cooled atoms in the $(F = 2, m_F = 2)$ state, which were transferred into a cigar-shaped magnetic trapping potential with trapping frequencies of $n_{radial} = 240$ Hz and $n_{axial} = 24$ Hz. Here F denotes the total angular momentum and m_F the magnetic quantum number of the state. Forced radio-frequency evaporation was used to create Bose-Einstein condensates with up to 2x10^5 atoms and no discernible thermal component. In order to form the three-dimensional lattice potential, three optical standing waves are aligned orthogonal to each other, with their crossing point positioned at the centre of the Bose-Einstein condensate. The resulting three-dimensional optical potential [16] for the atoms is then proportional to the sum of the intensities of the three standing waves, which leads to a simple cubic type geometry of the lattice: $V(x, y, z) = V_0 \left(\sin^2(kx) + \sin^2(ky) + \sin^2(kz)\right)$.

A theory for Multi-site Mean Field Theory or commonly nown as Cluster Mean Field Theory was given by T. McIntosh, P. Pisarski, R. J. Gooding, and E. Zaremba in their paper **Multisite mean-field theory for cold bosonic atoms in optical lattices**[11]. Through this theory inter-site correlations which allow for fluctuations of various physical variables could be captured, at least to some extent, by dividing the system into clusters of arbitrary size and using mean-field theory to decouple the clusters. The approach here is based on partitioning the lattice into small clusters which are decoupled by means of a mean-field approximation. This approximation invokes local superfluid order parameters defined for each of the boundary sites of the cluster.

The ability of bosons to hop in pairs in optical lattices has been theoretically realised by Xiang-Fa Zhou, Yong-Sheng Zhang, and Guang-Can Guo [10]. This study tries to bring an analogy between Bardeen-Cooper-Schrieffer (BCS) [17] superconductivity and Bose-Einstein condensation (BEC) of tightly bound pairs. This was done by realising a state dependent optical lattice. One can change the intensity of the laser beams, thus the relative well depth of the lattice can be adjusted. In addition variation of θ leads to change in the separation of the two lattice potentials. Therefore in such deep optical lattices Hamiltonian resembles that of the traditional Bose-Hubbard model except that the kinetic term is replaced with the pairing hopping of bosonic atoms in the lattices. It is also to be noted that competition between PSF-SF leads to a 1st order PSF(SF)-MI transition.

A perturbative approach to study bosons at Finite T to obtain simple analytical expressions for the occupation number and number fluctuations was done in 2004 by Plimak, L. I., Olsen, M. K. and Fleischhauer, M in their study titled **Occupation number and fluctuations in the finite-temperature Bose-Hubbard model**[4].

The Boson-Hubbard Model in 2 Dimension under the effect of Thermal FLuctuations (i.e Finite Temperature) was studied by K. W. Mahmud, E. N. Duchon, Y. Kato, N. Kawashima, R. T. Scalettar, and N. Trivedi in their paper titled **Finite temperature study of bosons in a two dimensional optical lattice**[8]. It was observed that in addition to the usual ground state SF and MI phases of the Bose Hubbard model, a new third phase had arisen which was the Normal Bose Liquid (NBL). It was reported that at higher temperature, regions develop which have incommensurate filling but also superfluid order parameter $\psi = 0$. This is called as Normal Bose Liquid (NBL) phase.

After the experimental observation of effective multibody interactions [18, 19], A team of Researchers, A. Safavi-Naini, J. von Stecher, B. Capogrosso Sansone, and Seth T. Rittenhouse in their paper **First-Order Phase Transitions in Optical Lattices with Tunable Three-Body Onsite Interaction**[6] have shown that the density two Mott lobe disappears and the system displays first-order phase transitions separating the $\rho = 1$ from the $\rho = 3$ lobes and the $\rho = 1$ and $\rho = 3$ Mott insulator from the superfluid in Optical Lattices with a tunable three-body interaction. The mechanism to control this on-site interaction is by an external rf pulse that couples the triply occupied state with a three-body bound state associated with an excited hyperfine state. This local three-body interaction then, only affects triply occupied sites leading to a modified BH Hamiltonian. In the region $|W| > U$, $\rho = 2$ MI lobe disappears and it was thought that a direct first-order phase transition at finite hopping occurs between the $\rho = 1$ and $\rho = 3$ MI lobes.

However, later in a paper titled **Anamolous pairing of bosons : Effect of multibody interactions in an optical lattice** by Manpreet Singh, Sebastian Greschner, Tapan Mishra were able to show that an unconventional pairing of bosons occurs due to the competing repulsive two-body and attractive three body interactions[7]. They showed this competition leads to a formation of PSF phase in between the $\rho = 1$ MI and $\rho = 3$ MI lobes as opposed to a direct first order jump as proposed in [6]. For any $0 < t \ll U, W$ between the MI-1 and MI-3 lobes, an intermediate region of pair superfluid is found. This pair SF phase was called as Anomolous Pair SF(PSF) phase.

The effect of Finite temperatures in Optical lattices with Three-body interactions has been reported by T.K. Kopeć and M.W. Szymański[9]. It was observed that Finite temperature smears the lobes and the effect is seen to be stronger for higher temperatures.

Recently, In a paper titled **Two-body repulsive bound pairs in a multibody interacting Bose-Hubbard model** Suman Mondal, Augustine Kshetrimayum and Tapan Mishra were able to show that PSF phase can be realsied even with an onsite 4-body interactions[13]. With $U_2 > 0, U_3 < 0$ and $U_4 > 0$ they were able to show that there is a formation of PSF phase in the region between the $\rho = 1$ MI and $\rho = 3$ MI lobes. By considering this two-body repulsion along with large three-body attraction and four-body repulsion they showed that bosons prefer to move in pairs. Also this pair formation was found to be not limited to $\rho = 1$ MI and $\rho = 3$ MI lobes but rather could be manifested between $\rho = 2$ MI and $\rho = 4$ MI lobes by employing a 5-body interaction. Along with this it was confirmed that for these set of multi-body interactions the PSF phase survives the thermal fluctuations.

1.2 Motivation

Ultracold atoms trapped in Optical lattice provide a neat platform to study interacting quantum phase transitions. Prominent example of such quantum phase transition is the SF to MI transition occurring in case of bosonic atoms trapped in optical lattice. This transition was predicted by solving Bose Hubbard model and was verified experimentally. By applying external RF pulses or radiations various two and three body interactions can be tuned in the optical lattice system. With three body attractive interaction, an anomalous pairing of bosons is predicted by use of DMRG and Cluster mean field theory. In such case two bosons pair up to hop through the lattice. All the predictions of this pair SF phase occurring in BH model with attractive three body interaction is at zero temperature.Cluster mean field theory is a simple numerical technique able to predict SF and MI phases qualitatively. This theory can be extended to do non zero temperature calculations. This serves as motivation of this report.

1.3 Objectives

The objectives are as follows

- To apply Cluster Mean Field Theory to BH model for studying SF-MI transition at zero temperature.
- To employ CMFT method to characterise and study PSF phase occurring due to attractive three body interactions in BH model.
- To study the effects of thermal fluctuations on the SF, MI and PSF phases.

Chapter 2

Model and Method

Here model and method for solving the model is discussed.

2.1 Model

With three-body interaction, the Bose-Hubbard Model in Eq. 1.3 is modified as

$$H = -J \sum_{<i,j>} (\hat{a_i}^\dagger \hat{a_j} + H.C) + \frac{U}{2} \sum_i \hat{n_i}(\hat{n_i} - 1) + W \sum_i \delta_{n_i,3} \tag{2.1}$$

where W is the on-site three-body interaction. $\delta_{n_i,3}$ is a function which is one if $n_i = 3$, or else is zero. The Hamiltonian in Eq. 2.1 cannot be solved exactly. One can apply Cluster Mean Field Theory to solve this model qualitatively. The method for solving is as follows.

2.2 Cluster Mean Field Theory

The entire lattice is divided into clusters of N_C number of sites. In this report cluster of four sites is considered. Hopping of bosons inside the cluster is treated exactly. And hopping of bosons outside the cluster is approximated by standard mean field decoupling. i.e. $\hat{a}_i = \psi_i + \delta\hat{a}_i$, where $\psi_i = \langle \hat{a}_i \rangle$ is the SF order parameter and $\delta\hat{a}_i$ is fluctuation over it. Using this and neglecting the terms which are quadratic in fluctuations we get

$$\hat{a}_i^\dagger \hat{a}_j \simeq \langle \hat{a}_i^\dagger \rangle \hat{a}_j + \hat{a}_i^\dagger \langle \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle \tag{2.2}$$

$$\hat{a}_i^\dagger \hat{a}_j \simeq \psi_i^* \hat{a}_j + \hat{a}_i^\dagger \psi_j - \psi_i^* \psi_j \tag{2.3}$$

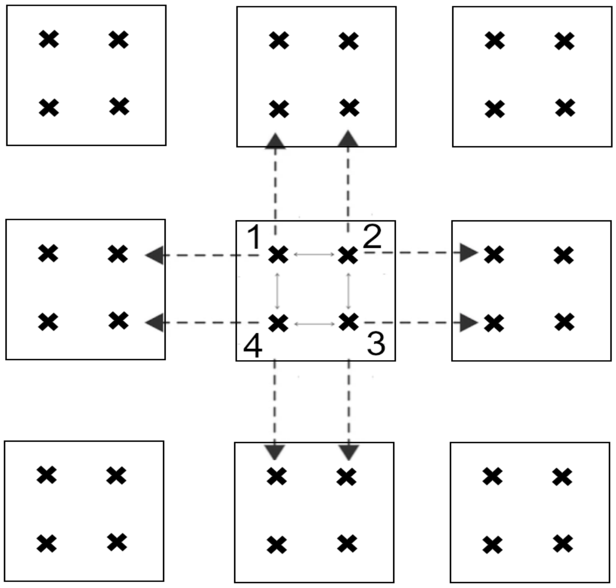

Figure 2.1: Illustration of a 4-site 2d cluster. The dashed arrows represent interaction outside the cluster which is approximated using mean field decoupling. Solid arrows represent hopping inside the cluster treated exactly.

We assume SF order parameter to be real. With this the Hamiltonian of 4 site cluster becomes

$$\begin{aligned} H^{Cluster} = & -J \sum_{<i,j>}^{4} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2} \sum_i^4 n_i(n_i - 1) + W \sum_i^4 \delta_{n_i,3} - \mu \sum_i^4 n_i \\ & - 2J \sum_i^4 (\hat{a_i}^\dagger \psi_j + \hat{a}_i \psi_j - \psi_i \psi_j) \end{aligned} \tag{2.4}$$

The first term represents hopping within the cluster. Second and third terms are on site two and three body interactions. Fourth term controls density of bosons on a site inside cluster. Fifth term is the mean field decoupled hopping. It represents hopping of bosons from a cluster to the sites in another neighbouring cluster. See Fig. 2.1.

.

Within this CMFT approach considered in Eq 2.4, it is difficult to determine a parameter describing the pairing of bosons. Therefore, second-order terms in tunneling in the Hamiltonian can be included. In the limit $J << U$ within second-order perturbation theory effective two particle hopping amplitude is $J_{eff} = \frac{J^2}{U-W}$. Such second-order tunneling terms is explicitly included in the CMFT approach in order to describe PSF phase. With this the Cluster Hamiltonian becomes

$$
\begin{aligned}
H^{Cluster} =& - J \sum_{<i,j>}^{4} (\hat{a}_i^{\dagger}\hat{a}_j + \hat{a}_j^{\dagger}\hat{a}_i) + \frac{U}{2}\sum_{i}^{4} n_i(n_i - 1) + W \sum_{i}^{4} \delta_{n_i,3} - \mu \sum_{i}^{4} n_i \\
& - 2J \sum_{i}^{4} (\hat{a}_i{}^{\dagger}\psi_j + \hat{a}_i\psi_j - \psi_i\psi_j) \\
& - J_{eff} \sum_{i}^{4} (\hat{a_i^2}^{\dagger}\phi_j + \hat{a_i^2}\phi_j - \phi_i\phi_j)
\end{aligned} \tag{2.5}
$$

where $\phi_i =< \hat{a_i^2} >$ is the PSF order parameter.

In this study energy scaling is done by setting $U = 1$. So, J,W and μ are dimensionless. We consider that bosons are trapped in a 2D optical lattice and sysyem is homogeneous. i.e $\psi_i = \psi$ and $\phi_i = \phi$.

Cluster Hamiltonian in Eq. 2.5 is solved self-consistently according to the Flow-Chart in Fig. 2.2. Brief explanation of each step is given below.

1. For U, W, μ and temperature T guess initial values of $\psi = \psi_i$ and $\phi = \phi_i$.

2. Using this values of ψ_i and ϕ_i construct Hamiltonian matrix by operating Hamiltonian in Eq. 2.5 on to number basis $|n_1, n_2, n_3, n_4\rangle$. Here $n_i = 0, 1, 2, \ldots, n_{max}$. Value of n_{max} is truncated such that it does not affect Free energy of the system. In our case we choose $n_{max} = 6$ as we work below $\rho = 4$. The Hamiltonian matrix has dimensions 7^4 x 7^4.

3. Diagonalize Hamiltonian matrix to obtain Eigen Energies E_α and Eigen vectors $|\alpha\rangle$.

4. Using these Eigen Energies and Eigenstes calculate Partition function $Z = \sum_\alpha e^{-\beta E_\alpha}$. Here $\beta = 1/k_B T$.

5. Calculate new order parameters $\psi_{new} = \langle \hat{a} \rangle_T$ and $\phi_{new} = \langle \hat{a} \rangle_T$. Where $\langle \hat{O} \rangle_T$ represents thermal average of operator $\hat{O}$ such that

$$
\langle \hat{O} \rangle_T = \sum_{\alpha} \frac{e^{-\beta E_\alpha} \langle \alpha | \hat{O} | \alpha \rangle}{Z} \tag{2.6}
$$

6. If $\psi_i \neq \psi_{new}$ and $\phi_i \neq \phi_{new}$ set $\psi_i = \psi_{new}$ and $\phi_i = \phi_{new}$ and repeat the above procedure from step-2 until they converge.

This convergence guarantees convergence of the Free energy $F = -k_B T ln(Z)$. After convergence following quantites are calcualted. Boson density

$$
\rho = \langle \hat{n}_i \rangle_T \tag{2.7}
$$

comressibility

$$\kappa = \frac{\delta \rho}{\delta \mu} \tag{2.8}$$

and thermodynamic Entropy

$$S = -k_B \sum_{\alpha} P_{\alpha} ln(P_{\alpha}) \tag{2.9}$$

where $P_{\alpha} = \frac{e^{-\beta E_{\alpha}}}{Z}$ is the probability to occupy $|\alpha\rangle$ sate.

SF,PSF, MI and NBL phases are characterised by using ψ, ϕ, ρ and κ. Table shows the characterisation.

Parameter/Phases	**SF**	**PSF**	**MI**	**NBL**
ψ	$\neq 0$	$= 0$	$= 0$	$= 0$
ϕ	$\neq 0$	$\neq 0$	$= 0$	$= 0$
ρ	Non-Integer	Non-Integer	Integer	Non-Integer
κ	$\neq 0$	$\neq 0$	$= 0$	$\neq 0$

Table 2.1: Characterisation of different phases of BH model

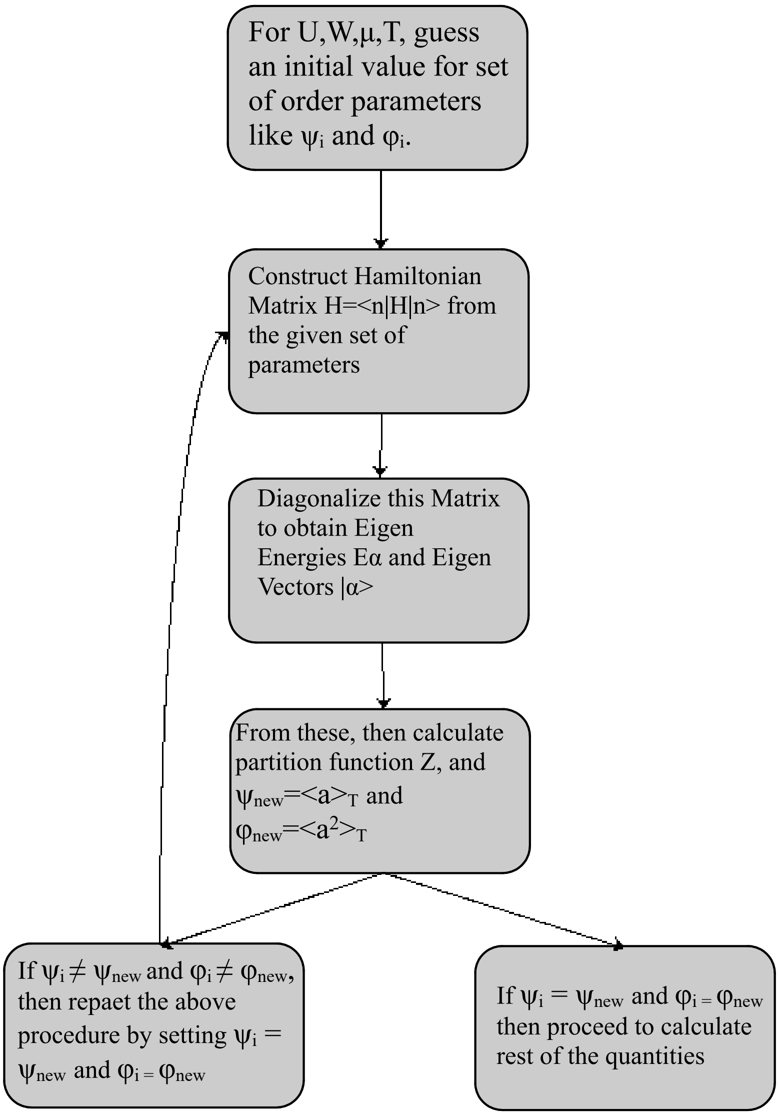

Figure 2.2: Flowchart depicting self-consistent CMFT calculations.

Chapter 3

Results

Results of CMFT calculations of BH models are presented here. First we concentrate on $T = 0$ case to emphasise role of quantum fluctuations on BH model. After clear understanding of zero temperature phases and phase transitions, nonzero temperature results are shown.

3.1 $W = 0$ and $T = 0$ case

At zero temperature and with no three-body interaction SF order parameters and boson densities are plotted in Fig. 3.1(a) and Fig. 3.1(b) respectively. For $J = 0.072$ (depicted by Yellow up triangles) SF order parameter is non zero for for all the values of μ representing SF phase throughout for $J = 0.072$. Boson density ρ increases with increase in μ. For $J = 0.040$ (depicted by Red squares) ψ is non zero except between $\mu = 0.25$ and $\mu = 0.6$. For the same μ values ρ is pinned to integer value 1. This represents $\rho = 1$ MI phase. With decrease in J to 0.008 we see that ψ is zero between $\mu = 0.0500$ to $\mu = 0.9$,$\mu = 1.1$ to $\mu = 1.75$ and from $\mu = 2.15$ to $\mu = 2.85$. At same μ values ρ is pinned to 1,2 and 3 depicting $\rho = 1$ MI, $\rho = 2$ MI and $\rho = 3$ MI. As value of J decreases, the on-site repulsion U between bosons dominate over the tunneling of bosons. Due to this increasing repulsive interaction, bosons avaoid hopping to their nearest sites and system undergoes a phase transition from SF to interaction driven MI.

Collecting the μ values for which $\psi = 0$, $\psi \neq 0$ and $\rho =$ integer as well as non-integer, $J - \mu$ phase diagram is plotted in Fig.3.2(a) and Fig.3.2(b) . White dots represent the SF-MI phase boundary. The color-map depicts the numerical value of ψ and ρ in (a) and (b). We can see that for low values of J, ψ is mostly zero with ρ being integer. This is because the repulsive interaction U dominates over boson tunneling amplitude J and the atoms are highly localised. (dark blue indicates zero value for ψ). However, as the tunneling amplitude J increases bosons are able to tunnel freely from one site to another and overcome the repulsion U to remain in SF phase.

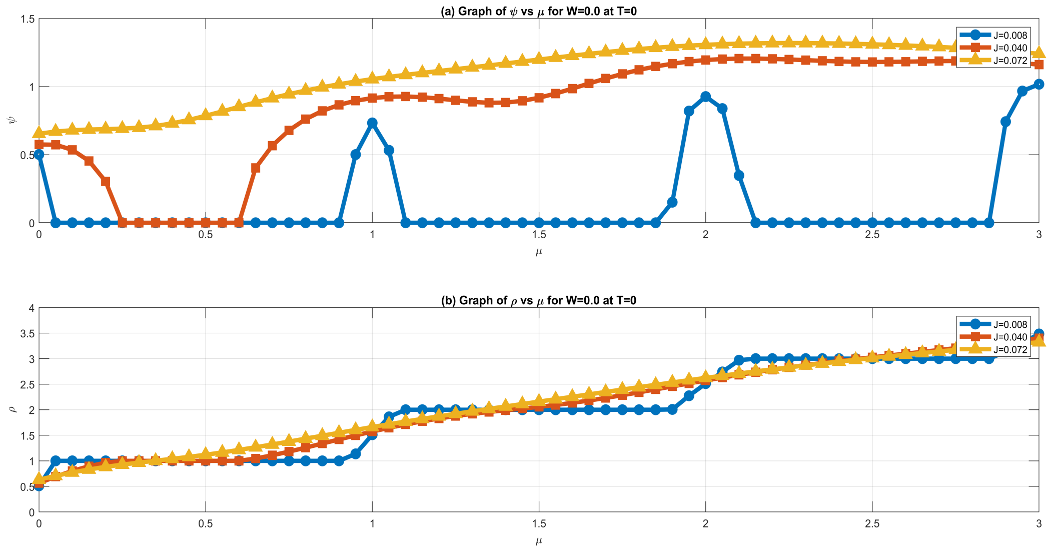

Figure 3.1: Graph of ψ and ρ against μ depicting SF-MI Transition for W=0 at T=0

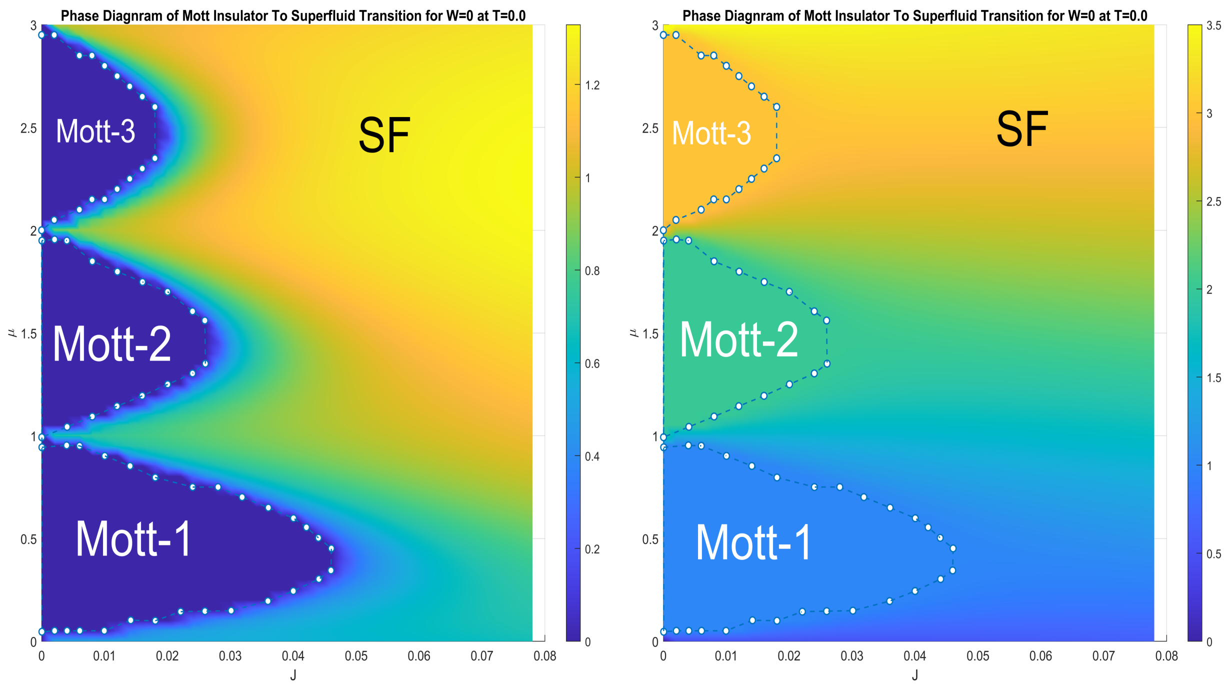

Figure 3.2: $J - \mu$ phase diagram for $W = 0$ and $T = 0$.

3.2 $W \neq 0$ and $T = 0$ case

Now To understand the role of three-body interaction W we plot ψ, ϕ and ρ against μ for different attractive three-body interaction strengths $W = 0, -0.5, -1.0$ and -2.0 at fixing $J = 0.01$ in Fig. 3.3(a),Fig. 3.3(b),Fig. 3.3(c) and Fig. 3.3(d) respectively. We see that at $W = 0$, ψ is zero for $\mu = 0.05$ to $\mu = 0.9$, $\mu = 1.1$ to $\mu = 1.85$ and $\mu = 2.15$ to $\mu = 2.8$. For the same values we observe that ρ

is pinned to integer values 1,2 and 3 respectively. This represents MI phases. Rest is the SF phase where $\psi \neq 0$. For W=-0.5 similar plots as in Fig. 3.3(a) are obtained wherein we see the three mott phases. But as W=-1.0 we see that $\psi \neq 0$ from $mu = 0.91$ to $mu = 1.13$ where we see that there is no $\rho = 2$ phase and hence there is dissapearence of Mott-2 lobe for this attractive repulsion. As we increase W to W=-2.0 we observe that $\psi = 0$ everywhere and ϕ, which is the pair super-fluid order parameter is non zero for $\mu = 0.499$ to $\mu = 0.501$. For these values ρ is non-integer, hence we assume this to be the PSF phase. There is no $rho = 2$ phase since bosons prefer hopping in pairs.

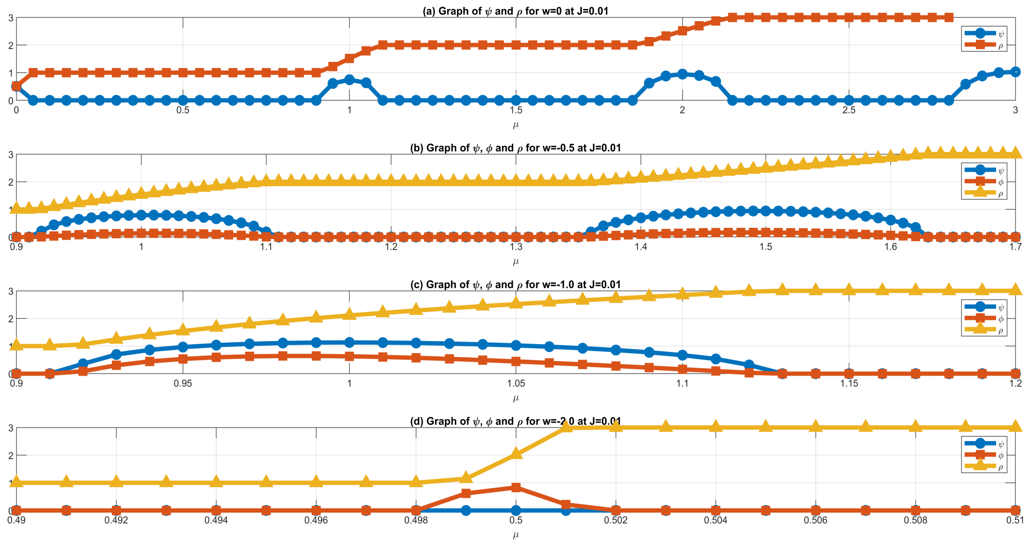

Figure 3.3: ψ,ϕ, and ρ plotted against μ for $W = 0$,-0.5,-1 and -2 for fixed $J = 0.01$

To understand the effect tunneling parameter J on PSF phase we plot ψ, ϕ and ρ for J=0.01, 0.04 and 0.075 at W=-2.0 against μ in Fig. 3.4(a),(b),(c). For J=0.01 we see that ψ is zero for most values of μ and, ϕ is non zero for $\mu = 0.499$ to $\mu = 0.501$. At these μ values ρ is non-integer and increases from 1 to 3. As we increase the J to J=0.04 we see that ψ is nonzero from $\mu = 0.45$ to $\mu = 0.6$. This means that as tunneling parameter is increased, bosons again can hop individually. Further increase in J to J=0.075 makes ψ non-zero everywhere up to $mu = 1.15$, after which system goes in density 3 MI. Since ψ is non zero before $\mu = 1.15$ we see no $\rho = 1$ and $\rho = 2$ phases. This is because J is high enough to overcome inter-body interactions.

We plot the $J - \mu$ phase diagram for $W = -2.0$ in Fig. 3.5. Here the white dots represent the phase boundary. The color map depicts numerical value of ψ in Fig.3.5(a) and numerical value of ϕ in Fig.3.5(b). We can see here that compared to W=0.0 case, $\rho = 3$ MI is enlarged and it engulfs $\rho = 2$ phase. Enlarged phase diagram of MI($\rho = 1$)-PSF-MI($\rho = 3$) is shown in Fig.3.5(b). Here we see PSF phase sandwiched between $\rho = 1$ MI and $\rho = 3$ MI. This was reported in [7].

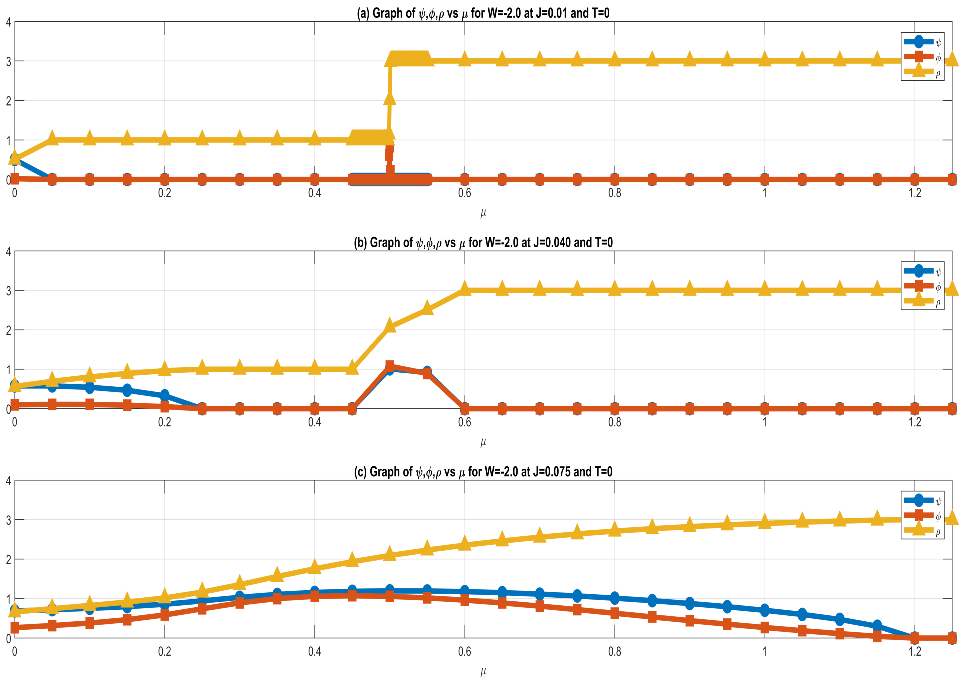

Figure 3.4: ψ,ϕ, and ρ plotted against μ for $W = -2$ for different J

After understanding SF, PSF and MI phase at zero temperature we present the non-zero temperature calculation results in next section.

3.3 $W = 0$ and $T > 0$ case

First we study the effect of thermal fluctuations on SF and MI phases of simple BH model, i.e. $W = 0$. At Temperature T=0.0,T=0.05 and T=0.1 ψ, ρ and Entropy S are plotted against μ for fixed J=0.016 in Fig. 3.6(a),(b),(c), respectively. At T=0.0 we have already seen that ψ is non zero over three ranges of μ. As we increase the temperature to T=0.05 ψ value is seen to decrease, i.e. superfluidity is reduced. Particularly, SF phase with $\rho < 1$ entirely vanishes. For $\mu = 0.75$ to $\mu = 0.9$ we see that $\psi = 0$ but the Entropy S is not zero. And hence this is not a Mott Phase but rather a Normal Bose Liquid phase. Similarly another NBL phase is observed from $\mu = 1.15$ to $\mu = 1.25$ between the $\rho = 1$ and $\rho = 2$ phase. ρ assumes non integer values in this μ range further confirming its not Mott insulator phase but rather NBL phase.

At T=0.1, ψ is almost zero everywhere until $\mu = 2.75$, after system goes in SF phase. From $\mu = 0$ to $\mu = 2.75$, Entropy is non zero everywhere along with $\psi = 0$, this shows a characteristics of NBL phase. Also ρ is non integer for this range. After $\mu = 2.75$ ψ is non zero, hence we characterize it as SF with non integer ρ values.

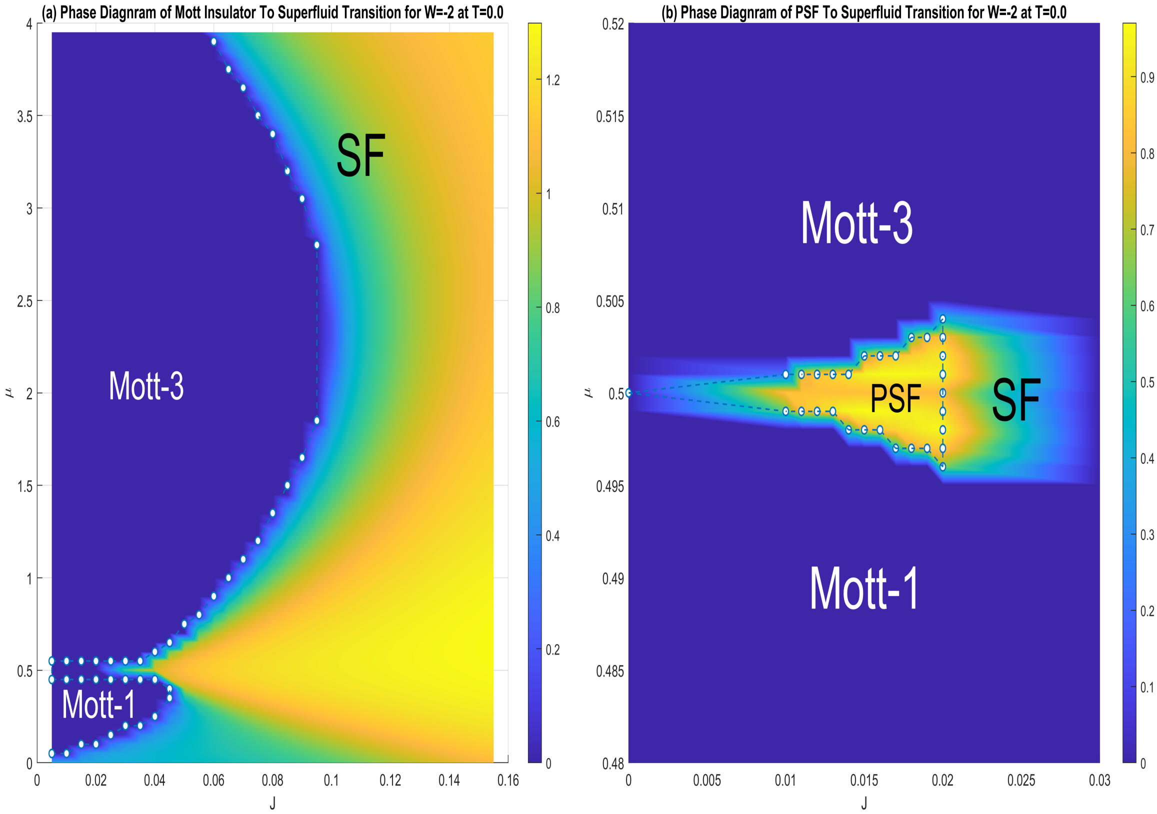

Figure 3.5: $j - \mu$ phase diagram of MI-PSF-SF phase with $W = -2$ and $T = 0$

We plot another $J - \mu$ phase diagram for W=0 case with different T with ψ numerical value as color map in Fig. 3.7. White dots represent the phase boundary. Whenever $\psi = 0$ system is in NBL or MI phase. With increase in temperature we can see that superfluidity decreases. The SF region sandwitched between two MI phases is suppressed dominantly with the temperature. The MI/NBL region is seen to be enlarged.

To differentiate between MI and NBL phase, values of compressibilty κ are depicted in Fig.3.8. The color map represents numerical value of κ. The Fig.3.8(a) is similar to that of 3.2. Fig.3.8(b) and Fig.3.8(c) depicts T=0.05 and T=0.1 case. For T=0.05 case, in between the Mott phases we see emergence of NBL phase, wherein $\psi = 0$ (Fig.3.7) but κ shows large values. For T=0.1 case, thermal fluctuations kill the MI phases and reduce the SF region keeping bosons in NBL phase.

Similar to the last figure Fig.3.8, we plot a $J - \mu$ phase diagram but this time the color map represents the numerical value of Entropy S. At T=0.05 Similar to compressibilty κ, Entropy is non zero in between the Mott phases wherein $\psi = 0$, hence we get a confirmation that there is NBL phase in between the Mott phase. And as J is increased we see that $\psi \neq 0$ (Fig.3.7) and Entropy S reduces. At T=0.1 we have non-zero entropy when J is small or $\psi = 0$ indicating vanishing of Mott Phase, again similar to our

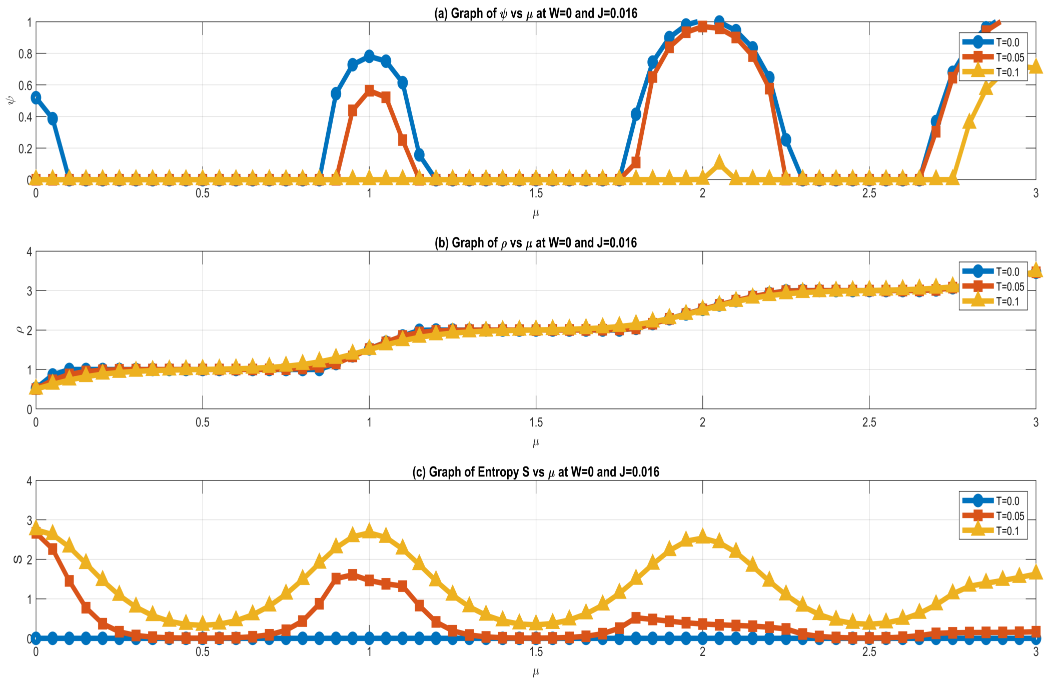

Figure 3.6: ψ, ρ and Entropy S plotted against μ at different temperatures at fixed $J = 0.016$.

compressibily κ result. As this J is increased again there is transition from NBL to SF phase characterised by $\psi \neq 0$ (Fig.3.7).

To study the effect thermal fluctuations on SF phase which is sandwiched between $\rho = 1$ and $\rho = 3$ MI phases for $W = 0$ we plot Fig. 3.10 and Fig. 3.11. When $T << J$ there is no effect on the SF nature. As T starts increasing, super fluidity starts decreasing and smoothly vanishes to become NBL. The critical temperature for this transition is seen to increase with increase in hopping amplitude J. The plot of T_C against J values shows that $T_C \propto J$. SF nature is due to the strength of hopping amplitude J. When thermal energy becomes comparable to J, bosons start loosing its SF nature. In case of Pair SF phase studied earlier, the PSF nature is due to strength of J_{eff}. It is a smaller quantity compared to J. Due to this, the Pair SF phase could be destroyed by feeble thermal fluctuations which are comparable to J_{eff}.

Note that if the cluster size is increased, the obtained critical temperatures will be more accurate but the trend show is expected to be same.

3.4 $W \neq 0$ and $T > 0$ case

To understand effect of thermal fluctuation on PSF phase we plot ψ, ϕ, ρ and Entropy S at T=0.0,T=0.001,T=0.01 against μ going from 0.48 to 0.52 at J=0.015 and $W = -2.0$ in Fig. 3.12. At T=0.001 both ψ and ϕ are zero everywhere but the Entropy S is non-zero for $\mu = 0.496$ to $\mu = 0.0.504$, hence for this μ range

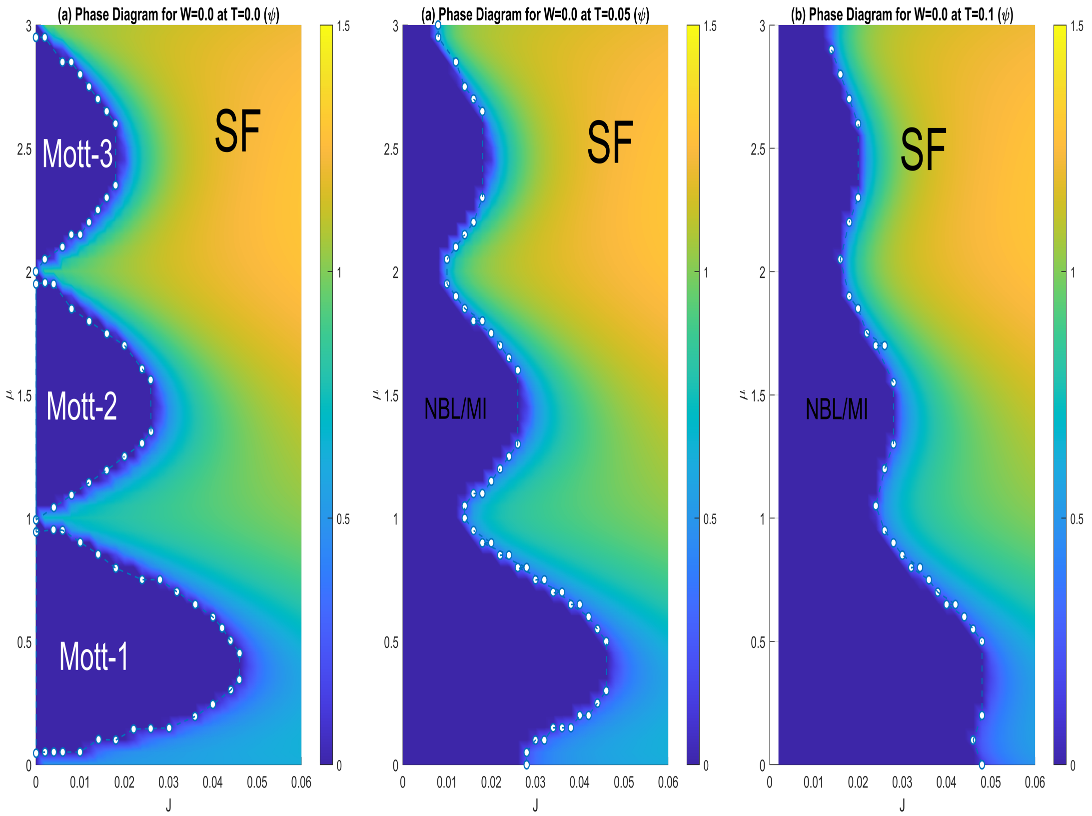

Figure 3.7: $J - \mu$ phase diagram with $W = 0$ at different T depicting MI, NBL and SF phases. Color map is with ψ values. White dots represents the MI/NBL-SF phase boundary.

where PSF phase has turned into NBL phase. Before $\mu = 0.496$, ρ is pinned to integer value of 1 and after $\mu = 0.504$, ρ is pinned to integer value 3, thus we can say that there is an NBL phase in between the Mott-1 and Mott-3 phase and no PSF phase at T=0.001. At T=0.01 it is observed that ψ and ϕ are zero everywhere, hence no SF or PSF phase. But over this μ range Entropy is non zero everywhere, hence it is entirely an NBL phase .i.e. NBL phase broadens with ρ assuming non integer values. The breaking of PSF can be explained from the fact that since the pairing in PSF atoms is not due to attractive interaction it can be easily broken with a slight thermal fluctuation.

We collect all the J and μ values to plot a $J - \mu$ phase diagram at T=0.001 and T=0.01 in Fig. 3.13. The color map represents the numerical value of compressibilty κ. At T=0.001 κ is non zero for a range of μ initially for small J, but as J is increased the NBL boundary increases but κ decreases. κ is zero everywhere else with $\rho = 1$ and $\rho = 3$ on either side of the NBL phase. At T=0.01 compressibility is non zero everywhere and hence there is no Mott phase. ALong with *psi* and *phi* being zero we can say the NBL has entirely engulfed the Mott phase and we have a region of that consist of only NBL. Compressibilty is high around $\mu = 0.5$ and slowly decreases as we move away from this center.

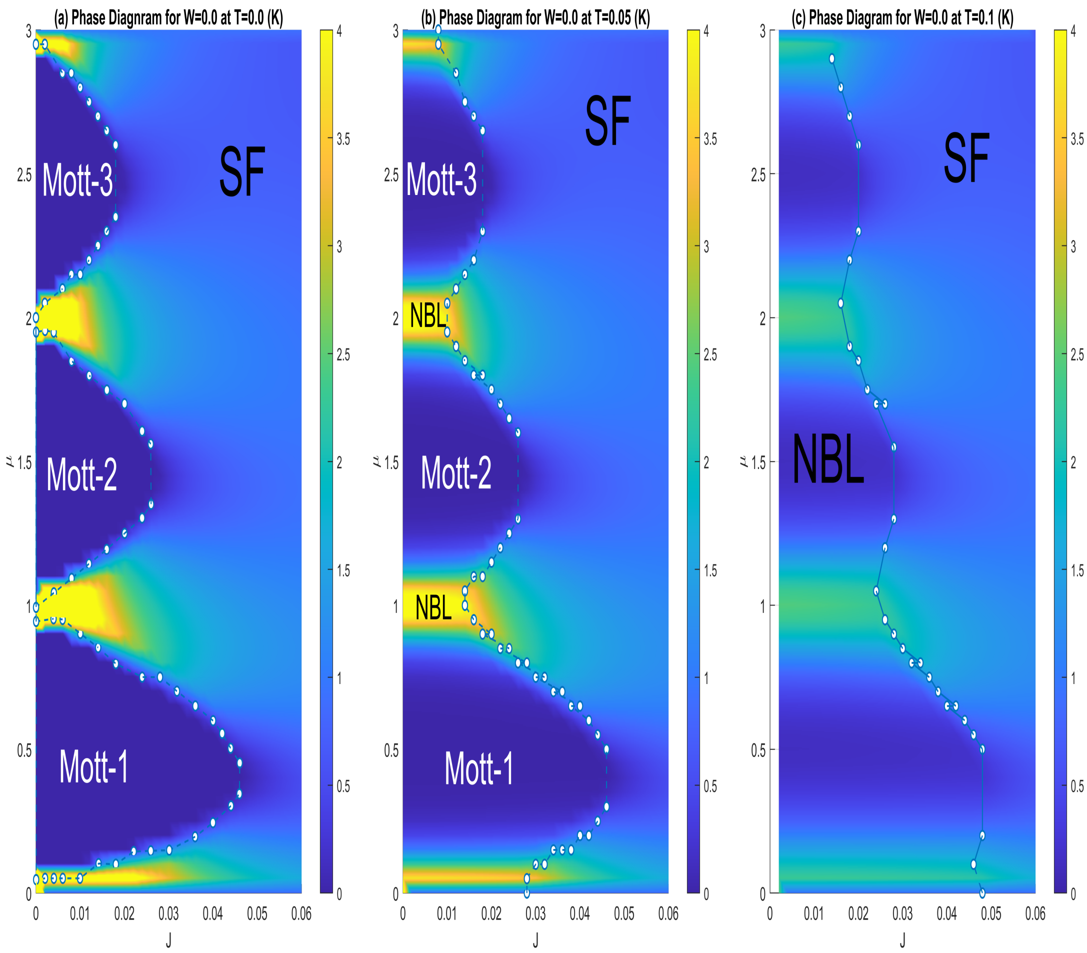

Figure 3.8: $J - \mu$ phase diagram with $W = 0$ at different T depicting MI, NBL and SF phases. Color map is with compressibility κ values. White dots represents the MI/NBL-SF phase boundary.

Similar figure to Fig.3.13 is plotted in Fig. 3.14 but in place of compressibilty κ, here the color map represents the numerical value of Entropy S. At T=0.001, Entropy is non zero for a range of mu between 0.495 to 0.505. And since ψ and ϕ both are zero we assume this region to NBL phase. Everywhere else Entropy is zero hence we say it is Mott Insulator phase characterised by $\rho = 1$ and $\rho = 3$ on either side of the NBL phase. This is in agreement with our compressibilty result. For T=0.01, this time the Entropy is non zero everywhere, hence no Mott Phase but rather whole region is just NBL with $\psi = 0$ and $\rho = 0$ for these parameters. Entropy also like compressibilty is high around $\mu = 0.5$ and decreases away from this value. With both Compressibilty and entropy results fully agreeing with each other we can say that there is no PSF phase observed at Finite T of T=0.001 and T=0.01 because the pairing in PSF atoms is not due to attractive interaction it can be easily broken with a slight thermal fluctuation.

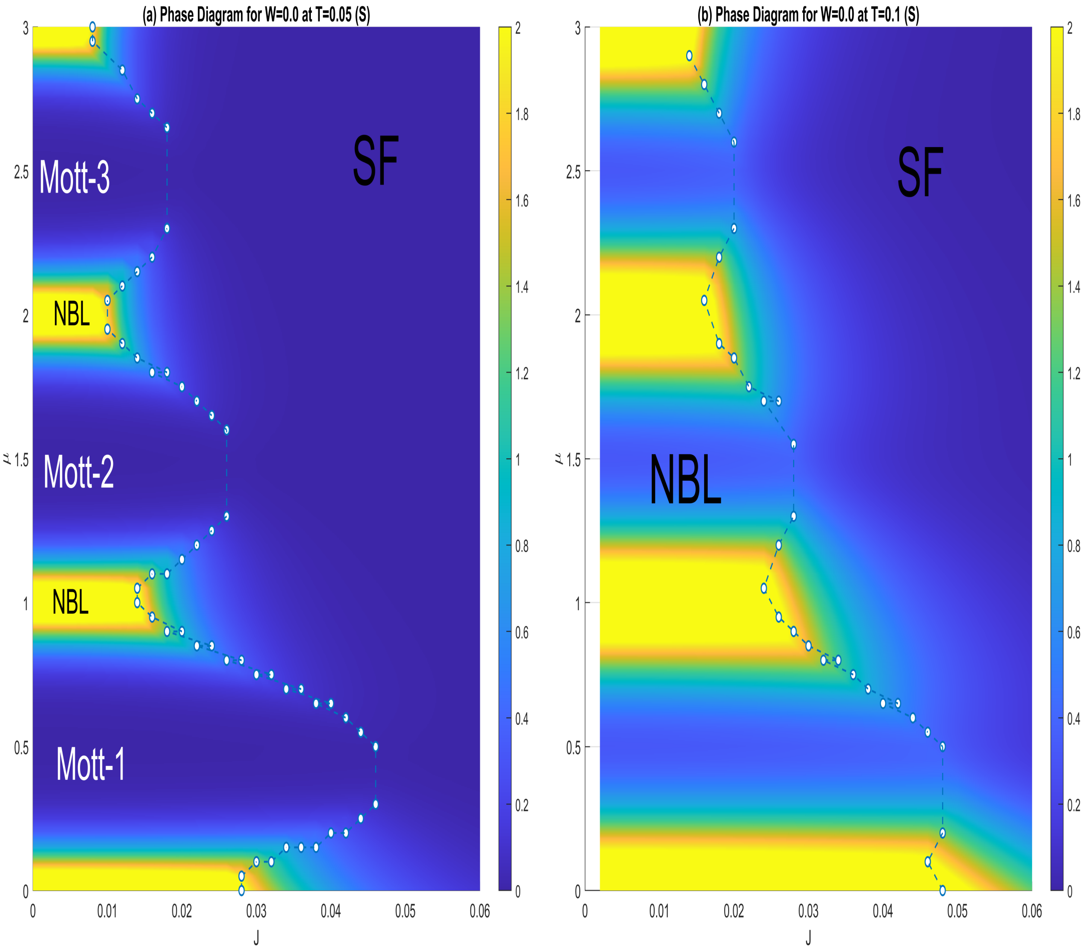

Figure 3.9: $J - \mu$ phase diagram with $W = 0$ at different T depicting MI, NBL and SF phases. Color map is with Entropy S values. White dots represents the MI/NBL-SF phase boundary.

We plot a graph of ψ, ϕ and ρ vs T/Jeff for J=0.015 and μ=0.5. For this μ, $\psi = 0.0$ everywhere but initially for smaller T, ϕ is non zero with ρ around 2, but as T is increased, ϕ begins to decrease slowly and at T/Jeff=12, ϕ becomes zero along with ρ shooting way above 2. This is a crucial Graph to understand the critical value of Thermal Fluctuation T needed for termination of PSF phase for a particular J value. From the figure we understand that the ratio of T to Tunneling element Jeff has to be equal to 12 for the PSF phase to vanish .i.e the critical temperature T_C needed to terminate PSF is $T_c = 12J_{eff}$

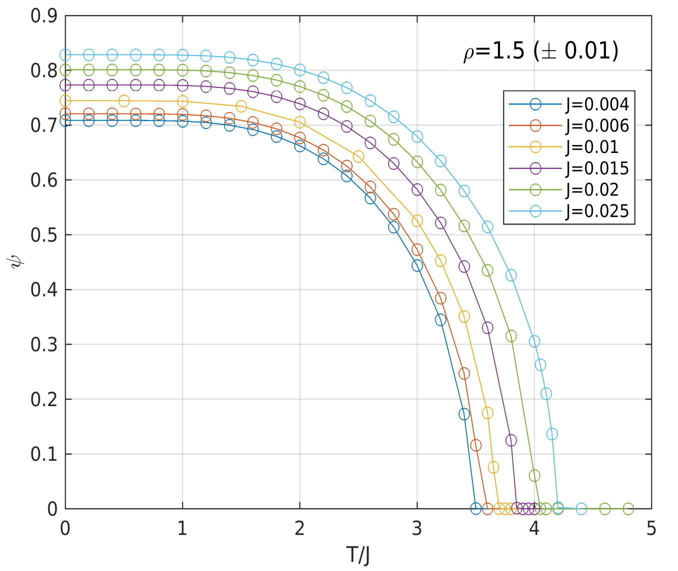

Figure 3.10: SF order parameter plotted against T/J at fixed boson density $\rho = 1.5$ for different values of J

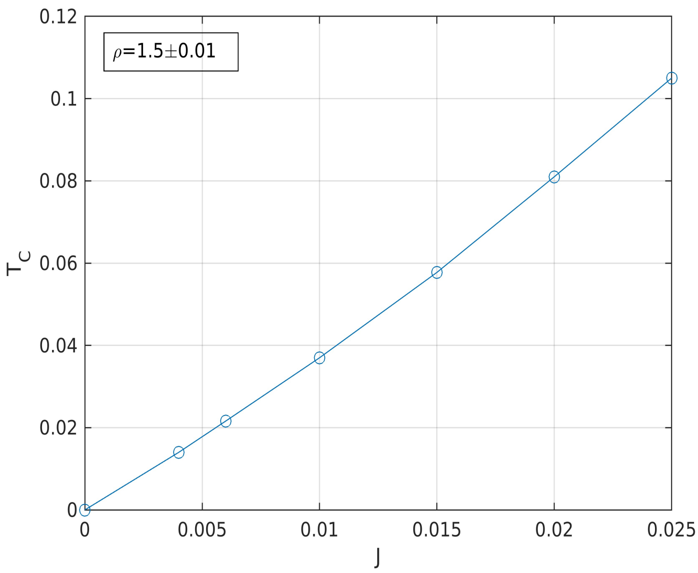

Figure 3.11: Critical Temperature T_C for SF-NBL phase transition for different J values. Boson desity is fixed to $\rho = 1.5$.

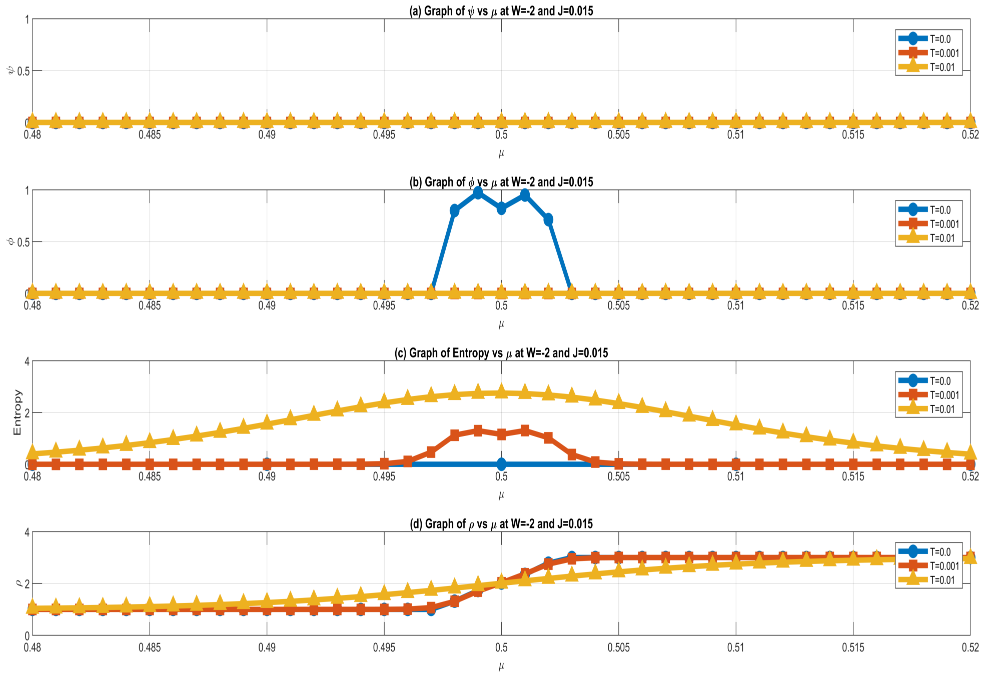

Figure 3.12: ψ, ϕ, ρ and S plotted against μ for three different temperatures. J is fixed to 0.015

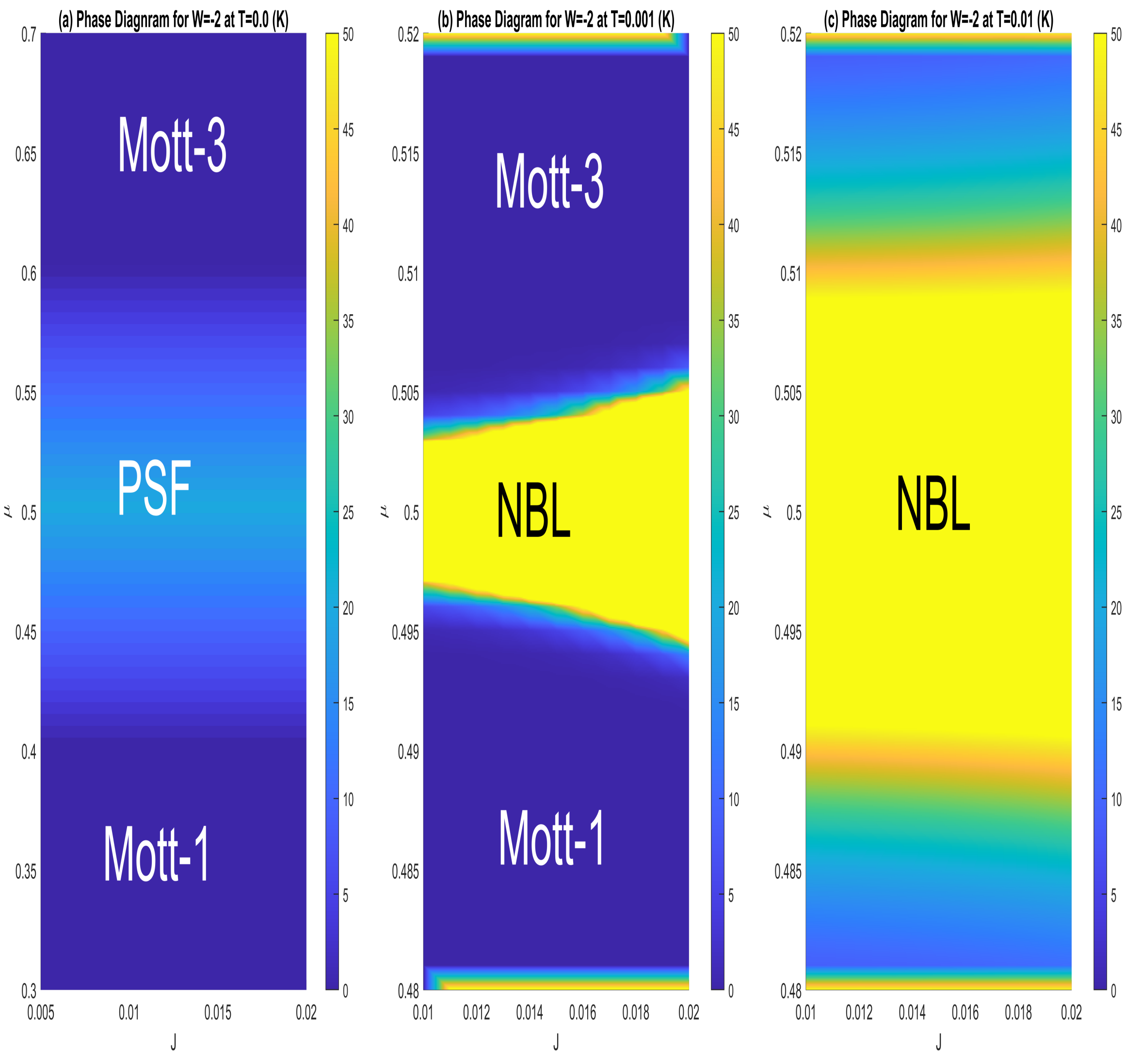

Figure 3.13: $J - \mu$ phase diagram with $W = -2$ at different T depicting MI, NBL and PSF phases. Color map is with compressibility κ values.

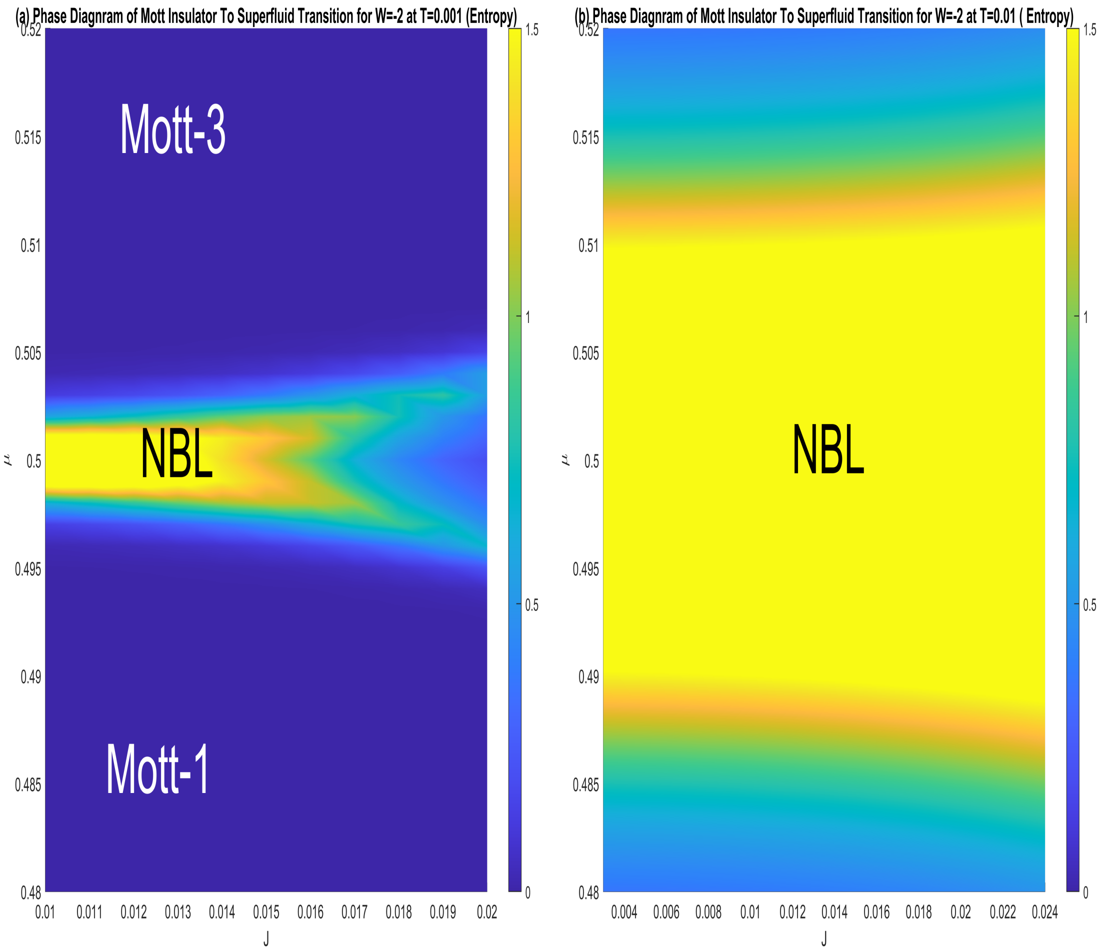

Figure 3.14: $J - \mu$ phase diagram with $W = -2$ at different T depicting MI, NBL and PSF phases. Color map is with Entropy S values.

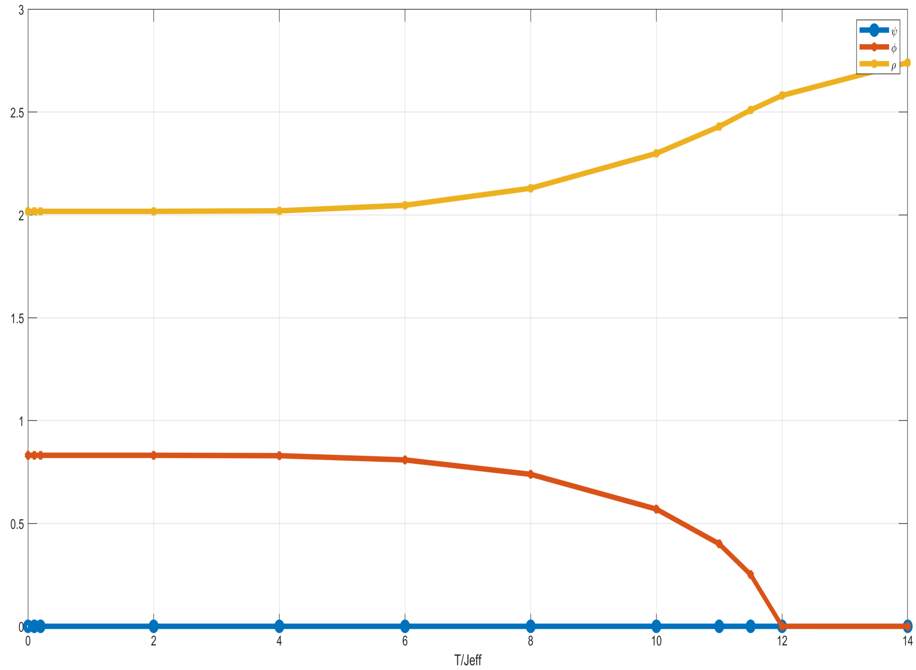

Figure 3.15: Critical Temperature For J=0.015 μ=0.5

Chapter 4

Conclusion

Bose Hubbard model with and without three body interactions was studied using Cluster Mean Field Theory. These calculations were done at zero and non-zero temperatures and several interesting results were obtained. By changing the J/U ratio this model predicts SF-MI phase transition. It has been experimentally verified for the Bosonic atoms loaded in Optical Lattice. With inclusion of attractive hard core three body interaction W, Mott-3 lobe enlarges and an anomalous PSF phase is seen between MI-1 and MI-3 phase. Bosons hop here as pairs. Such repulsively bound pair of atoms has been realised in optical lattice systems[20] in deep MI phase. To study the effect of thermal fluctuations on this PSF phase, first BH model without three body interactions was studied. It was seen that with increase in temperature the SF phase sandwiched between two Mott phases appears fragile towards the thermal fluctuations. The critical temperatures need to destroy SF nature here was seen to be proportional to the hopping amplitude. Such behaviour was seen through Monte-Carlo studies too[8]. The PSF phase is seen to exist between MI-1 and MI-3 phase at very small values of J. Due to this, slight thermal fluctuations can destroy the repulsively bound anomalous PSF phase. Overall, studies done here have given $J-\mu-T$ phase diagrams which are or primary importance in Optical lattice systems.

Future aspects of this work will be to study the role of attractive three body interaction strength with temperature on the MI phases. Effect of disorder can also be studied in this framework.

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