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Random Phase Approximation and Cluster Mean Field Studies of Hard Core Bose Hubbard Model

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Abstract. We investigate zero temperature and finite temperature properties of the Bose Hubbard Model in the hard core limit using Random Phase Approximation (RPA) and Cluster Mean Field Theory (CMFT). We show that our RPA calculations are able to capture quantum and thermal fluctuations significantly better than CMFT.

INTRODUCTION

Superfluid (SF) to Mott Insulator (MI) quantum phase transition occurring in optical lattices has received great interest since its theoretical prediction [1] and followed by its experimental realization [2, 3]. Techniques like Density Matrix Renormalization Group, Quantum Monte Carlo, Mean field approximation etc have been used to study the phase diagrams of ultra cold bosons in optical lattices quantitatively and qualitatively. Even with this, direct comparison of theoretical results to that of experiments is difficult due to (i) restriction of lattice sites under consideration because of exponential growth in the Hilbert space in theoretical calculations, (ii) presence of small but finite thermal fluctuation in experiments and (iii) in-homogeneity in lattices. The quest to find technique which can account for at least two of the above difficulties simultaneously forms a challenge for theoretical condensed matter physicists.

The minimal model which describes bosons in such optical lattices is Bose Hubbard Model (BHM). When repulsive interaction between two bosons on same site is infinite, this model is termed as Hard Core Bose Hubbard Model (HC-BHM). This model has gained vast attention due to its analogs in spin and fermionic systems. The overall phase diagram predicted by this model at zero temperature comprises of, (i) vacuum state: where all lattice sites are empty, (ii) superfluid (SF): where bosons tunnel into neighboring lattice sites easily making incommensurate boson filling per site and non-zero superfluid density and (iii) Mott Insulator (MI): where tunneling of bosons costs infinite energy and hence there is exactly one boson localized per site. In presence of thermal fluctuations, SF melts to Normal Bose liquid (NBL).

Aim of this letter is to solve this HC-BHM using two different methods: Random Phase Approximation (RPA) [4] and Cluster Mean Field Theory (CMFT) [5] at zero and finite temperatures. Both of these techniques rely over mean field approximation. CMFT, an extension of standard mean field theory (MFT), accounts for some of the neglected fluctuations in MFT by increasing number of sites under consideration. Whereas RPA calculation demands solving equation of motion for the Green's function in terms of Standard Basis Operators [6] build over single site MFT states. Our RPA results for HC-BHM are complete, in contrast to work done by A.S Sajna et.al [7] for BHM, as we are able to investigate properties in deep SF phase.

In next section we present the model and the procedure used to solve HC-BHM using both the techniques. In third section we unfold the results obtained followed by the conclusion in fourth section.

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MODEL AND METHOD

Bose Hubbard Hamiltonian is defined as

$$H = -t\sum_{<i,j>}(a_i^+ a_j + h.c) + \frac{U}{2}\sum_i n_i(n_i - 1) - \mu\sum_i n_i \quad (1)$$

where t is the hopping amplitude between nearest neighboring sites $\langle i,j\rangle$. $a_i^+(a_i)$ and n_i are, respectively, the boson creation (annihilation) and number operators at site i. U represent the onsite two body repulsion interaction between bosons and μ is the chemical potential which controls boson density in the system. When the repulsive interaction strength is infinite ($U \to \infty$), U term in equation (1) can be dropped restricting only zero or one boson per site. The resultant Hamiltonian is termed as Hard Core Bose Hubbard Hamiltonian and defined as

$$H = -t\sum_{<i,j>}(a_i^+ a_j + h.c) - \mu\sum_i n_i \quad (2)$$

This Hamiltonian is solved using RPA and CMFT as shown in following subsections.

Random Phase Approximation

We start with writing creation (annihilation) operators in model (2) in terms of an average value and fluctuations over it, i.e. $a_i^+ = \langle a_i^+\rangle + \delta a_i^+$ $(a_i = \langle a_i\rangle + \delta a_i)$. Introducing superfluid order parameter $\psi_i = \langle a_i\rangle$, which we treat as a real quantity, model (1) can be re-written as $H = \sum_i H_i^{MF} - t\sum_{<i,j>}\left(\delta a_i^+ \delta a_j + H.C.\right)$ where $H_i^{MF} = -zt(a_i^+ + a_i)\psi_i - \mu n_i + zt\psi_i^2$ and z is the coordination number of the lattice. Energy scaling is done by setting $zt = 1$. Mean field Hamiltonian H_i^{MF} which is now a single site Hamiltonian is diagonalized in Fock's basis $|0\rangle$ and $|1\rangle$ (referring to zero and one boson state) to give eigen energies E_α and eigenstates $|i\alpha\rangle$ where $\alpha \in 0,1$ (corresponding to first (ground state) and second (excited state) eigenvectors) . We use these eigenstates to construct the standard basis operator $L^i_{\alpha\alpha'} = |i\alpha\rangle\langle i\alpha'|$ and the Green function in terms of these operators is given by $G^{ij}_{\alpha\alpha'\beta\beta'}(t) = -i\theta(t)\langle\left[L^i_{\alpha\alpha'}(t), L^j_{\beta\beta'}(0)\right]\rangle$. Here $\theta(t)$ is Heaviside step function. Solving equation of motion for $G^{ij}_{\alpha\alpha'\beta\beta'}(t)$ within Random Phase Approximation and Fourier transforming it into momentum and energy space, we get

$$(\omega - E_\alpha + E_{\alpha'})G_{\alpha\alpha'\beta\beta'}(k,\omega) = \frac{1}{2\pi}P_{\alpha\alpha'}\delta_{\alpha\beta'}\delta_{\alpha'\beta} + \varepsilon_k P_{\alpha\alpha'}\sum_{\mu\mu'}\tilde{T}_{\alpha'\alpha\mu\mu'}G_{\mu\mu'\beta\beta'}(k,\omega) + \sum_{\mu\mu'}P_\mu\left(\tilde{T}_{\mu\mu\mu'\alpha'}G_{\mu'\alpha'\beta\beta'}(k,\omega) - \tilde{T}_{\mu\mu\alpha'\mu'}G_{\alpha\mu'\beta\beta'}(k,\omega)\right) \quad (3)$$

where $P_{\alpha\alpha'} = \langle L_{\alpha\alpha}\rangle - \langle L_{\alpha'\alpha'}\rangle$ and $P_\alpha = \langle L_{\alpha\alpha}\rangle$ is the occupational probability of state α. $\tilde{T}_{\alpha\alpha'\beta\beta'} = t(T^{ij}_{\alpha\alpha'\beta\beta'} + T^{ij}_{\beta\beta'\alpha\alpha'})$ with $T^{ij}_{\alpha\alpha'\beta\beta'} = \langle i\alpha|a_i^+|i\alpha'\rangle\langle j\beta|a_j|j\beta'\rangle$ and $\varepsilon_k = 2\sum_{j=x,y,z}\cos(\pi k_j)$. Solution of Eq. (3) can be written as $G_{\alpha\alpha'\beta\beta'}(k,\omega) = \sum_r \frac{A_r(k)}{\omega - \omega_r(k)}$ where $\omega_r(k)$ is the r^{th} excitation energy and $A_r(k)$ is corresponding spectral weight. It should be noted that both excitation energy and spectral weight are dependent on occupational probabilities P_α [7] which can be solved self consistently using the relation $P_\alpha = \frac{1}{(2\pi)^3}\sum_{r,k}A_r(k)f(\omega_r)$ where $f(\omega) = \left(e^{\omega/T} - 1\right)^{-1}$ is the Bose distribution function. We have taken Boltzmann constant $k_B = 1$. Using the self consistent solution to P_α, the superfluid order parameter $\psi = \sum_{\alpha\in 0,1}P_\alpha\langle\alpha|\hat{a}|\alpha\rangle$ is also obtained self consistently. From these solutions superfluid density $\rho_{SF} = |\psi|^2$ and boson density $\rho = \sum_{\alpha\in 0,1}P_\alpha\langle\alpha|\hat{n}|\alpha\rangle$ are also calculated. Different phases are identified in the following manner: superfluid phase corresponds if $\rho_{SF} \neq 0$, vacuum is $\rho_{SF} = 0$ and $\rho = 0$, Mott insulator $\rho_{SF} = 0$ and $\rho = 1$ and Normal Bose Liquid state (NBL) when $\rho_{SF} = 0$ and $0 < \rho < 1$.

Cluster Mean Field Theory

To solve HC-BHM using CMFT, whole lattice is partitioned into clusters with N_C number of sites each. Each cluster is decoupled from others using standard mean field approximation i.e., by approximating $a_i^+ a_j + a_i a_j^+ \cong a_i^+\psi_j + a_i\psi_j - \psi_i\psi_j$ where i is the site belonging to edge of cluster under consideration and j to the nearest cluster. ψ_i is

the SF order parameter of site i. Hopping term inside the cluster is treated exactly. The resultant cluster Hamiltonian is given as

$$H^{Cluster} = -t\sum_{<i,j>}^{N_C}(a_i^+ a_j + a_i a_j^+) - t\sum_i^{N_C}\sum_j'(a_i^+ \psi_j + a_i\psi_j - \psi_i\psi_j) - \mu\sum_i^{N_C} n_i \quad (4).$$

First term represents hopping of bosons within cluster, whereas in second term $\sum_j'$, runs over all sites which are nearest neighbor to i and belonging to neighboring clusters. To match with our RPA results above, energy scaling is done such that $zt = 1$. We solve $H^{Cluster}$ in following steps. First we construct the Hamiltonian matrix in Fock's basis $|N_1, N_2, \dots, N_C\rangle$ assuming initial guess for ψ. Here $|N_i\rangle \in \{0,1\}$ and we dropped site index in the superfluid order parameter due to homogeneity of the lattice. Diagonalizing this matrix, we obtain eigenvalues E_α, eigenvectors $|\alpha\rangle = \sum_{N_1,N_2\dots N_C} C_{N_1,N_2\dots N_C}|N_1, N_2, \dots, N_C\rangle$ and the partition function $Z = \sum_\alpha e^{-\frac{E_\alpha}{T}}$ where we assume $k_B = 1$. Superfluid order parameter is given by $\psi = \sum_\alpha e^{-\frac{E_\alpha}{T}}\langle\alpha|a|\alpha\rangle/Z$ which is solved self consistently. Further SF density $\rho_{SF} = |\psi|^2$ and boson density $\rho = \sum_\alpha e^{-\frac{E_\alpha}{T}}\langle\alpha|n|\alpha\rangle/Z$ are calculated.

RESULTS

Here we discuss the results obtained by both methods. In CMFT calculations we choose cluster sizes of $N_C = 8\,(2\times2\times2$ cube) denoted by CMFT in plots. Single site Mean field theory ($N_C = 1$) denoted by MFT is also plotted for the sake of completeness. In FIGURE 1 we plot SF density ρ_{SF} versus chemical potential μ at T=0. Inset show boson density ρ for the same parameters. For ≤ -1 ($\mu \geq 1$) , $\rho_{SF} = 0$ and $\rho = 0$ ($\rho = 1$) which shows a vacuum (Mott Insulator) state. For $-1 < \mu < 1$, ρ is seen to increases as μ increases from 0 to 1. Superfluid density ρ_{SF} increases up to $\rho = 0.5$ and then reduces to zero smoothly. MFT shows maximum $\rho_{SF} = 0.25$, and CMFT, which accounts for some neglected quantum fluctuations from MFT shows $\rho_{SF} = 0.241$. Whereas RPA predicts $\rho_{SF} = 0.229$. This shows RPA has captured quantum fluctuations better than CMFT.

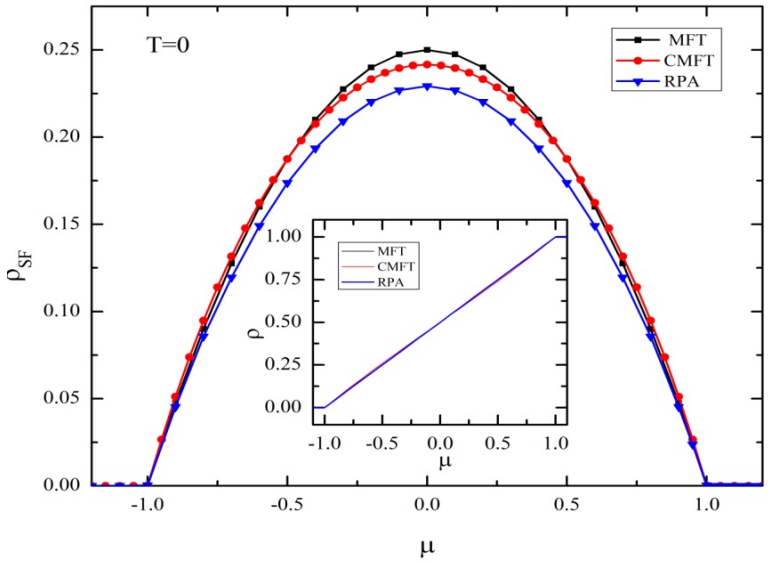

FIGURE 1. (Color online) SF density ρ_{SF} calculated by using MFT(black curve), CMFT(red) and RPA(blue) are plotted against chemical potential μ at *T=0* . (Inset) Boson density ρ is plotted against chemical potential μ with same color coding. Calculated ρ is almost same with all methods, whereas RPA shows reduction of ρ_{SF} compared to that of CMFT and MFT.

In FIGURE 2(a) ρ_{SF} for $\rho = 0.5$ is plotted against temperature T. For very low temperatures, RPA has captured both quantum and thermal (small but finite) fluctuations better (reflected in reduction of ρ_{SF}) than CMFT and MFT. As T increases ρ_{SF} decreases and vanishes, yielding a transition from SF to NBL. For $\rho = 0.5$, the critical temperature T_C for SF-NBL transition is, respectively, equal to $0.425, 0.45$ and 0.51 for RPA, CMFT and MFT.

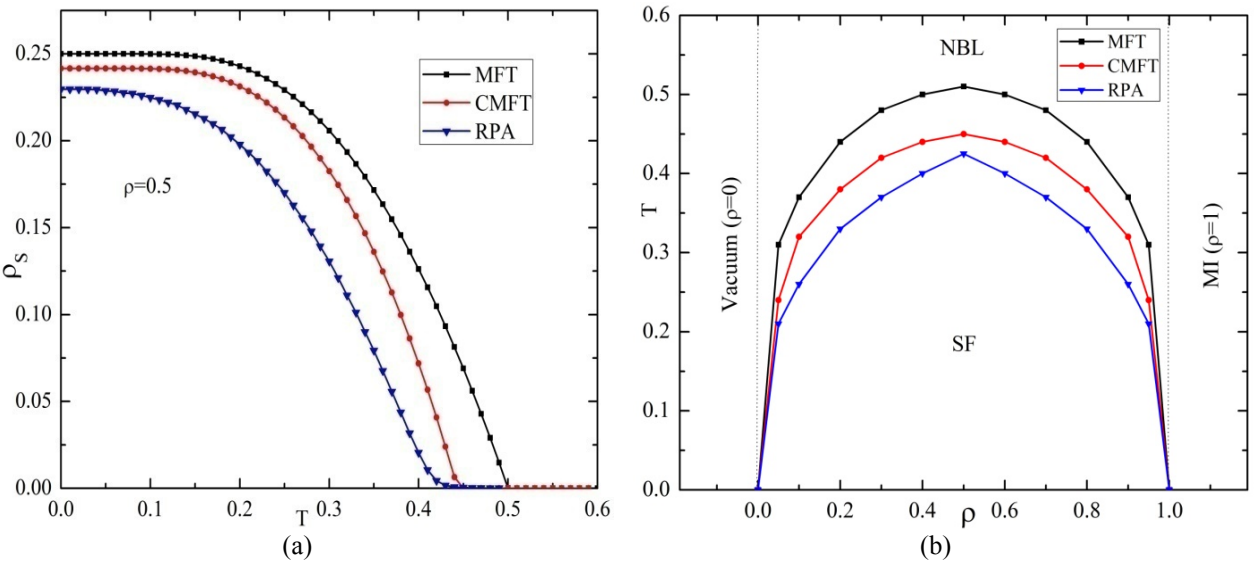

FIGURE 2. (Color online) (a) Calculated SF density ρ_{SF} by MFT (Black curve), CMFT (Red) and RPA (Blue) is plotted against T. (b) Critical temperatures for SF to NBL transition predicted from MFT (Black), CMFT (Red) and RPA (Blue) calculations for different boson densities ρ.

Using the transition temperature for different densities, we plot phase diagram for HC-BHM in FIGURE 2(b). Overall phase diagram shows that critical temperatures for SF-NBL transition as predicted by RPA, are significantly lesser compared to CMFT and MFT results.

CONCLUSION

We solved HC-BHM using two different methods; RPA and CMFT both build over mean field approximation. RPA which relies on single site standard basis operators and assumes random phases of operators in correlation functions has captured quantum and thermal fluctuations significantly better than CMFT which suffers exponential growth in Hilbert space in order capture these fluctuations. Our results yield valuable insights and a starting point for extending this RPA method for soft core and other Bose Hubbard Models.

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