Melting of Mott Phases in Spin-1 Bose Hubbard Model

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Abstract: The Cluster Mean Field theory calculation is extended for finite temperatures to study the combined effect of quantum and thermal fluctuations on various phases arising in the spin-1 Bose Hubbard model. This investigation finds that the polar nature of the superfluid phase persists, and the density of bosons with spin component $\sigma = 0$ increases with the temperature. The phase diagram is obtained and compared with that of the single-site mean-field theory. Compressibility shows a signature of divergence at the transition from the polar superfluid phase to the normal boson liquid phase. Small thermal fluctuations are sufficient to destroy the anti-ferromagnetic, maximally entangled odd density Mott insulator phase, whereas large thermal fluctuations are needed to break the singlet formed in the even density Mott insulator phase. However, in both the cases, the insulators melt to normal boson liquid at the same temperature.

INTRODUCTION

Ultra-cold atoms loaded in an optical lattice have served as excellent testing grounds for studying Quantum Phase Transitions (QPT) \cite{1-3}. The study of superfluid (SF) to Mott insulator (MI) transition occurring in bosonic atoms is the most eminent in this field. Bosonic atoms like $^{23}$Na, $^{87}$Rb have hyperfine spin F=1. If these atoms are trapped in purely optical potential, they exhibit much interesting degenerate magnetic phases along with SF and MI phases \cite{4}. Spin-1 Bose Hubbard Model describes spinor bosons in an optical lattice. Hamiltonian used in Spin-1 Bose Hubbard Model is given below.

\begin{equation}
H = -t \sum_{\langle i,j \rangle, \sigma}(a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + \frac{u_0}{2} \sum_i n_i(n_i - 1) + \frac{u_2}{2} \sum_i (F_i^2 - 2n_i) - \mu \sum_i n_i
\end{equation}

where $\sigma \in \{1, 0, -1\}$ are the spin components, summation $\langle i,j \rangle$ run over all nearest neighbor sites, $a_{i,\sigma}^\dagger (a_{i,\sigma})$ is the creation (annihilation) operation of boson with spin component $\sigma$ at site $i$, $n_i = \sum_\sigma n_{i,\sigma}$, $F_i = \sum_\sigma S_{\alpha,\sigma}^\dagger a_{i,\sigma} S_{\sigma,\alpha}$ and $S_{\alpha,\sigma}$ represents the standard spin-1 matrices. Here $t, U_0, U_2$ and $\mu$ are the hopping amplitude, spin independent interaction, spin dependent interaction and chemical potential respectively. Ratio $U_2/U_0$ can be tuned in experiments. It can take positive (negative) value, resulting in Anti-Ferromagnetic (Ferromagnetic) spin dependent interaction.

The earlier work \cite{5} of this model using the Cluster Mean Field Theory (CMFT) focused on the zero temperature properties. Some of the salient features of this study are: i) the CMFT captures some of the neglected quantum fluctuations in the mean-field theory and addresses all the magnetic phases arising in this model, ii) for anti-ferromagnetic spin-dependent interaction, SF shows polar nature (Polar SF), iii) the density $\rho = 1$ MI is Nematic and the transition from Polar SF to MI phase is continuous, iv) the $\rho = 2$ MI is singlet or Nematic depending upon the strength of the anti-ferromagnetic interaction, and transition from Polar SF to singlet (Nematic) MI transition is of first-order (continuous), and iv) Bosons in Nematic MI phase are highly entangled which lowers the total magnetic moment. Since effects of thermal fluctuations on all these phases are of great interest, an attempt is made to examine this issue by extending the CMFT calculations to study the finite temperature properties of the two dimensional spin-1 Bose Hubbard Model.

In section 2 we present outline of CMFT formalism. Section 3 contains the predictions of the formalism and the relevant discussions. This calculation is restricted to anti-ferromagnetic case ($U_2 > 0$) with cluster size of $N_c = 1, 2$. Conclusion is presented in the section 4.
METHOD

In the CMFT, the lattice is divided into clusters of \( N_c \) sites and the hopping term between nearest neighboring clusters is decoupled using mean field approximation i.e. \( a_{i,+}^\dagger a_{j,-} + a_{i,-}a_{j,+}^\dagger \equiv a_{i,+}^\dagger \psi_{j,+} + a_{i,-} \psi_{j,-} - |\psi_{i,+}|^2 \). Here \( \psi_{i,+} = \langle a_{i,+} \rangle \) is the superfluid order parameter of spin component \( \sigma \) at site \( i \). Hopping term inside the cluster, however, is treated exactly. The resultant cluster Hamiltonian is given by

\[
H_{\text{Cluster}} = -t \sum_{(i,j)\sigma} (a_{i,+}^\dagger a_{j,-} + a_{i,-}^\dagger a_{j,+}) - t \sum_{i,j} (a_{i,+}^\dagger \psi_{j,+} + a_{i,-} \psi_{j,-} - |\psi_{i,+}|^2) + \frac{u_b}{2} \sum_{i} n_i (n_i - 1) + \frac{u_c}{2} \sum_{i} (F_i^2 - 2n_i) - \mu \sum_{i} n_i.
\]

(2)

First term represents hopping of bosons within the cluster and \( j \) in the second term runs over all sites which are nearest neighbor to \( i \) and belonging to neighboring clusters. In order to calculate the ground state of \( H_{\text{Cluster}} \), the Hamiltonian matrix is constructed in the Fock’s basis \( |N_1 \rangle \otimes |N_2 \rangle \) assuming an initial guess for \( \{ \psi_{1,+}, \psi_{1,-}, \psi_{1,-} \} \). Here \( |N_1 \rangle \equiv |N_{1,1}, N_{1,0}, N_{1,-1} \rangle \) with \( N_{i,+} \) representing number of bosons with spin component \( \sigma \) at site \( i \). In this calculation, we restrict the maximum total number of bosons per site: \( \sum_i N_{i,+} = 3 \). Energy scaling is done by setting \( t = 1 \). We diagonalize the Hamiltonian matrix to obtain the eigenvalues \( E_\alpha \) and the eigenvectors \( |\alpha \rangle \equiv \sum_i n_i \psi_{i,+} \). The partition function \( Z = \sum_\alpha e^{-\frac{E_\alpha}{T}} \), where \( T \) stands for temperature and the Boltzmann constant \( k_B \) is scaled to 1. For self-consistency, we re-estimate the superfluid order parameters using the relation \( \psi_{\sigma} = \langle \alpha_\sigma \rangle \). In this calculation, the thermal average of any operator \( O \) is given as: \( \langle O \rangle = \frac{1}{Z} \sum_\alpha e^{-\frac{E_\alpha}{T}} \langle \alpha \rangle |O| \langle \alpha \rangle \). The SF order parameters are obtained using self consistent calculation. The site index \( i \) is dropped due to homogeneity of the lattice.

The superfluid density \( \rho_s = \sum_\sigma |\psi_{\sigma}|^2 \) and the boson density \( \rho = \sum_\sigma \rho_\sigma \) where \( \rho_\sigma = \langle n_\sigma \rangle \) are calculated from the self-consistent ground state. Ground state is a superfluid phase if \( \rho_\sigma \neq 0 \) and compressibility \( \kappa = \frac{d\rho}{d\mu} \neq 0 \). \( \rho_s = 0 \), and \( \kappa = 0 \) with density \( \rho \) pinned to an integer depicts MI phase. At finite temperatures, system also exhibit normal bose liquid (NBL) phase which is characterized by \( \rho_s = 0 \) and \( \kappa \neq 0 \). To study magnetic properties of the ground state we calculate magnetic moment of a site \( \langle F_i^2 \rangle \) and singlet density \( \rho_{SD} = \langle A_{SD}^\dagger A_{SD} \rangle \), where \( A_{SD}^\dagger = \frac{1}{\sqrt{6}} (2a_{i,+}^\dagger a_{-1}^\dagger - a_{0,+}^\dagger a_{0,-}^\dagger) \) is the singlet creation operator. Magnetic moment of a cluster is calculated from two site operator \( \langle F_i^2 \rangle = \langle F_{i,+}^2 + F_{i,-}^2 + 2F_i^2 \rangle \). The order parameter which characterizes the Nematic phase is given by \( Q_{aa} = \langle F_{a,i}^2 + \frac{1}{3} F_i^2 \rangle \), where \( a = x,y,z \). Nematic order exists if \( Q_{aa} \neq 0 \).

RESULTS

In the Fig. 1, we present the phase diagram in the \( \mu - T \) plane for \( U_2/U_0 = 0.03 \) and \( U_0 = 24 \). Single site mean field phase diagram (labeled with \( N_c = 1 \)) is also plotted in the same figure for comparison. At very low temperatures (\( T \sim 0.01 \)), polar SF to MI (\( \rho = 1 \)) transition is second order, and the Mott phase region is enlarged due to the inclusion of fluctuations [5]. As the temperature increases, the polar SF to MI (\( \rho = 1 \)) transition is changed to first order and the Mott phase region remains same. It is evident from the Fig. 1 that the MI phases start melting to normal bose liquid phase with increasing temperature. The SF to NBL transition is continuous. Thus the present study using CMFT improves the phase diagram compare to the single site mean field theory. It is interesting to note that both \( \rho = 1 \) and \( \rho = 2 \) Mott insulators melt at the same temperature, even though \( \rho = 2 \) MI is known to be more stable than \( \rho = 1 \) MI.
The evolution of the SF order parameters $\psi_\sigma$ and the boson densities $\rho_\sigma$ as a function of temperature in the SF phase at fixed density $\rho = 1.5$ is shown in the Fig. 2. At $T = 0$, we have $\psi_1 = \psi_{-1} \neq 0$ and $\psi_0 = 0$ depicting the polar nature of the superfluid phase. The existence of small but non-zero $\rho_0$ implies bosons with spin component $\sigma = 0$ are in the NBL state. As $T$ increases, $\rho_{\pm 1}$ decreases and vanishes at the SF to NBL transition. The $\psi_0$ however, remains zero. Thus, the polar nature of the superfluid phase persists even at finite temperatures. It is interesting to note that $\rho_0$ increases while $\rho_{\pm 1}$ decreases with increase in the temperature. In the NBL phase we find $\rho_{\pm 1} = \rho_0$ and the compressibility shows a maximum at the SF to NBL transition.

Figure 3(a) shows the total magnetization of the cluster $\langle F^2_{\text{tot}} \rangle$ as a function of $T$ deep inside the $\rho = 1$ MI phase. At low values of temperature we find $\langle F^2_{\text{tot}} \rangle$ are closed to zero. This state is predicted to be maximally entangled via quantum fluctuations [5]. For small values of $U_2/U_0$ ratio, relatively low temperature is sufficient to break this arrangement, resulting abrupt increase in $\langle F^2_{\text{tot}} \rangle$. For relatively large $U_2/U_0$ values, higher temperature is
needed to increase $\langle F_t^2 \rangle$. Other parameters like magnetic moment of site $\langle F_t^2 \rangle$ and Nematic order parameter $Q_{zz}$ do not change significantly in the $\rho = 1$ MI phase.

![Figure 3](image)

**FIGURE 3.** (Color online) (a) Magnetization of cluster $\langle F_{tot}^2 \rangle$ for different $U_2/U_0$ against $T$ in $\rho = 1$ MI. (b1)-(b4) plots, respectively, $\langle F_t^2 \rangle$, $\rho_{sd}$, $\langle F_{tot}^2 \rangle$ and $Q_{zz}$ as a function of $T$ for different $U_2/U_0$ ratios in $\rho = 2$ MI phase.

In the Figs. 3, we present the plots of magnetic moment of a site (b1), singlet density (b2), magnetization of cluster (b3), and Nematic order (b4) as a function of $T$ for different values of $U_2/U_0$ in $\rho = 2$ MI phase. As temperature increases, the singlet state in the $\rho = 2$ MI breaks which leads to increase in the Nematic order parameter.

**CONCLUSION**

In the present work, an attempt is made to study the effects of quantum and thermal fluctuations in the Spin-1 Bose Hubbard Model using CMFT. These calculations show improvement in predicting the critical point for the polar SF to NBL transition with that of single-site mean-field studies. This study finds the polar nature of the SF phase persists at finite temperatures, and the density of bosons with spin component $s = 0$ increases with temperature. Compressibility shows a signature of divergence at the polar SF to NBL transition. In the case of the $\rho = 1$ MI phase, a small thermal fluctuation is sufficient to destroy the anti-ferromagnetic ground state of the cluster; however, it requires a large thermal fluctuation to break the singlet pairs in the $\rho = 2$ MI. It is interesting to note that both Mott insulators melt at the same temperatures even though different temperatures are needed to break their magnetic ground state. To conclude, the inclusion of quantum and thermal fluctuations in our CMFT formalism allows us to study all the phases and respective phase transitions.

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