

Quantum Phase Transitions in a Dimerized Bose-Hubbard Model: A DMRG Study

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Abstract. - We investigate the phase diagram of a dimerized Bose-Hubbard model, using density matrix renormalization group technique. We find a new phase, which is the coexistence of superfluid and bond-wave phases, due to the effect of dimerization. Experimentally dimerization in optical lattice can be realized by using two counter propagating laser beams of different wavelengths. Apart from the conventional superfluid to Mott insulator transition, we find a new quantum phase transition: from superfluid-bond-wave to Mott insulator-bond wave phase. Our study suggests a rich phase diagram which can be easily probed.

Introduction. – Over the last decade, there have been a large number of interesting theoretical predictions on the rich physics of strongly correlated optical lattice systems [1–3]. The spectacular experiment by Greiner *et al.* [4] has opened a new frontier, as it convincingly demonstrates that at low temperature, the cold atoms trapped in an optical lattice undergo a quantum phase transition from the delocalized superfluid (SF) state to the localized Mott insulator (MI) state. The unprecedented control in experiment over the theoretical parameters provides a good opportunity to study the various competing phases in this class of lattice systems.

The theory of the underlying quantum phase transition of strongly interacting bosons confined in an optical lattice is described by the well-known Bose-Hubbard (BH) model [5]. The BH Hamiltonian is given by

$$H_{BH} = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) + U \sum_i n_i(n_i - 1)/2 \quad (1)$$

where t is the hopping parameter, b_i (b_i^\dagger) are the annihilation (creation) operators of bosons on site i and $n_i = b_i^\dagger b_i$ represents the number of bosons on site i . U is the repulsion between a pair of bosons occupying the same site. Experimentally, the ratio t/U is varied by tuning the laser intensity, thus the depth of the optical potential can be adjusted. When $U/t \ll 1$ *i.e.*, the optical trap is very shallow,

the hopping between different lattice sites dominates, making the atomic wave functions completely delocalized, giving rise to a superfluid phase. As U/t is increased, the depth of the optical trap increases and the system is driven towards Mott insulator phase. In this regime, since fluctuations in the boson number become energetically costly, bosons localize at different lattice sites. Thus there are fixed number of bosons at each site.

The BH Hamiltonian has been studied extensively using mean-field theory [3,5,6], quantum Monte Carlo techniques [2,7–9] and density matrix renormalization group (DMRG) [10,11] method. DMRG is a very promising and powerful numerical technique for low dimensional interacting systems. This gives accurate results with a very good precision at low temperature. It is useful for finding accurate approximations of the ground state and the low-lying excited states of strongly interacting quantum lattice systems. DMRG has been proved to be successful for bosonic [12–14], fermionic [15] and spin [16,17] systems.

Dimerized BH model. – We employ DMRG method to study one-dimensional (1D) system of interacting bosons in presence of onsite repulsion and hopping dimerization. The basic physics which governs the bosons trapped in optical lattice is the competition between the kinetic energy and the onsite repulsive potential energy.

The kinetic energy can be controlled by laser field modulation. If two counter propagating laser beams of different wavelengths are used, the hopping amplitude can be modulated as weaker and stronger in consecutive sites in a lattice. This is because the laser induced optical trap can be tuned with the wavelengths of the counter propagating laser beams so that they generate deeper and shallower traps in alternate optical lattice sites. For such a dimerization in hopping strengths, while the Hubbard U term localizes the particles in lattice sites, dimerization would lead to an insulating phase. In fact, the dimerization is one reason why no one-dimensional lattice system can be metallic [18]. In one-dimension, for Fermionic systems, the potential energy $\frac{1}{2}kx^2$ from the springs competes with the dimerization. Whether tuning of well depth stabilizes a one-dimensional optical lattice and what would be the effect of dimerization on superfluid to Mott insulator transition have not been studied before.

In this letter, we consider dimerization in hopping integral to describe basic physics associated with such a term. The Bose-Hubbard model with dimerization can be written as

$$H = \sum_i [t + (-1)^{i+1}\delta] (b_i^\dagger b_{i+1} + h.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) \quad (2)$$

where δ is the dimerization parameter which creates hopping strengths $t + \delta$ and $t - \delta$ at alternate sites keeping the total length of the one-dimensional lattice the same. We set $t = 1$ in all our calculations and express energy in units of t .

In DMRG, with open boundary condition, we vary the density matrix cut-off so as to get the converged result. Although, there is no restriction on the maximum number (n) of bosons per site, for computational purpose n has to be truncated at a finite value. We choose $n = 3$, *i.e.*, with 0, 1 and 2 bosons per site. We have checked the convergence of our results with $n = 4$ and 5 also. In literature, estimation of critical point (U_c) for SF to MI transition has been obtained by using different methods. Kühner *et. al.* [14] have used finite-size DMRG with open boundary condition and estimated U_c as 3.37 ± 0.1 by studying the decay of the correlation function. There are also other methods like Bethe Ansatz [19] ($U_c \simeq 3.46$), exact diagonalization and renormalization group [9] ($U_c \simeq 3.29 \pm 0.01$) and Quantum Monte Carlo [20] ($U_c \simeq 3.33 \pm 0.05$) by which the critical point has been estimated.

In this letter, we focus on the δ vs. U phase diagram. The interesting physics which is revealed due to the effect of hopping dimerization, is the appearance of a new phase; bond-wave (BW) phase, coupled with the existence of conventional superfluid and Mott insulator phases. There are many suggestions and examples of supersolid (SS) phases where superfluid order coexists with modulation of the boson density [2, 3, 21]. Our central result points towards existence of a new phase where we find simultaneous presence of superfluid order and modulation of bond kinetic

energy. We can draw an analogy of our model with the Boson-Hubbard model with an additional ‘superlattice’ potential, in which the confining potential has multiple minima [22]. In some recent experiments, the ‘superlattice’ potential has already been implemented [23–25]. Similar to the consequence of dimerization which results in a bond wave order that breaks translation invariance, the superlattice potential likewise causes the formation of a density order pattern which can compete with or coexist with a superfluid phase [22].

In the Fermionic Hubbard model at half-filling, there are examples of coexistence of density wave (DW) with bond-wave phases [26]. In this context, since kinetic energy controls density alternation, its modulation leads to BW phase and in a periodic system, both DW and BW order parameters are equivalent in the momentum space. We find that along the U -line ($\delta = 0$), the phase transition is from superfluid to Mott insulator phase, while along the $\delta=1$ line the superfluid phase vanishes, since the dimerized hopping breaks the optical lattice into disconnected dimers. We also estimate the critical line and the complete phase diagram in the two-dimensional $U - \delta$ parameter space.

Results and Discussions. – To obtain a clear insight into the complete phase diagram in the $U - \delta$ plane, we have calculated ground state energy, excitation gap and various correlation functions. For the well known BH Hamiltonian with $\delta = 0.0$, we find the excitation to be gapless in the superfluid phase, whereas a small gap opens up at the SF to MI transition point as found previously. The critical point, however, can not be solely determined from the gap and since inclusion of δ opens up a dimerized gap, we define an order parameter for the SF phase, the asymptotic value of the quantity $\langle b_i^\dagger b_j \rangle^{1/2}$ as $|i - j| \rightarrow \infty$, and estimate the critical U_c at which this quantity vanishes. For $\delta = 0$, the critical U -value is found to be 3.37 ± 0.1 in agreement with [14].

To bring out the effect of dimerization, we first study bond-wave phase. The bond-wave phase is characterized by the alternating strengths of the expectation value of the kinetic energy operator on the bonds. This quantity, $\langle b_i^\dagger b_{i+1} + h.c. \rangle$, against the bond index, i , is shown in Fig. 1(a) for a range of U values and for $\delta = 0.1$ and $\delta = 0$. As can be seen, for $\delta = 0$, there is equal strength of kinetic energy on each bond, but for finite value of δ , the kinetic energy strength alternates characterizing the BW phase. Interestingly, the alternation is found to be stronger for larger U values. In Fig. 1(b), we plot the thermodynamic stabilization energies per site with respect to the undimerized system against δ for small and large U values. For all the cases, we find that the stabilization energy varies as $A\delta^2$, where A depends on U . The prefactor A turns out to be 0.158, 0.252 and 0.267 for $U = 0.5, 3.0$ and 5.0 respectively. This shows that the stabilization energy gained by the system is of the same power in distortion as the lattice term. Thus, the stabilization is conditional and depends

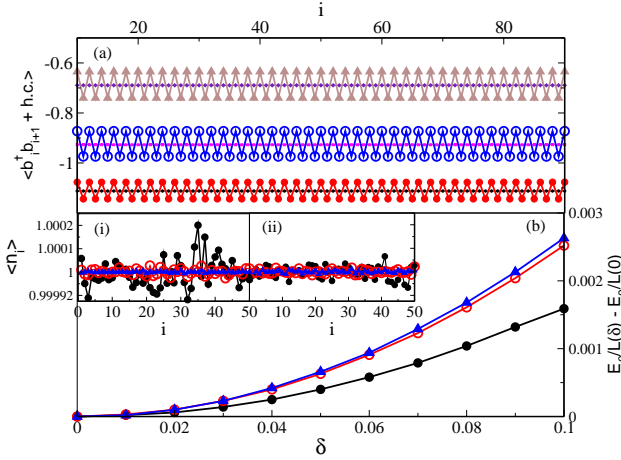


Fig. 1: (color online) (a) Plot of expectation values of kinetic energy operator against the bond index for $\delta = 0.1$ and $U = 0.5$ (filled circle), 3.0 (open circle) and 5.0 (triangle). The points along the middle of each present the same for $\delta = 0$. (b) Variation of stabilization energy against δ for $U = 0.5$ (filled circle), 3.0 (open circle) and 5.0 (triangle). The points are joined by lines to guide the eye. Inset: Plot of local density against the site index (i) for (i) $\delta = 0.0$ and (ii) $\delta = 0.5$. In each case the U values are 0.5 (filled circle), 3.0 (open circle) and 5.0 (triangle).

crucially on the width of the optical trap potential. Moreover, for a particular value of δ , the stabilization energy is more for larger U values. The SF phase is characterized by fluctuations in particle numbers, while in MI phase, in a given site, the particle number is fixed as it becomes energetically costly for the particle to hop. To understand such a variation, we plot the local density, $\langle n_i \rangle$, as a function of lattice site in the inset (of Fig. 1(b)) for small and large U values and for two different δ s. As can be seen, when the system is in SF phase, it is easier for the bosons to hop between sites, hence there is a large fluctuation of this quantity. On contrary, in MI phase the bosons are localized and so the fluctuation in $\langle b_i^\dagger b_i \rangle$ reduces with increase in correlation strength. It is also interesting to note that with increase in dimerization strength, the particle number fluctuations reduce considerably, giving an indication that even δ drives the system out of SF phase.

The other quantity that varies considerably near the SF to MI phase transition is the extent to which the lattice sites are correlated. Whether dimerization also reduces the correlation length, we study the hopping correlation function, $\langle b_0^\dagger b_r \rangle$, with the distance $r = |i - j|$ for a range of values in the $U - \delta$ plane. For three U values, we plot $\langle b_0^\dagger b_r \rangle$ for the undistorted as well for system with increasing dimerization in Fig. 2. As can be seen, when the system is in superfluid phase, *i.e.*, for small U , the correlation function shows a quasi long range order. In this regime, the decay of the correlation function obeys a power law behavior $\sim r^{-K/2}$ (K is the Luttinger liquid parameter). In SF phase we find $K \geq 2$. As it is clear from

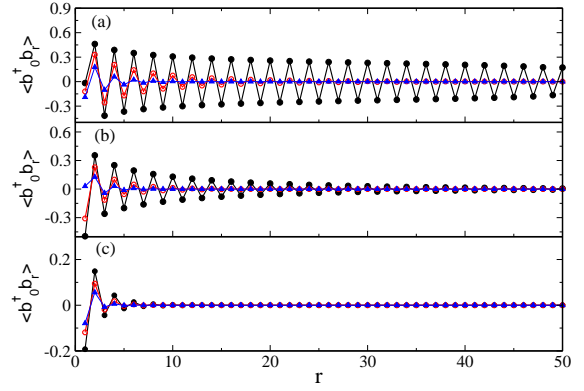


Fig. 2: (color online) Plot of hopping correlation function against $r = |i - j|$ for (a) $\delta = 0.0$ (b) $\delta = 0.5$ and (c) $\delta = 0.8$. In each case the U values are 0.5 (filled circle), 3.0 (open circle) and 5.0 (triangle).

the figure, with increase in onsite repulsion, *i.e.*, when the system transits to the MI phase, the decay of the correlation function becomes faster. In MI phase, the particles are pinned at each lattice sites, so the ordering becomes short ranged. We find that in MI phase, the decay of the correlation function is exponential, which is given by $e^{-r/\xi}$; ξ being the correlation length. For $U = 5.0$, this ξ comes out to be 2.38, 2.35, 2.34, 2.10, 1.68 and 1.46 for $\delta = 0.0, 0.05, 0.1, 0.3, 0.5$ and 0.7 respectively. So there is a gradual decrease of correlation length with increase in dimerization. It is to be noted that with increase in dimerization, the decay of the correlation function becomes faster and in Fig. 2(c) even for $U = 0.5$, the decay of the correlation function is exponential. Thus, as the system becomes more dimerized, the SF to MI transition occurs at smaller U value. Note that, for nonzero δ value, both the SF and MI phases coexist with BW order, since nonzero δ inherently introduces bond energy fluctuations.

In Fig. 3 we present the asymptotic value of the order parameter, $\langle b_i^\dagger b_j \rangle^{1/2}$, against U for different δ values. In all cases the order parameter vanishes (attains $\sim 10^{-9}$) at some critical U values. The critical points have been determined through opening up of the excitation gap, density fluctuations data and estimation of correlation length. However, the error in estimating the critical points can be minimized if we determine the transition points where the asymptotic ($|i - j| \rightarrow \infty$) value of $\langle b_i^\dagger b_j \rangle^{1/2}$ vanishes. In all cases, the critical U value deviates of the order of ± 0.1 . We find that with increase in δ , the order parameter vanishes at a smaller U -value.

In Fig. 4, we present the δ vs. U phase diagram. The critical line is shown with a width which corresponds to the uncertainties in determining the critical U values. The phase diagram shows that as the system becomes more dimerized the critical point shifts to a lower U value. Near the δ -line beyond $\delta = 0.6$ the critical values of U becomes very small to determine. Infact, there exists an

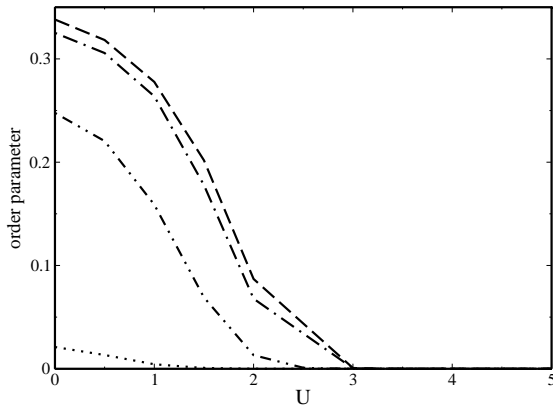


Fig. 3: Plot of superfluid order parameter (asymptotic value of $\langle b_i^\dagger b_j \rangle^{1/2}$ such that $|i - j| \rightarrow \infty$) against U for $\delta = 0.0$ (dashed line), 0.1 (dashed dotted line), 0.3 (dash dot dot) and 0.5 (dotted line).

extremely narrow region beyond $\delta > 0.6$ where superfluid and bond-wave phase coexist and the phase boundary touches asymptotically the point $\delta = 1$. In fact, along $\delta=1$ line, the system essentially breaks into disconnected dimers and the superfluid phase ceases to exist. It should be mentioned clearly here that at $U = 0$ and $\delta = 1$ (marked by a star to avoid confusion with the filled circles which correspond to critical point for transition) there is no phase transition, as along $\delta=1$ line the system consists of dimers only. The underlying physics is quite simple. The correlation length or the characteristic length of the system decreases as we increase δ as the bond strength alternates. Beyond $\delta = 0.6$, the correlation length becomes too small to even estimate. If we consider a dimer (correlation length is smaller than 1), it corresponds to $\delta = 1.0$ in the Hamiltonian. For unit filling, the matrix eigen values are U , $\frac{U - \sqrt{32 + U^2}}{2}$ and $\frac{U + \sqrt{32 + U^2}}{2}$. Expanding the lowest excitation gap for small U gives an estimate of $\frac{U}{2} + 2\sqrt{2} + \frac{\sqrt{2}U^2}{32}$ as the gap value. Thus even for $U = 0.0$, there is a finite gap (for a dimer) which prevents SF phase to exist. In fact, beyond $\delta = 0.6$, the correlation length becomes so small that even a small (but finite) U can drive the system to an insulating phase. In the phase diagram, the $\delta = 0$ line (broken line) corresponds to pure SF phase below the critical point and above U_c , it corresponds to pure MI phase. However, for non-zero value of δ , the phase transition is from superfluid-bond-wave (SF-BW) phase to Mott insulator-bond-wave (MI-BW) phase. The main point is that dimerization reduces the correlation length which in turn destabilizes the SF phase. Note that, in this sense both the many-body repulsion and dimerization in kinetic energy drive the system into insulating phase.

Conclusion. – In conclusion, we have studied the δ - U phase diagram of a system of bosons in a one-dimensional optical lattice by density matrix renormalization group method. Our investigation reveals the existence of a new phase, where superfluid phase coexists with bond-

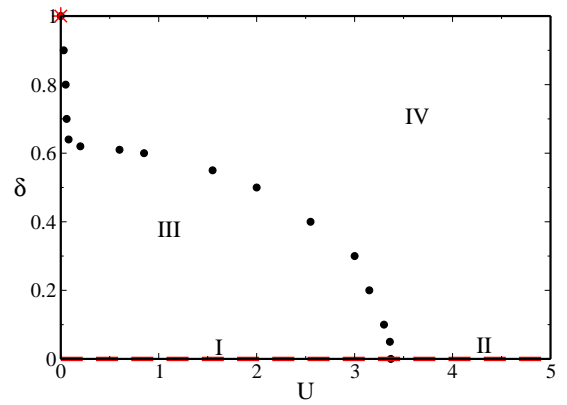


Fig. 4: (color online) Phase diagram of δ vs. U . The $\delta = 0$ line (broken line) corresponds to SF to MI transition only. The different phases are (I) pure SF phase, (II) pure MI phase (along the $\delta = 0$ line), (III) SF-BW phase and (IV) MI-BW phase.

wave phase due to the effect of dimerization in hopping strengths. We have observed two types of phase transitions: conventional superfluid to Mott insulator phase and superfluid-bond-wave to Mott insulator-bond wave phase. We have also calculated the critical point at which the transitions occur. However, note that in our model the bond-wave symmetry breaking is imposed “externally” by the Hamiltonian itself. Whether any new phase will appear due to the effect of next nearest neighbor hopping is currently under study.

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