Phase separation in a two species Bose mixture

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We study the ground state quantum phase diagram for a two species Bose mixture in a one-dimensional optical lattice using the finite size density matrix renormalization group(FSDMRG) method. We discuss our results for different combinations of inter and intra species interaction strengths with commensurate and incommensurate fillings of the bosons. The phases we have obtained are superfluid, Mott insulator and a novel phase separation, where different species reside in spatially separate regions. The spatially separated phase is further classified into phase separated superfluid(PS-SF) and Mott insulator(PS-MI). The phase separation appears for all the fillings we have considered, whenever the inter-species interaction is slightly larger than the intra-species interactions.

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Studies of quantum phase transitions are currently of great interest as they provide important insights into a wide variety of many-body systems [1, 2]. The pioneering observation of the superfluid (SF) to Mott insulator (MI) transition in an optical lattice using cold bosonic atoms [3], which had been predicted by Jaksch et. al. [4], highlights the exquisite control of the inter atomic interactions that is possible in such systems. In that experiment, performed using ^{87}Rb atoms, the tunneling of the atoms to neighboring sites and also the strength of the on-site interactions was controlled by tuning and/or detuning the laser intensity in order to achieve the transition from the SF phase(random distribution of atoms) to MI phase where there are a fixed number of atoms per site [3]. Recent developments involving the manipulation of ultracold atoms have led to the realization of genuine one dimensional systems such as the Tonks-Girardeau gas [5]. Several interesting phenomena including the SF-MI transition have been observed in a one-dimensional optical lattices [6].

In the past few years, on the theoretical side, many investigations have been carried out using a single species of bosonic atoms in optical lattices [7, 8]. Recently cold bosonic mixtures [9], fermions [10] and Bose-Fermi mixtures [11, 12] in optical lattices have attracted much attention. Mixtures of different species are very interesting since additional phases could appear due to the inter-species interactions [13, 14].

In this Letter, we consider a system with two species of bosonic atoms or equivalently, bosonic atoms with two relevant internal states. The two species shall be called a and b type respectively. The low-energy Hamiltonian is then given by the Bose-Hubbard model for the two boson species:

$$\begin{aligned} H &= -t^a \sum_{<i,j>} (a_i^\dagger a_j + h.c) - t^b \sum_{<i,j>} (b_i^\dagger b_j + h.c) \\ &+ \frac{U^a}{2} \sum_i n_i^a (n_i^a - 1) + \frac{U^b}{2} \sum_i n_i^b (n_i^b - 1) \\ &+ U^{ab} \sum_i n_i^a n_i^b. \end{aligned} \quad (1)$$

Here a_i (b_i) is bosonic annihilation operator for bosonic atoms of a (b) type localized on site i. $n_i^a = a_i^\dagger a_i$ and $n_i^b = b_i^\dagger b_i$ are the number operators. t^a (t^b) and U^a (U^b) are the hopping amplitudes between adjacent sites $\langle ij \rangle$ and the on-site repulsive energies, respectively for a (b) type of atom. The inter-species interaction is given by U^{ab}. In this work we consider inter-exchange symmetry $a \longleftrightarrow b$, implying $t^a = t^b = t$ and $U^a = U^b = U$ and study the effect of inter-species interaction using finite size density matrix renormalization group(FSDMRG) method[15]. We set our energy scale by $t = 1$.

The model (1) has been studied earlier using the Monte-Carlo [13] and the Bosonization methods [14] and this has resulted in the prediction of the basic structure of its ground state phase diagram. The Bosonization study predicts phase separation (PS) for large values of the inter-species interaction U^{ab} by considering one species of bosons to be hard core and the other to be in the intermediate to hard core regime [14]. Phase separation is also seen using a variational method based on the multi orbital best mean field ansatz [16]. However, a clear picture of the transitions pertaining to the SF, MI and PS phases has not emerged so far. In order to achieve this, we consider the influence of the inter-species interaction U^{ab} on these phases, by carrying out a systematic study of its effect on the ground state of model (1) in one-dimension using the finite size density matrix renormalization method [8, 15]. This method is very well suited for performing studies in one-dimensional

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lattice systems [17]. It involves the iterative diagonalization of a Hamiltonian in a restricted Hilbert Space to obtain the wavefunction and the energy of a particular state (target state) of a many-body system. The size of this space is determined by an appropriate number of eigenvalues and eigenvectors of the density matrix.

Before proceeding further we give a brief summary of our results. The various parameters that we calculate to study the ground state properties of model (1) are the energy gap G_L, which is the difference between the energies needed to add and remove one atom from a system of atoms,i.e.,

$$G_L = E_L(N_a+1, N_b) + E_L(N_a-1, N_b) - 2E_L(N_a, N_b) \quad (2)$$

and the on-site density correlation function

$$\langle n_i^\alpha \rangle = \langle \psi_{0LN_aN_b} | n_i^\alpha | \psi_{0LN_aN_b} \rangle. \quad (3)$$

Here α, is an index representing type a or b bosons, $E_L(N_a, N_b)$ is the ground-state energy for a system of size L with N_a (N_b) number of a (b) type bosons and $|\psi_{0LN_aN_b}\rangle$ is the corresponding ground-state wavefunction, which are obtained from the FSDMRG method [18]. Defining the ratio of inter and intra species interaction $\Delta = U^{ab}/U$, we study the ground state of model (1) for $\Delta < 1$ and $\Delta > 1$. The ground state exhibits some similarities as well as differences when $\Delta < 1$ and $\Delta > 1$. When the kinetic energy is the dominant term in the model, the ground state is in 2SF (both a and b species are in the SF phase) state for all Δ. This similarity is, however, lost when the interactions dominates. For $\Delta < 1$, i.e., $U^{ab} < U$, the large U phase is Mott insulator with non-zero energy gap in the ground state. This state has an uniform local density of bosons for each species, i.e., $\langle n_i^a \rangle = \langle n_i^b \rangle$ for all i. The 2SF to MI transition is possible only when the total density $\rho = \rho_a + \rho_b$ is an integer. Since we have chosen $U^{ab} \sim U$ in this work ($\Delta = 0.95$ and 1.05), the 2SF-MI transition for model (1) is similar to SF-MI transition for single species bosons with the same density of bosons. For $\Delta > 1$ and for small values of U, the ground state is a 2SF state. However, when U increases, the ground state first goes into superfluid phase with a and b bosons spatially separated into different regions of the lattice. This is the case when $\rho_a = \rho_b = 1/2$. This phase may be called the phase separated superfluid(PS-SF). There is no gap in the ground state energy spectrum and the phase separation order parameter defined as

$$O_{PS} = \frac{1}{L} \sum_i \langle \psi_{0LN_aN_b} | (|n_i^a - n_i^b|) | \psi_{0LN_aN_b} \rangle. \quad (4)$$

is non-zero. A further increase in U results in opening up of the gap in the energy spectrum. This Mott insulator has a non-zero phase separation order parameter and it may be called the phase separated Mott-Insulator(PS-MI). The total local density $\langle n_i \rangle (= \langle (n_i^a + n_i^b) \rangle) = \rho$ remain uniform across the lattice. When the densities are different, for example $\rho_a = 1$, $\rho_b = 1/2$, no PS-MI is found and the ground state has only 2SF and PS-SF phases. When $\rho_a = 1$, $\rho_b = 1$ we find, for the $\Delta = 1.05$, no PS-SF phase and the transition is directly from 2SF to PS-MI. We now discuss the details of the present work.

In $d = 1$, the appearance of the MI phase is signaled by the opening up of the gap $G_{L\to\infty}$. However, G_L is finite for finite systems and we must extrapolate to the $L \to \infty$ limit, which is best done by using finite-size scaling [8]. In the critical region, i.e., SF region, the gap

$$G_L \approx L^{-1} f(L/\xi), \quad (5)$$

where the scaling function $f(x) \sim x$, $x \to 0$ and ξ is the correlation length. $\xi \to \infty$ in the SF region. Thus plots of LG_L versus U, for different system sizes L, consist of curves that intersect at the critical point at which the correlation length for $L = \infty$ diverges and gap G_∞ vanishes.

In the absence of the inter-species interaction U^{ab}, the ground state of model (1) is a simple independent mixture of the individual species of bosons. In order to investigate the influence of U^{ab} on its ground state, we consider two cases $\Delta = 0.95$ and 1.05. In each of these two cases, we consider three different ranges of densities.

(i)$\rho_a = \rho_b = 1/2$:

It should be noted that in the single species model with only the on-site interaction, the MI phase is possible only for integer densities. Thus when $\rho_a = \rho_b = 1/2$, the MI phase is absent when $U^{ab} = 0$ and the model (1) will have only SF phase. Figure (1) shows a plot of scaling of gap LG_L versus U for $\Delta = 0.95$. Curves for different values of L coalesce for $U \le U_c \simeq 3.4$ indicates a MI phase for $U > U_c$. The emergence of MI phase here is due to the combined interactions of both species of bosons, i.e., U and U^{ab}. The fact that $U_c \simeq 3.4$, indicates that the model (1) when $\Delta \approx 1$ behaves like a single species Bose-Hubbard model at density 1. These results are in the expected lines because, when $U^{ab} \approx U$, every boson in the system interact with all the other bosons, irrespective of whether they are of a or b types, with the same strength and therefore species index become irrelevant. However, the situation changes when the inter-species interaction $U^{ab} > U$. The on-site densities $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ are plotted in Fig. (2) for $\Delta = 1.05$ clearly demonstrates a spatial separation between a and b species of bosons for $U = 4$ and no spatial separation for $U = 1$. This reveals a Phase Separation (PS) transition as a function of U. The question then arises whether this spatially separated phase is superfluid or Mott Insulator. In order to sort this out, we plot both the scaling of the gap LG_L and the order parameter O_{PS} for phase separation in Fig. (3). It is evident that the phase transition to MI happens at around $U_c \simeq 3.4$ while that to spatially separated phase is around $U_c \simeq 1.3$. The gap remains zero for $1.3 < U < 3.4$. Thus for the case $\rho_a = \rho_b = 1/2$ and

$\Delta = 1.05$, there are three phases: the superfluid phase (2SF) for $U < 1.3$, superfluid, but phase separated (PS-SF) for $1.3 < U < 3.4$ and finally Mott Insulator, but again phase separated (PS-MI) for $U > 3.4$. The range of U for each phase, however, will depend on the value of Δ. The detailed phase diagram in the $\Delta - U$ plane and the nature of different phase transitions will be reported elsewhere.

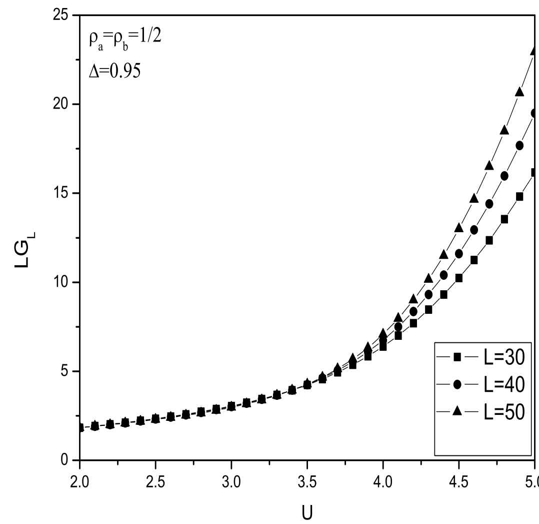

FIG. 1: Scaling of gap LG_L is plotted as a function of U for different system sizes for $\Delta = 0.95$. The coalescence of different curve for $U \simeq 3.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

(ii)$\rho_a = 1, \rho_b = 1/2$:
In this case, when $U^{ab} = 0$ the species a has a superfluid to Mott insulator transition at $U_c \simeq 3.4$ by virtue of having density one, while the b species, having density 1/2, remain in the superfluid phase. However, when $U^{ab} \sim U$, no transition from SF to MI was found for either of the two species. In the Fig. (4(a)), we plot the length dependence of gap G_L for different U, which clearly indicates that the gap vanishes at $L \to \infty$. This emphasizes the fact that as far as transition to the Mott insulator is concerned, when $U^{ab} \sim U$, it is the total density that matters, which has to be an integer irrespective of the densities of the individual species of bosons.

The phase separation, however, happens when $U^{ab} > U$. The local density distribution of different species of bosons are given in Fig. (4(b)) for $U = 1$, 4 and $\Delta = 1.05$. For $U = 1$, we find no phase separation. However, for $U = 4$, the a and b species bosons are phase separated. They rearrange in such a manner that the average total density remains a constant. For example, when $\rho_a = 1$ and $\rho_b = 1/2$, one-third of the region is occupied by the b species and two-third by the a species. The total density being 3/2, the distribution of the a and b species

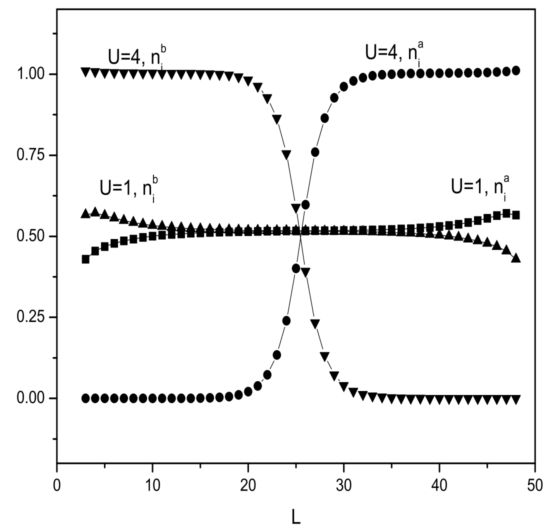

FIG. 2: Plots of $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ versus i for $U = 1$ and $U = 4$. These plots are for $\rho_a = \rho_b = 1/2$, $\Delta = 0.95$ and for system size $L = 50$. The deviation in $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ near the boundaries for $U = 1$ is due to the open boundary condition used in our FSDMRG

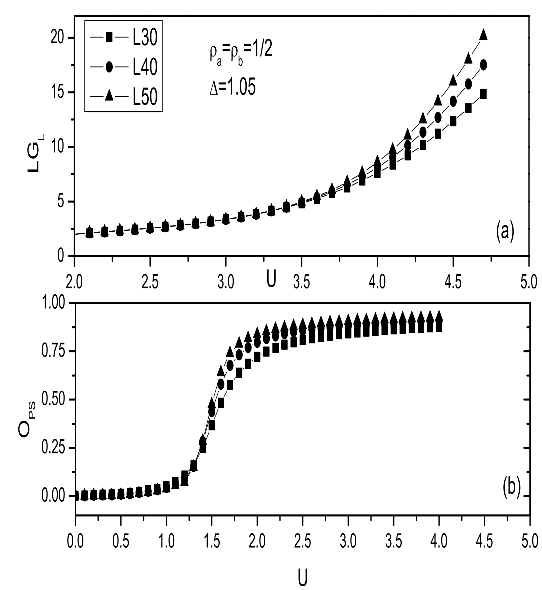

FIG. 3: Plots of LG_L (a) and O_{PS} (b) versus U demonstrate various phases in the case $\rho_a = \rho_b = 1/2$ and $\Delta = 1.05$.

of bosons follow the ratio of their densities.

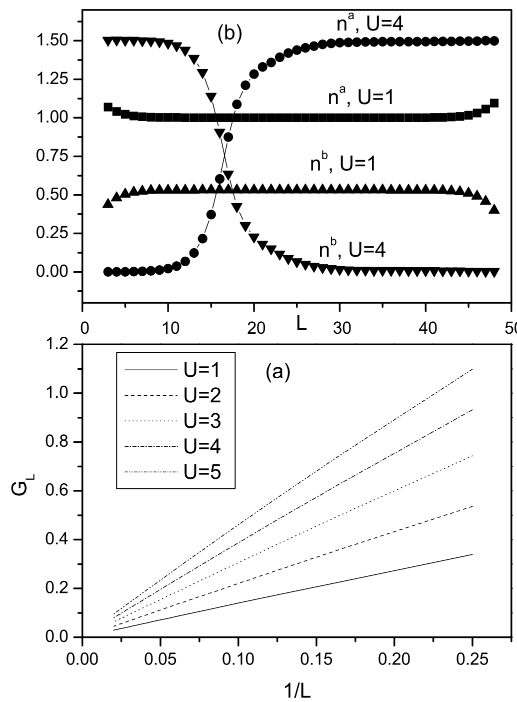

FIG. 4: (a)Plots of gap G_L versus $1/L$ for different values of U. The gap goes to zero linearly when $L \to \infty$ for all the values of U considered. Here $\rho_a = 1$, $\rho_b = 1/2$ and $\Delta = 1.05$. (b) Local density distribution $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ for the same case but for two different $U = 1, 4$.

(iii)$\rho_a = 1, \rho_b = 1$:
We now consider a double commensurate case where both the species of bosons undergo SF to MI phase transition in the absence of U^{ab} (for $\rho_a = \rho_b = 1$, $U_c \sim 3.4$). In Fig. (5(a)), we plot the scaling of the gap LG_L for $\Delta = 1.05$. It is clear from these figures and from a similar one for $\Delta = 0.95$ that for $U^{ab} \sim U$, the transition from SF to MI occurs at a much higher value of $U \sim 5.7$, which corresponds to the SF-MI transition in single Bose-Hubbard model for $\rho = 2$. This is consistent to what we had observed in the earlier cases also. For $U^{ab} \sim U$, the superfluid to Mott Insulator transition is due to the collective intra and inter species interactions. The phase separation transition, however, occurs for $\Delta > 1$ as given in the Fig. (5(b)). In this case the transitions to phase separation and to the Mott insulator occur around same $U_c \sim 5.7$. In other words we did not find a PS-SF phase sandwiched between 2SF and PS-MI for this case.

Finally from these three cases discussed here, the following conclusions can be drawn. For the values of the interaction strengths and the densities considered here, we obtain several phases: 2SF, MI, PS-SF and PS-MI. For $U^{ab} \leq U$, the Mott Insulator phase is possible only when the total density is an integer. The superfluid to Mott Insulator transition in model (1) is then similar to the single species Bose-Hubbard model with the same total density. The deviation from this behavior, however, occurs for $U^{ab} > U$, where we observe a phase separation. The Mott insulator phase is then phase separated. In the case of $\rho_a = \rho_b = 1/2$, we observe a phase separated superfluid PS-SF sandwiched between 2SF and PS-MI. However, for $\rho_a = \rho_b = 1$, no SF-PS was found and the transition is directly from 2SF to MI-PS. It would indeed be worthwhile to devise experiments to test our findings.

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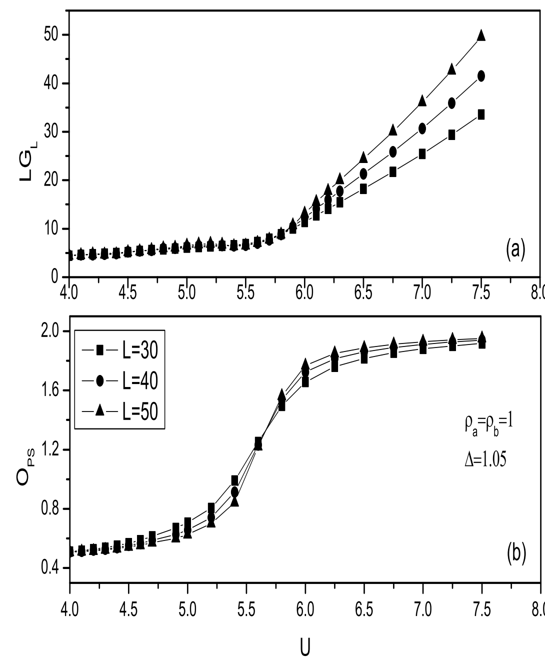

FIG. 5: Plots of LG_L (a) and O_{PS} (b) versus U demonstrate various phases in the case of $\rho_a = \rho_b = 1$, $\Delta = 1.05$.

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