Phase separation in a two-species Bose mixture

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We obtain 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 method. We discuss our results for different combinations of inter- and intraspecies interaction strengths with commensurate and incommensurate fillings of the bosons. The phases we have obtained are a superfluid and a Mott insulator, and a phase separation where the two different species reside in spatially separate regions. The spatially separated phase is further classified into phase-separated superfluid and Mott insulator. The phase separation appears for all the fillings we have considered, whenever the interspecies interaction is slightly larger than the intraspecies interactions.

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I. INTRODUCTION

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 interatomic 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 were controlled by tuning and/or detuning the laser intensity in order to achieve the transition from the SF phase (random distribution of atoms) to the 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 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 interspecies interactions [13,14].

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

$$H = - t^a \sum_{\langle i,j\rangle} (a_i^\dagger a_j + \text{H.c.}) - t^b \sum_{\langle i,j\rangle} (b_i^\dagger b_j + \text{H.c.}) + \frac{U}{2}^a \sum_i n_i^a(n_i^a - 1) + \frac{U}{2}^b \sum_i n_i^b(n_i^b - 1) + U^{ab} \sum_i n_i^a n_i^b . \quad (1)$$

Here a_i (b_i) is the 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 intraspecies repulsive energies, respectively, for the a (b) type of atom. The interspecies interaction is given by U^{ab}. The hopping amplitudes (t^a, t^b) and interaction parameters (U^a, U^b, U^{ab}) are related to the depth of the optical potential, the recoil energy, and the scattering lengths of the atoms. The ratio $U^{ab}/U^{a,b}$ can be controlled to a wide range of values [15] experimentally. In this work we consider interspecies exchange symmetry $a \leftrightarrow b$, implying $t^a = t^b = t$ and $U^a = U^b = U$ and study the effect of interspecies interaction on the ground state of model (1) in one dimension. We set our energy scale by $t=1$.

The model (1) is not exactly solvable even in one dimension, and one must therefore use a numerical or an approximate method to obtain its ground-state wave function and energy, which are needed for studies on quantum phase transitions. The model (1) has been studied earlier using Monte Carlo simulations [13], bosonization methods [14], and the mean-field theory [15]. These studies have resulted in the prediction of the basic structure of the ground-state phase diagram, which consist of 2SF (both a and b type bosons in the SF phase), SF+MI (a boson in the SF and b in the MI phase, or vice versa) and 2MI (both a and b bosons in the MI phase). In addition to these phases Kuklov *et al.* [13] predict a superfluid counterflow (SCF) phase for $U^{ab} > 0$. The bosonization study predicts phase separation for large values of the interspecies 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 has also been found using a variational method based on the

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multiorbital best mean-field ansatz [16]. Unlike in the case of fermions, phase-separated bosons can form a superfluid or Mott insulator. The exact nature of the ground state of the phase-separated phase has not been discussed before to our knowledge. In order to obtain a clear picture of the transitions pertaining to the SF, MI, and PS phases, we consider the influence of the interspecies 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 group (FSDMRG) method [8,17]. This method is arguably the best method for the numerical study of one-dimensional lattice systems. The numerical solutions provided by this method will give important insights into the ground state of the model, which can then be used to understand its general features in higher dimensions. The possibility of making a genuine one-dimensional system in an optical lattice makes this problem interesting on its own merits.

The rest of the paper is organized as follows. Section II contains the details of our finite-size density matrix renormalization method. Section III contains our results. We end with concluding remarks in Sec. IV.

II. FSDMRG CALCULATIONS

The finite-size density-matrix renormalization group (FSDMRG) method has proven to be very useful in studies of one-dimensional quantum systems [8,17]. The details of this method are given in a recent review by Schollwöck [18]. The open boundary condition is preferred over the periodic boundary condition for this method because the loss of accuracy, which increases with the size of the system, is much less in the former than the latter. In the conventional FSDMRG method, the lattice is first built to the desired length (L) using the infinite-system density-matrix renormalization method. The finite-size sweeping is done only for this desired lattice size L. We use a slightly modified form of the FSDMRG, where we sweep at every step of the procedure and not just for the case that corresponds to the largest value of L. This enables one to obtain accurate correlation functions. Furthermore, since the superfluid phase in models such as Eq. (1), in $d=1$ and at $T=0$, is critical and has a correlation length that diverges with the system size L, finite-size effects must be eliminated by using finite-size scaling, as we show later. For this purpose, the energies and the correlation functions, obtained from a DMRG calculation, should converge satisfactorily for each system size L. It is important, therefore, that we use the FSDMRG method as opposed to the infinite-system DMRG method, especially in the vicinities of continuous phase transitions.

In the FSDMRG method, the bases used for left- and right-block Hamiltonians are truncated by neglecting the eigenstates of the density matrix corresponding to small eigenvalues, which leads to truncation errors. If we retain M states, the density-matrix weight of the discarded states is $P_M=\Sigma_{\alpha=1}^{M}(1-\omega_\alpha)$, where ω_α are the eigenvalues of density matrix. P_M provides a convenient measure of the truncation errors. We find that these errors depend on the order parameter and correlation length for a given phase. For a fixed M, we find very small truncation errors in the gapped phase and the truncation errors are largest for the SF phase. In our calculations we choose M such that the truncation error is always less than 5×10^{-5} and we find that $M=128$ suffices.

The number of possible states per site in the model (1) is infinite, since there can be any number of a and b species bosons on a site. In a practical FSDMRG calculation we must truncate the number of states n_{max} allowed per site. The value of n_{max}, of course, will depend on the on-site interaction U. The smaller the value of U the larger must be n_{max}. From our earlier calculation [8] on related models, we find that $n_{max}=4$ is sufficient for the value of U considered here. This implies, for model (1), four states each per site for a and b species bosons and a total of 16 states per site. This corresponds to a truncation of bases of the left (right) block from $16M$ to M in each FSDMRG iteration.

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) a (b) type bosons, and $|\psi_{0LN_aN_b}\rangle$ is the corresponding ground-state wave function, obtained by the FSDMRG method. 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., the SF region, the gap

$$G_L \approx L^{-1} f(L/\xi), \quad (4)$$

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.

Defining the ratio of inter- and intraspecies interactions $\Delta=U^{ab}/U$, we study the ground state of model (1) for $\Delta<1$, $\Delta=1$, and $\Delta>1$. The ground state exhibits some similarities as well as differences in each of the cases. When the kinetic energy is the dominant term in the model, the ground state is in the 2SF (both a and b species are in the SF phase) state for all Δ. This similarity is, however, lost when the interactions dominate. For $\Delta\le 1$, i.e., $U^{ab}\le U$, the large-U phase is the Mott insulator with nonzero energy gap in the ground state. This state has a 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. For $U^{ab}\sim U$, the 2SF-MI transition for model (1) is similar to the 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 the 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 (PSSF). There is no gap in the ground-state energy spectrum and the phase separation order parameter defined as

$$O_{PS}=\frac{1}{L}\sum_i \langle\psi_{0LN_aN_b}|(|n_i^a-n_i^b|)|\psi_{0LN_aN_b}\rangle \qquad (5)$$

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

III. RESULTS AND DISCUSSION

In the absence of the interspecies interaction U^{ab}, model (1) is an independent mixture of the individual species of bosons. So the nature of the ground state of model (1) depends only on the densities of the individual species of bosons: ρ_a, ρ_b, and U $(=U^a=U^b)$, the on-site interactions. For example, if $\rho_a\neq n$, $\rho_b\neq n$, where n is an integer, the ground state is always in the superfluid phase irrespective of the strength of the on-site interaction U. The Mott insulator is possible only when either $\rho_a=n$ or $\rho_b=n$. Based on the values of ρ_a, ρ_b, and U, the ground state is categorized as 2SF (both a and b type bosons in the SF phase), SF+MI (a boson in the SF and b in the MI phase, or vice versa), or 2MI (both a and b bosons in the MI phase). For $\rho_a\neq n$, $\rho_b\neq n$, or for any values of ρ_a, ρ_b with $U<U_c$, where U_c is the critical on-site interaction for the SF to MI transition, the ground state is always in the 2SF phase. The SF+MI phase is possible for $\rho_a\neq n$, $\rho_b=n$ (or vice versa), and $U>U_c$. If both $\rho_a=\rho_b=n$ and $U>U_C$, we have the 2MI phase. In order to investigate the influence of U^{ab} on these ground states, we consider three cases: $\Delta<1$, $\Delta=1$, and $\Delta>1$, where $\Delta=U^{ab}/U$. In each of these three cases, we consider three different ranges of densities: (i) $\rho_a=\rho_b=1/2$, (ii) $\rho_a=1,\rho_b=1/2$, and (iii) $\rho_a=\rho_b=1$. The choices of these three cases are made to understand the effect of the interspecies interaction on the 2SF, SF+MI, and 2MI phases. We now discuss each case below.

A. $\rho_a=\rho_b=1/2$

As discussed in the previous paragraph, for this case, there is no MI phase if $U^{ab}=0$ and the model (1) has only the 2SF phase. However, with the introduction of interspecies interaction, the 2SF phase is destroyed. For example, Fig. 1 shows a plot of the scaling of the gap LG_L versus U for $\Delta=1$. Curves for different values of L coalesce for $U\leq U_c\simeq 3.4$, indicating a gapped MI phase for $U>U_c$. The emergence of this phase is due to the intraspecies as well as interspecies interaction strengths. The fact that $U_c\simeq 3.4$ indicates that the model (1) when $\Delta=1$ behaves like a single species of bosons at unit density [8]. These results are along the expected lines because, when $U^{ab}=U$, every boson in the system interacts with the rest of the bosons, irrespective of whether they are of type a or b, with the same strength, and therefore the species index becomes irrelevant. However, the situation changes when the interspecies interaction $U^{ab}\neq U$.

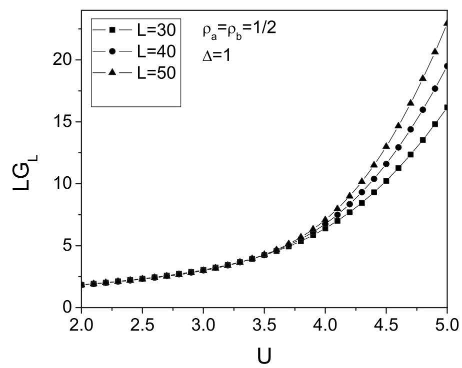

FIG. 1. Scaling of gap LG_L is plotted as a function of U for different system sizes for $\rho_a=\rho_b=1/2$, $\Delta=1$. The coalescence of the different curves for $U\leq 3.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition. This transition is similar to the SF-MI transition for the single-species Bose-Hubbard model for $\rho=1$ [8].

For $\Delta<1$, i.e., $U^{ab}<U$, the system still undergoes the 2SF-MI transition when the on-site repulsion increases, but with a higher U_c. For example Fig. 2 shows a plot of scaling of the gap LG_L versus U for $\Delta=0.5$. The critical $U_c(\Delta=0.5)\sim 5.4$ is substantially greater than $U_c(\Delta=1)\sim 3.4$. The ground state of the model (1) for $\rho_a=\rho_b=1/2$, $\Delta<1$ consists only of 2SF and MI phases. The transition from 2SF to MI is of Kosterlitz-Thouless type.

Kuklov *et al.* [13] predict the possibility of a superfluid counterflow phase in addition to 2SF, SF+MI, and MI+MI phases for $U^{ab}>0$. The superfluid order parameters $\langle\psi_a\rangle$ and $\langle\psi_b\rangle$ are zero in the SCF ground state but $\langle\psi_a\psi_b^\dagger\rangle\neq 0$. This suggests a finite gap for a and b bosons in their energy spectrum, but no gap when flipping an a boson into a b boson. The MI phase that we predict has this property, and would

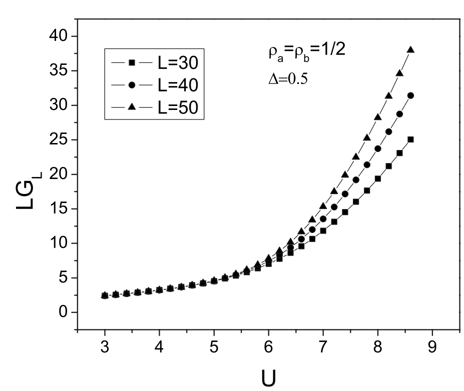

FIG. 2. Scaling of gap LG_L is plotted as a function of U for different system sizes for $\rho_a=\rho_b=1/2$, $\Delta=0.5$. The coalescence of different curves for $U\simeq 5.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

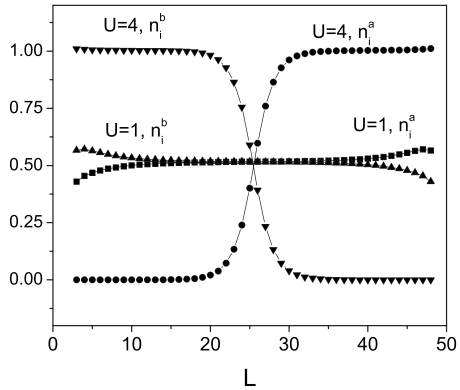

FIG. 3. $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ versus i for $U=1$ and 4. These plots are for $\rho_a=\rho_b=1/2$, $\Delta=1.05$, and for system size $L=50$. The deviation in $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ near the boundaries for $U=1$ is due to the open boundary condition used in our FSDMRG calculations.

correspond to a SCF. However, we would prefer calling it a MI for the following reason. The two-boson mixture model can be generalized to multiboson mixtures and the Mott insulator phase is possible whenever the total density of bosons equals an integer. Consider a three-boson mixture, where the 3SF to MI transition is possible when the density of individual bosons equals 1/3 and the on-site interaction $U > U_c \sim 3.4$. Cancellation of the superfluidity by the counterflow as discussed in Ref. [13] is not clearly explained in this case. So we prefer to call this phase a Mott insulator. Moreover we extend this study to understand the possibility of phase separation as discussed below.

When $\Delta > 1$, the scenario is drastically different from the one seen above. The on-site densities $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ are plotted in Fig. 3 for $\Delta=1.05$. It is clear from this figure that there is a spatial separation between the two different species of bosons for $U=4$ and no spatial separation for $U=1$. This highlights a phase separation transition as a function of U. The question then arises whether this spatially separated phase is a superfluid or a 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. 4. It is evident from these figures that the transition to the MI phase happens

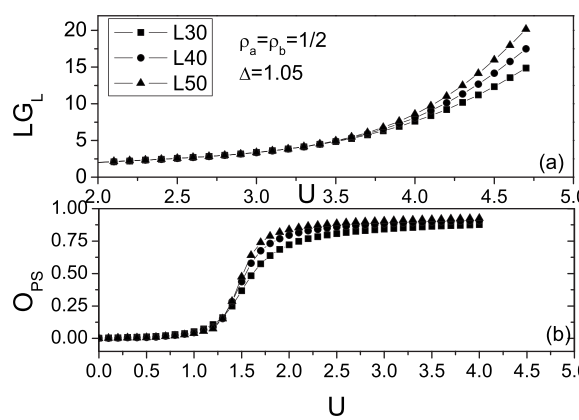

FIG. 4. Scaling of gap LG_L (a) and order parameter for phase separation O_{PS} (b) versus U demonstrating various phases for the case $\rho_a=\rho_b=1/2$ and $\Delta=1.05$.

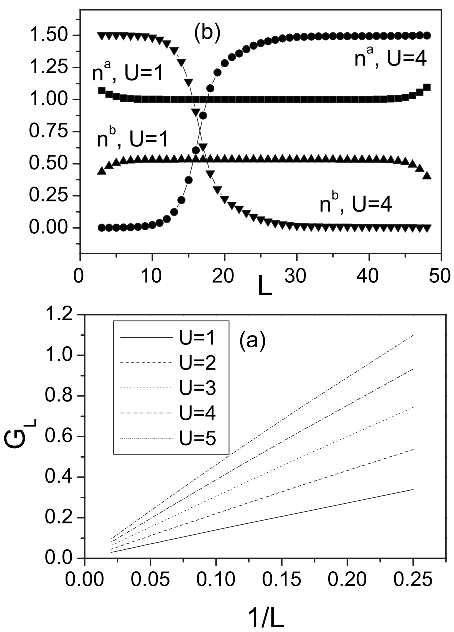

FIG. 5. (a) Gap G_L versus $1/L$ for different values of U. The gap goes to zero linearly when $L \to \infty$ for all the values of U considered. Here $\rho_a=1$, $\rho_b=1/2$, and $\Delta=0.95$. (b) Local density distribution $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ for $\rho_a=1$, $\rho_b=1/2$, and $\Delta=1.05$ for two different $U=1,4$.

at around $U_c \simeq 3.4$ and to the spatially separated phase 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 for $1.3<U<3.4$, and finally Mott insulator, but again phase separated for $U>3.4$. It should be noted that the total density of bosons $\rho=\rho_a+\rho_b$ remain constant through out the lattice, though bosons are space separated. The critical values of the 2SF to PSSF and PSSF to PSMI transitions depend on the value of Δ. The detailed phase diagram in the Δ-U plane and the nature of the different phase transitions will be reported elsewhere.

The bosonization method [14] has predicted phase separation for model (1). The authors have considered the hard-core limit for both species of bosons, or one of them in the hard-core limit while the other is in the intermediate- to hard-core limit, and predicted phase separation. In this work we have considered soft-core bosons where U is finite. It should be noted that phase separation is possible only when $U^{ab} > U$. So no phase separation should be seen for the hard-core bosons because in this limit $U^{ab} < U$.

B. $\rho_a=1, \rho_b=1/2$

In this case, when $U^{ab}=0$ species a bosons undergo a superfluid to Mott insulator transition at $U_c \simeq 3.4$ by virtue of having density $\rho_a=1$, while the b bosons, which have density $\rho_b=1/2$, remains in the superfluid phase. However, when $U^{ab} \leq U$, no transition from the SF to MI phase was found for either of the two species of bosons. The Mott insulator phase of the a bosons is completely lost. In the Fig. 5(a), we plot the length dependence of the gap G_L for different U,

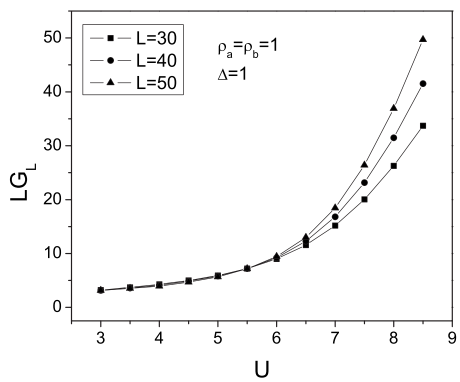

FIG. 6. Scaling of gap LG_L as a function of U for different system sizes for $\rho_a=\rho_b=1$ and $\Delta=1.0$. The coalescence of different curves for $U\simeq 5.7$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

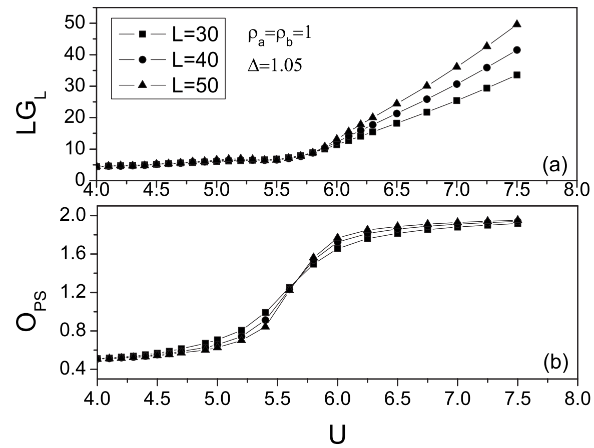

FIG. 7. LG_L (a) and O_{PS} (b) versus U demonstrating various phases in the case of $\rho_a=\rho_b=1$, $\Delta=1.05$.

which clearly indicates that the gap vanishes at $L\to\infty$ for all values of U considered. This emphasizes the fact that, as far as the transition to the Mott insulator is concerned, when $U^{ab}\leq U$, the total density must be an integer irrespective of the densities of the individual species of bosons; and it is this condition that really matters. This condition remains the same for $U^{ab}>U$. Thus, when the interspecies interaction is nonzero as in the present case and the total density $\rho\neq n$, no Mott insulator phase is observed.

The phase separation, however, happens when $U^{ab}>U$. The local density distributions of different species of bosons are given in Fig. 5(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 total density $\rho=\rho_a+\rho_b$ remains a constant. For example, when $\rho_a=1$ and $\rho_b=1/2$, one-third of the region is occupied by the species b and two-thirds by the species a. The total density ρ being 3/2, the distributions of the a and b types of bosons follow the ratio of their densities.

C. $\rho_a=1,\rho_b=1$

Finally, we consider the doubly commensurate case where both the species of bosons undergo the SF to MI phase transition in the absence of U^{ab}. It may be noted that for $\rho_a=\rho_b=1$, $U_c\sim 3.4$ for $U^{ab}=0$. In Fig. 6, we plot the scaling of the gap LG_L for $\Delta=1.0$. From this figure and from similar ones for $\Delta\leq 1$, i.e., $U^{ab}\leq U$, we find that the transition from 2SF to MI occurs at a much higher value of $U=U_c\sim 5.7$. No SF-MI transition observed at $U\sim 3.4$. Due to the collective intra- and interspecies interactions in model (1), the species index become irrelevant for the phase transition. For $U^{ab}\sim U$, the phase transition from 2SF to MI is similar to the SF-MI transition in single-species bosons with density $\rho=2$. This is consistent with the similar observations made for the case of $\rho_a=\rho_b=1/2$.

The phase separation transition, however, occurs for $\Delta>1$ as given in Fig. 7. In this case the transitions to phase separation and to the Mott insulator occur around the same $U_c\sim 5.7$. In other words we did not find a PSSF phase sandwiched between the 2SF and PSMI phases for this case.

IV. CONCLUSIONS

We have studied the ground state of a two-species Bose mixture in one dimension using the finite-size density-matrix renormalization group method. We have considered three sets of densities $\{\rho_a,\rho_b\}=\{1/2,1/2\},\{1,1/2\},\{1,1\}$. Analyzing the scaling of the gap in the energy spectrum and the order parameter for phase separation we have obtained several phases: 2SF, MI, PSSF, and PSMI. For $U^{ab}\leq U$, the Mott insulator phase is possible only when the total density $\rho=\rho_a+\rho_b=n$ is an integer. The superfluid to Mott insulator transition in model (1) is then similar to that in the single-species Bose-Hubbard model with the same total density ρ. The critical on-site interaction for the 2SF-MI transition, however, depends on the value of Δ. The lower the value of Δ, the larger the value of U_c. For $\rho\neq n$, the Mott insulator phase is not found. Phase separation occurs for $U^{ab}>U$ irrespective of the value of density. For $\rho=n$ and for all the values of Δ that we have considered, we found a phase-separated Mott insulator phase. In the case of $\rho_a=\rho_b=1/2$, we observe a phase-separated superfluid phase sandwiched between the 2SF and PSMI phases. However, for $\rho_a=\rho_b=1$, no PSSF was found and the transition is directly from 2SF to PSMI. For $\rho_a=1,\rho_b=1/2$ we found a transition from 2SF to PSSF for $\Delta>1$ and only the 2SF phase for $\Delta\leq 1$. It would indeed be worthwhile to devise experiments to test our findings.

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