Phase separated charge density wave phase in two species extended Bose-Hubbard model

Tapan Mishra*
Indian Institute of Astrophysics, II Block, Kormangala, Bangalore, 560 034, India.

B. K. Sahoo†
KVI, University of Groningen, NL-9747 AA Groningen, The Nederlands

Ramesh V. Pai‡
Department of Physics, Goa University, Taleigao Plateau, Goa 403 206, India.

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We study the quantum phase transitions in a two component bose-mixture in a one-dimensional optical lattice. The calculations have been performed in the framework of the extended Bose-Hubbard model using the finite size density matrix renormalization group method. We obtain different phase transitions for the system for integer filling. When the inter-species on-site and the nearest neighbor interactions are larger than the intra-species on-site and also the nearest neighbor interactions, the system exhibits a phase separated charge density wave (PSCDW) order that is characterized by the two species being spatially separated and existing in the density wave phases.

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I. INTRODUCTION

Ultra cold atoms in the optical lattices can provide new insights into quantum phase transitions [1]. The remarkable control of the interaction strengths between the atoms by tuning the laser intensity [2] leads to the experimental realization of the superfluid (SF) to Mott insulator (MI) transition which was predicted by Jaksch *et al* [3]. The observation of the SF to MI transition in the one-dimensional (1D) optical lattice [4] has further enhanced the interest in the search for new quantum phases in the low dimensional bosonic systems. Recent realization of Bose-Einstein condensation (BEC) in strongly dipolar ^{52}Cr atoms [5] has enlarged the domain of interaction space to investigate various quantum phase transitions and other possible subtle characters of bosons at different limit that can be experimentally observed. When atoms with large dipole moments loaded into the optical lattices, the long range interaction between the atoms plays very important role, in addition to the onsite interaction, in the determination of the ground state. This system can be described by the extended Bose-Hubbard (EBH) model, which includes the nearest neighbor interaction along with the onsite repulsion, exhibiting many new phases such as charge density wave (CDW) (sometime known as mass density wave (MDW)) [6, 7], Haldane insulator order[8] and exotic supersolid [9] et cetera..

On the other hand, the study of mixtures of atoms such as bose-bose [10, 11], bose-fermi [12, 13] and fermi-fermi [14, 15] have attracted much attention in recent years because of the successful realization of such systems in optical lattices. In the case of bose-bose mixture, the theoretical models take on-site intra- and inter-species interactions into consideration to describe the system in a large domain of system parameters and the competition between them opens-up many new possible quantum phases [16, 17, 18, 19]. Recent studies in the one-dimensional two species bose mixtures have revealed a spatially phase separated (PS) phase [20, 21], when the inter-species interaction is greater than the intra-species interaction. This phase separation can either of SF or MI type depending upon the strong interplay between the on-site intra-species and inter-species interactions [20]. In this context, it is very interesting and relevant to study the bose mixtures of dipolar atoms to investigate the underlying influence of long range interactions on these phases. Prior theoretical studies of such systems will be helpful to guide the direction of experimental investigations. Our aim of this work is to extend the search for new possible phases by taking into account the nearest neighbor interactions along with the onsite intra- and inter- species interactions in the two species bose mixture which we have studied earlier [20]. We employ the finite size density matrix renormalization group (FS-DMRG) method to study the system.

We have organized the remaining part of the paper in the following way. In Sec. II, we present the theoretical model that we have considered, followed by the method of calculations. We have given a brief discussions of the cases that we have taken into account in this work and a detailed analysis of the results in Sec. III and Sec. IV, respectively. Finally, we conclude our findings in the last section.

*Electronic address: tapan@iiap.res.in
†Electronic address: B.K.Sahoo@rug.nl
‡Electronic address: rvpai@unigoa.ac.in

II. MODEL HAMILTONIAN AND METHOD OF CALCULATIONS

In this work, we consider bose mixtures of dipolar atoms in an 1D optical lattice. The corresponding effective Hamiltonian for such systems can be expressed as

$$\mathcal{H} = \sum_{c=a,b} \left\{ \sum_i \frac{U^c}{2} n_i^c (n_i^c - 1) + \sum_{<i,j>} \left[-t^c (c_i^\dagger c_j + h.c.) + V^c n_i^c n_j^c \right] \right\} + \sum_i U^{ab} n_i^a n_i^b + V^{ab} \sum_{<i,j>} n_i^a n_j^b, \quad (1)$$

where c_i and $c_i^\dagger$ (with $c = a, b$) represent the annihilation and creation operators, respectively, for bosonic atoms of a or b types on site i whose number operators are defined by $n_i^c = c_i^\dagger c_i$. In the above equation, t^c, U^c and V^c are the amplitudes for the hopping between nearest neighboring sites, the on-site and nearest neighbor intra-species repulsive interactions, respectively. The inter-species on-site and nearest neighbor interactions are represented by U^{ab} and V^{ab}, respectively. It is obvious from Eq. (1) that there are at least 8 independent parameters in the model. Since it is not possible to vary all these parameters at a time to grasp the underlying physics of the above model, we restrict ourselves to some special range of parameters which are guided by some cases that have already been studied earlier [6, 20]. We also keep the symmetry between both the a and b types of bosons by assuming $t^a = t^b = t$, $U^a = U^b = U$ and $V^a = V^b = V$. We scale the energy of the whole system with respect to t by setting its value as unity.

In our earlier study in the absence of nearest neighbor interactions; i.e. $V = V^{ab} = 0$, many interesting phases had been predicted. In particular, our work revealed the possible existence of both the species being in SF phases, the system as a whole existing as a MI and phase separated superfluid (PSSF) and phase separated Mott insulator (PSMI) [20] by varying the onsite interaction strengths of both a and b type bosons. It was shown that a phase separation between SF phases of a and b is possible when U^{ab} is considered (slightly) larger than U. When the total density of the system was an integer ($\rho = 1$) with density of each species equal to half ($\rho_a = \rho_b = 1/2$), we had predicted SF, PSSF and PSMI phases in the U and U^{ab} phase space. Furthermore, in the incommensurate densities with $\rho_a = 1$, $\rho_b = 1/2$ and $\rho = 3/2$, we had found only the SF and PSSF phases. In contrast to this case, when $U^{ab} \leq U$ was considered, only the SF phase was possible for the incommensurate densities while signatures of both the SF and MI phases with a continuous SF to MI phase transitions were found for the commensurate densities.

The aim of this work is to investigate how these phases evolve in the presence of intra- and inter-species nearest neighbor interactions. For a better analysis of a particular situation, we restrict ourselves to the commensurate densities, especially the case when $\rho_a = \rho_b = 1/2$ with $\rho = 1$. This choice is governed by the knowledge that we have acquired from the following studies in the phase diagram of (i) the extended Bose Hubbard model for density $\rho = 1$ [6] for a single species boson and (ii) the two species Bose Hubbard model for densities $\rho_a = \rho_b = 1/2$ and $\rho = 1$ [20]. Our analysis of the results from the present study is based upon the findings of the above two cases and conclusions are drawn with respect to them.

Model (1) is a difficult problem to study analytically. We have employed FS-DMRG method with open-boundary condition to determine the ground state. This method has been proved to be one of the most powerful techniques for 1D systems [6, 22, 23]. We have considered a soft-core case by keeping the number of bosonic states per site for each species as four (4). We allow up to 128 states in the density matrix of the left and right blocks in each iteration of the FS-DMRG calculations. The weight of the states neglected in the density matrix of left and right blocks are less than 10^{-6}. To get a better convergence of the ground state energies of various phases, especially for larger values of intra- and inter-species nearest neighbor interactions, we have performed the finite size sweeping procedure [6] twice in each iteration of the FS-DMRG method.

To identify the ground states of various phases of the model Hamiltonian given by Eq. (1), we calculate the single particle excitation gap G_L defined as the difference between the energies needed to add and remove one atom from a system of atoms; i.e.

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

We also calculate the on-site number density as

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

Here c, as mentioned before, is an index representing type a or b bosons, with N_a (N_b) corresponds to total number of a (b) bosons in the ground state $|\psi_{LN_aN_b}\rangle$ of a system of length L with the ground state energy $E_L(N_a, N_b)$.

In $1D$ the appearance the SF phase is signaled by $G_L \to 0$ for $L \to \infty$. However, for a finite system G_L is

finite, and we must extrapolate to $L \to \infty$ limit, which is best done by finite size scaling of gap[6, 24]. In the critical region

$$G_L \equiv L^{-1} f(L/\xi) \tag{4}$$

where ξ is the correlation length which diverges in the SF phase. Thus plots of LG_L versus interaction for different values of L coalesce in the SF phase. On the other hand, when this trend does not follow then the system can be said to be in the MI phase.

We also define the CDW order parameter for the bosons as

$$O^c_{CDW} = \frac{1}{L}\sum_i \langle \psi_{LN_aN_b} | (|n^c_i - \rho|) | \psi_{LN_aN_b} \rangle. \tag{5}$$

So when the CDW order parameter of the system is finite then the system is assumed to be in the CDW phase. Since ρ of the system is constant, it is clear from the above equation that the density of the bosons will oscillate when they are in the CDW phase.

To find whether the ground state is in the spatially phase separated, we calculate the PS order parameter, which is given by

$$O_{PS} = \frac{1}{L}\sum_i \langle \psi_{LN_aN_b} | (|n^a_i - n^b_i|) | \psi_{LN_aN_b} \rangle. \tag{6}$$

When O_{PS} is finite, the system is said to be in the PS phase. Therefore, the system can be simultaneously in PS and one of the SF, MI or CDW phases which can be distinguished by determining both O_{PS} and one of the above properties to identify the other corresponding phase.

III. PRE-ANALYSIS OF RESULTS

Before presenting the details of our results, we first summarize the main features of our study here. In this study, our main focus is to understand the effects of intra- and inter-species nearest neighbor interactions between the atoms on the PSMI phase. As mentioned earlier, the PSMI phase is possible only if $\Delta U \equiv U^{ab}/U > 1$, when $V = V^{ab} = 0$. As we show below there is a stringent condition for the PSMI phases when the nearest neighbor interactions are finite. In the present work, we fix $\Delta U = 1.05$ and consider two values of intra-species on-site interaction $U = 6$ and 9. Our previous study [20] had yielded the ground state of model (1) with $\rho_a = \rho_b = 1/2$ is in PSMI phase for these values of intra- and inter-species on-site interactions. Similarly, the phase diagram of the single species EBH model [6] shows that ground state for $U = 6$ varies first from MI to SF as the nearest neighbor interaction V increases from zero and then to the CDW phase for the larger values of V. However, for $U = 9$, there is no SF phase sandwiched between the MI and CDW phases and the transition between them is direct. We present below the results obtained from this investigation, where the nearest neighbor interactions are finite.

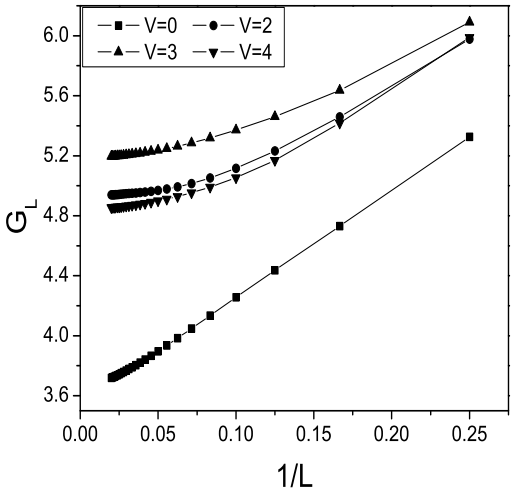

FIG. 1: Gap G_L versus $1/L$ for different values of V for $U = 9$, $\Delta U = 1.05$ and $\Delta V = 0.5$. $G_{L\to\infty}$ converges to a finite values signaling Mott insulator phase.

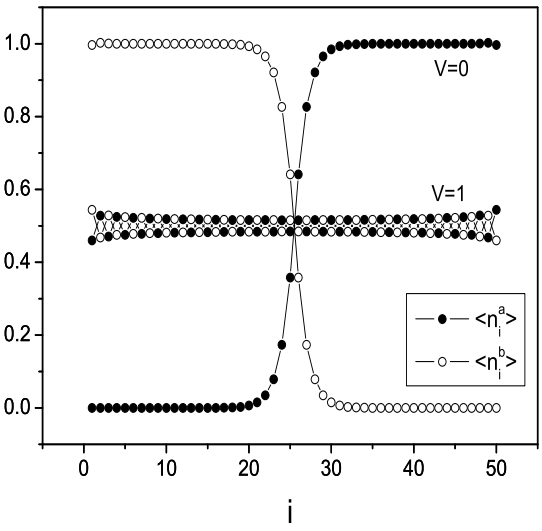

FIG. 2: Plots of $\langle n^a_i \rangle$ and $\langle n^b_i \rangle$ versus i for $V = 0$ and 1, respectively, showing PSMI and MI phases.

One feature which emerges from our study is that when intra- and inter-species nearest neighbor interactions are finite, the PSMI phase is possible only for $V^{ab} > V$. We find that for a fixed $\Delta V = V^{ab}/V = 1.25$ and $U = 6$, the ground state evolves from PSMI to PSSF phases as V steadily increases from an initial value of zero and at

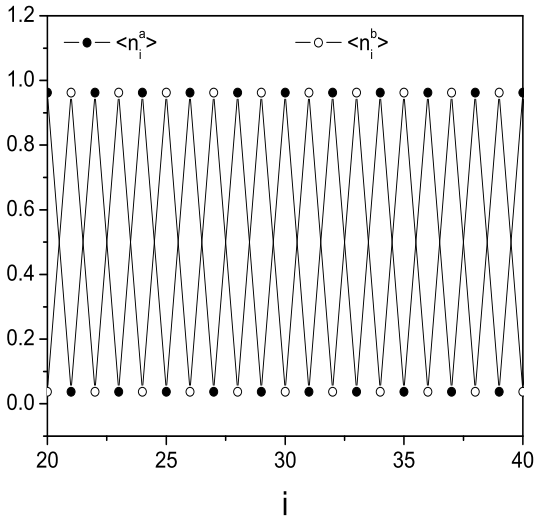

FIG. 3: Plots of $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ versus i for $V = 4$ showing intermingled CDW phases for a and b types of bosons.

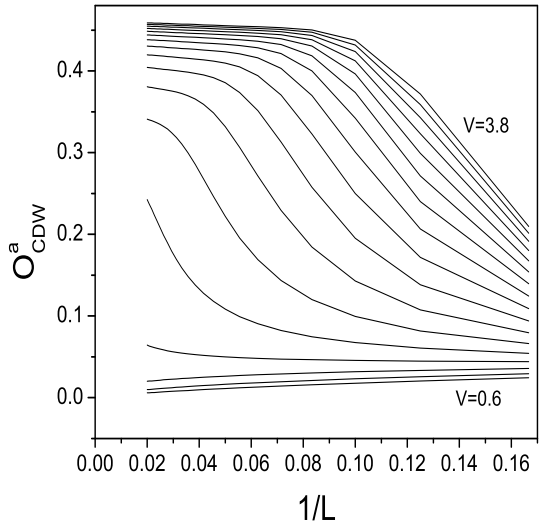

FIG. 4: Plot of CDW order parameter O^a_{CDW} for a-type atoms as a function of $1/L$ for values of V ranging from 0.6 to 3.8 in steps of 0.2. The O^a_{CDW} goes to zero for $V < V_C \simeq 1.2$ where as it is nonzero for higher values of V which shows the transition to CDW phase at $V_C \simeq 1.2$.

some critical value it evolves into the PSCDW phase, where a and b species of atoms reside in the opposite sides of the lattice and each of them showing a density oscillation as expected in the CDW phase. However, for $U = 9$, the transition from PSMI to PSCDW phase is direct with no PSSF phase sandwiched between them. In other words for $\Delta U > 1$ and $\Delta V > 1$, each type of bosons are phase separated, thus minimizing the energy corresponding to inter-species on-site and nearest neighbor interactions and the PS regions behave like a single species EBH model.

However, for $V^{ab} < V$, small value of V is sufficient enough to destroy the PSMI phase and the system evolves into the MI phase where the densities of a and b bosons are equal, but with a finite gap in the single particle energy spectrum. As V increases further the system evolves into a CDW phase with densities of both a and b type atoms exhibiting oscillations. However, these oscillations are shifted by one lattice site. This behavior is distinctly different from the single species EBH model.

IV. RESULTS AND DISCUSSIONS

We now present the details of our results. We begin with the case $\Delta U = 1.05$, $\Delta V = 0.5$, $U = 9$. Calculating the gap in the energy spectrum using Eq. (2), we observe that the system is always gapped for the entire range of V. Figure (1) shows a plot of gap G_L versus $1/L$ for few values of V. A finite gap is a signature of the insulator phase in the system.

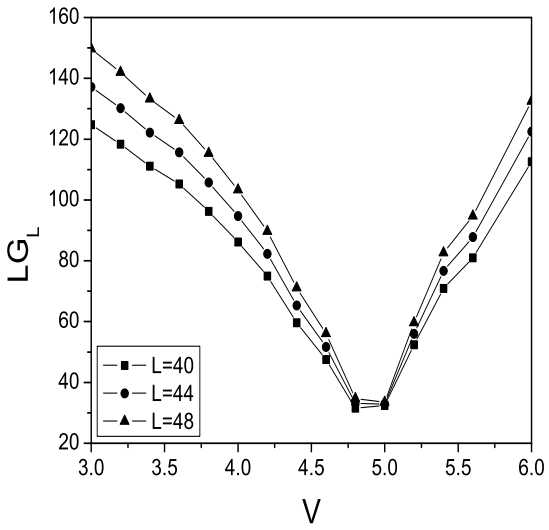

FIG. 5: Scaling of gap LG_L is plotted as a function of V for different system sizes for $\Delta U = 1.05$, $\Delta V = 1.25$ and $U = 9$. Gap remain finite for all the values of V and shows the PSMI-PSCDW transition at $V_C \simeq 4.7$.

In order to investigate the nature of this insulator phase, we further obtain the density distributions $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ of both a and b species bosons using Eq. (3) and they are plotted in Fig. 2 and Fig. 3 respectively. When V is equal to zero or very small, the insulator phase as shown in Fig.2 has a and b atoms spatially separated; i.e. it is in the PSMI phase. For small V, the system behaves like a two species Bose-Hubbard model. As V increases,

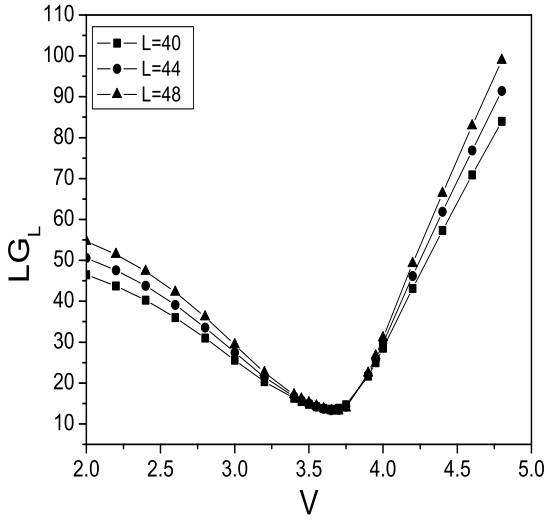

FIG. 6: Scaling of gap LG_L is plotted as a function of V for different system sizes for $\Delta U = 1.05$, $\Delta V = 1.25$ and $U = 6$. Coalescence of different plots between $3.4 < V < 3.9$ shows a gapless PSSF phase sandwiched between PSMI and PSCDW phases.

further the species distribute themselves through the lattice (see Fig.2) thereby destroying the phase separation. Since there is a gap in the excitation spectrum, this corresponds to the MI phase. The critical value of V for this PSMI to MI transition is 0.2 for $\Delta U = 1.05$, $\Delta V = 0.5$ and $U = 9$. Further increase of V drives the system to a phase where the two like atoms cannot occupy the adjacent sites because of large V. The competition between intra- and inter species interactions leads to an energetically favored state where the atoms arrange themselves as shown in Fig. 3. Both a and b type bosons exhibits CDW oscillations, however, they share adjacent sites to minimize the effect of on-site inter species interactions. The oscillation in $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ increases and then stabilizes at a higher V. This is a CDW phase and the density oscillations of a and b species atoms are shifted by one lattice site. The phase transition from MI to this intermingled CDW phase has a critical value of $V_C \approx 1.2$, which is obtained by plotting the CDW order parameter O^a_{CDW}, for different values of V ranging from 0.6 to 3.8 in steps of 0.2, versus $1/L$ as shown in Fig. (4). We notice that the O^a_{CDW} goes to zero for $V < V_C \simeq 1.2$ where it is finite for higher values of V. It should be noted that for the single species extended Bose Hubbard model, the V_C for MI to CDW transition was found to be approximately equal to 4.7 [6]. Thus for $\Delta U = 1.05$, $\Delta V = 0.5$ and $U = 9$, the nearest neighbor interaction between the species favors a CDW over a MI phase. The similar behavior is also seen for $U = 6$. So we arrive at the conclusion at this juncture that for $\Delta U > 1$ and $\Delta V < 1$, the PSMI phase is unstable in the presence of a small inter species nearest neighbor interaction. The phase diagram will then consist of PSMI, MI and CDW phases. However, it is interesting to note that the CDW phase is in fact two intermingled CDW, each for the two different species.

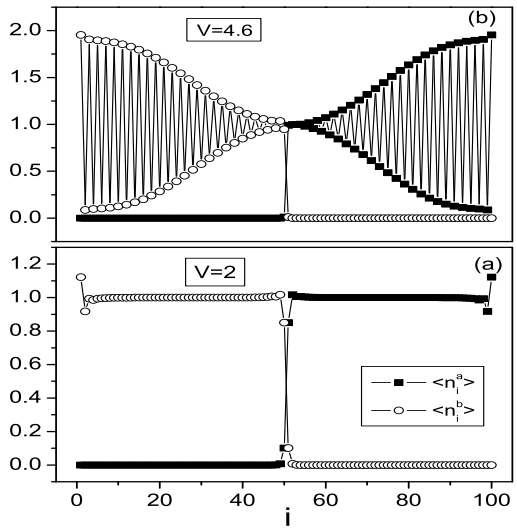

FIG. 7: Plots of $\langle n^a \rangle$ and $\langle n^b \rangle$ versus L for $U = 6$ and two different vales of V; (a) $V = 2$ showing PSMI phase and (b) $V = 4.6$ showing PSCDW phase.

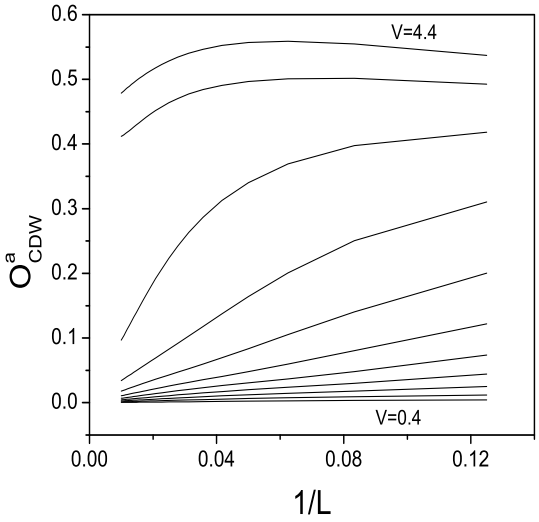

FIG. 8: Plot of O^a_{CDW} as a function of $1/L$ for values of V ranging from 0.4 to 4.4 in steps of 0.4.

Now, we proceed to discuss the other situation when $\Delta V > 1$. Considering $\Delta = 1.25$, we obtain the gap G_L, local density distributions ($\langle n_i^a \rangle$ and $\langle n_i^b \rangle$) and the

CDW order parameters for both $U = 6$ and 9. The most important feature seen in this case is that the phase separation survives for all the considered values of V. a and b species of atoms are present in the opposite sides of the lattice. Since the inter-species (both on-site and nearest neighbor) interactions are larger than the intra-species interactions, the PS phase is always energetically favored compared to the uniform case since the chances of a and b atoms sharing the same site or the nearest neighboring sites are minimized. In other words, the importance of U^{ab} and V^{ab} in the present system is minimized by the PS phase and only interactions left to compete with each other are the on-site and nearest neighbor intra-species interactions. That means both a and b atoms in the PS phase behave like a single species EBH model. We establish these results below by analyzing the gap, local densities and CDW order parameters.

In Fig. 5, we plot the scaling of gap LG_L as a function of V for on-site interaction $U = 9$. The curves for different lengths L do not coalesce anywhere in the figure which is the signature of the finite gap in the single particle energy spectrum [6]. This implies that the phase will be either a PSMI or a PSCDW. In contrast, different LG_L curves coalesce for $3.4 < V < 3.9$ for $U = 6$ as shown in Fig. 6 suggesting the existence of SF phase [6] sandwiched between two gapped phases. To understand the nature of these phases, we plot, in Fig. 7, $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ for two specific values of V, one each representing PSMI and PSCDW phases. Phase separation can be clearly seen in these figures. Plots of these kind yield a PSMI phase for $V < 3.4$. The phase separated phase has the average density $\rho_a = \rho_b = 1$ (see Fig.7(a)). For $3.4 < V < 3.8$, the gap vanishes but the phase separation order parameter remains finite, giving rise to a PSSF phase. And finally for larger value of V, we have a clear PSCDW phase (See Fig.7(b)). The CDW order parameters plotted in Fig.8 remain non-zero for the PSCDW phase. It may be noted that in the PS phase when calculating the CDW order parameter, say O^a_{CDW} for a bosons, only the spatially separated regions; i.e. right hand side of the lattice is considered since the density of a bosons is zero in the left part of the lattice. Therefore, for $U = 6$, we have a transition from PSMI to PSSF as V increases. On further increase of V leads to a transition from the PSSF to the PSCDW phase. However, the transition from PSMI to PSCDW is direct for $U = 9$ as seen from Fig.5. So we conclude here that for $U^{ab} > U$ and $V^{ab} > V$, the system has a PS phase for all values of V and it behaves like a single species BH model in this PS region.

V. CONCLUSIONS

We have investigated the ground state properties of a two species extended Bose-Hubbard model using the finite size density matrix renormalization group method. We study the system for integer filling; i.e. $\rho = \rho_a + \rho_b = 1$ with $\rho_a = \rho_b = 1/2$. Starting with a phase separated Mott insulator phase (i.e. keeping $U^{ab} > U$) and varying the nearest neighbor interaction strengths, we predict a transition from phase separated Mott insulator to Mott insulator and then to charge density wave phase for $V^{ab} < V$. The charge density wave phase in this case is actually an intermingled charge density wave phase, where both a and b species of atoms show density oscillations, but are shifted by one lattice site. For $V^{ab} < V$ the phase separation breaks for a very small nearest neighbor interaction strength. However when $V^{ab} > V$, the phase separation is robust. For large values of U, the ground state evolves from phase separated Mott insulator to phase separated charge density wave phase with a direct transition between them. This is expected to be a first order phase transition [6]. For smaller values of U, a phase separated superfluid phase is sandwiched between the phase separated Mott insulator and phase separated charge density wave phases. This is similar to that of a single species extended Bose-Hubbard model except that the two species are phase separated. We hope the present results will stimulate future experiments.

VI. ACKNOWLEDGMENTS

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