Density-Matrix Renormalization Group studies of mixture of two different ultracold bosonic atoms

2007 J. Phys.: Conf. Ser. 80 012039

(http://iopscience.iop.org/1742-6596/80/1/012039)

Journal of Physics: Conference Series **80** (2007) 012039 doi:10.1088/1742-6596/80/1/012039

Density-Matrix Renormalization Group studies of mixture of two different ultracold bosonic atoms

Tapan Mishra[1], **Ramesh V Pai**[2], **B P Das**[1]

[1]Indian Institute of Astrophysics, II Block, Kormangala, Bangalore, 560 034, India
[2]Department of Physics, Goa University, Taleigao Plateau, Goa 403 206, India

E-mail: tapan@iiap.res.in, rvpai@unigoa.ac.in, das@iiap.res.in

Abstract. We investigate the ground state 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 present our result for different combinations of inter and intra-species repulsion strengths with a commensurate filling factor. We obtain a superfluid(SF) to Mott insulator(MI) transition when the inter species interaction term is less than the intra-species interaction term. However, when the former is slightly greater than the latter we find that the two different species reside in spatially separate regions.

1. Introduction

Ultracold atoms in optical lattices are ideally suited for studying quantum phase transitions in many particle systems because of the unprecedented control of the inter atomic interactions that is possible in such a system. This was exploited by Griener *et al* [1] to observe the superfluid (SF) to Mott insulator (MI) transition in a three dimensional optical lattice. The quantum phase transition was subsequently observed in a one dimensional optical lattice [2]. A number of theoretical investigations have been carried out on a single species of ultracold bosonic atoms in one-dimensional optical lattices [3, 4]. In addition, several interesting predictions have been made for different types of mixtures of cold bosonic atoms [5], fermions [6] and bose-fermi mixture [7, 8] using a variety of approaches.

In this paper we present a numerical study of a two species bosonic mixture in a one dimensional optical lattice. It has been well established that the Bose-Hubbard(BH) model is appropriate for explaining the behaviour of ultracold Bose gases in optical lattices [9]. The different phases in a two species Bose mixture are determined by the competition between the kinetic energy, the on-site interactions and the interspecies interactions between the bosons. The Hamiltonian for such a system is given by:

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

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 corresponding to adjacent sites $\langle ij \rangle$ and the intra-species repulsive interaction 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 $U^a = U^b = U$. We set our energy scale by $t = 1$.

We have carried out our investigations of quantum phase transitions in the above system by using the Finite-Size Density Matrix Renormalization Group(FSDMRG) method[10, 11] which is clearly one of the most powerful approaches to study one dimensional lattice systems. We first summarize our results. We obtain the transition from the superfluid phase (where the atoms are randomly distributed across the lattice) to the Mott insulator phase (where equal number of atoms are localized at different lattice sites) whenever the inter species interaction is less than the intra-species interaction. However, in the opposite case, i.e., when the inter species interaction is larger than the intra-species interaction, we obtain a novel phase separation where the two species reside in spatially separated regions. The individual species of bosons in this spatially separated region may be in the superfluid or Mott insulator phase depending on the strength of the inter species interaction.

The remaining part of this paper is organized as follows. Section 2 contains the details of the FSDMRG calculation. Section 3 contains our results. We end with concluding remarks in Section 4.

2. FSDMRG method

The finite size density matrix renormalization group method has proven to be one of the most powerful methods to study one dimensional interacting quantum systems [4, 10]. Open boundary conditions would be appropriate for such an approach since the error in the calculations would be significantly less than in the case periodic boundary conditions as the size of the system increases. We present below the salient features of this method

Each iteration of our FSDMRG method consists of the following two steps:

(i) The system size is increased from L to $L + 2$ by adding two sites as in the case of the infinite-system density-matrix renormalization group method (DMRG).

(ii) The system size L is held fixed, but the energy of a target state is improved iteratively by a sweeping procedure, described below, till convergence is obtained.

For a model represented by Eq. (1) we first construct the Hamiltonian matrix of the superblock configuration $\mathbf{B}_1^\ell \bullet \bullet \mathbf{B}_1^r$, where $\mathbf{B}_1^\ell$ and $\mathbf{B}_1^r$ represent left- and right-block Hamiltonians, respectively, and each one of the $\bullet$ represents a single-site Hamiltonian. In the first step of the DMRG iteration both $\mathbf{B}_1^\ell$ and $\mathbf{B}_1^r$ also represent single sites, so, at this step, we have a four-site chain. The number of possible states per site in the Bose-Hubbard model Eq. (1) is infinite since there can be any number of bosons on a site. In a practical DMRG calculation we must restrict the number n_{max} of states or bosons allowed per site. The smaller the interaction parameter U, the larger must n_{max} be. As in earlier calculations [4] on related models, we find that $n_{max} = 4$ is sufficient for the values of U considered here. This means that there are $4 \times 4 = 16$ (4 each a and b type bosons) states per every single site.

We now diagonalize the Hamiltonian matrix of the superblock and obtain the energy and the eigenfunction of a *target state*. In our study the target state is the ground state of the system of size L with either $N^a = L,\ N^b = L$ or $N^a = L \pm 1,\ N^b = L$ bosons. Here $N^a(N^b)$ represents total number of $a(b)$ type of bosons. The latter is required for obtaining the gap in the energy spectrum. We now divide the superblock into two equal halves, the left and the right parts, which are treated, respectively, as the *system* and the *universe*. The density matrix for this *system*, namely, $\mathbf{B}_2^\ell \equiv \mathbf{B}_1^\ell \bullet$, is calculated from the *target state*. If we write the *target state* as

$\mid \psi\rangle = \sum_{i,j} \psi_{i,j} \mid i\rangle \mid j\rangle$, where $\mid i\rangle$ and $\mid j\rangle$ are, respectively, the basis states of the *system* and the *universe*, then the density matrix for the *system* has elements $\rho_{i,i'} = \sum_j \psi_{i,j}\psi_{i',j}$. The eigenvalues of this density matrix measure the weight of each of its eigenstates in the *target state*. The optimal states for describing the *system* are the ones with the largest eigenvalues of the associated density matrix. In the first step of the DMRG the superblock, and hence the dimension of the density matrix, is small, so all the states can be retained. However, in subsequent steps, when the sizes of the superblocks and density matrices increase, only the most significant states are retained, i.e. the ones corresponding to the largest M eigenvalues of the density matrix (in our studies we choose $M = 128$). We then obtain the effective Hamiltonian for the *system* $\mathbf{B}_2^\ell$ in the basis of the significant eigenstates of the density matrix; this is used in turn as the left block for the next DMRG iteration. In the same manner we obtain the effective Hamiltonian for the right block, i.e., $\mathbf{B}_2^r \equiv \bullet\mathbf{B}_1^r$. In the next step of the DMRG we construct the Hamiltonian matrix for the superblock $\mathbf{B}_2^\ell\bullet\bullet\,\mathbf{B}_2^r$, so the size of the system increases from $L = 4$ to $L = 6$. For a system of size L, we continue, as in the first step, by diagonalizing the Hamiltonian matrix for the configuration $\mathbf{B}^\ell_{\frac{L}{2}-1}\bullet\bullet\mathbf{B}^r_{\frac{L}{2}-1}$ and setting $\mathbf{B}^\ell_{\frac{L}{2}} \equiv \mathbf{B}^\ell_{\frac{L}{2}-1}\bullet$ and $\mathbf{B}^r_{\frac{L}{2}} \equiv \bullet\mathbf{B}^r_{\frac{L}{2}-1}$ in the next step of the DMRG iteration. Thus at each step of the DMRG iteration the left and right blocks increase in length by one site and the total length L of the chain increases by 2.

In the infinite-system DMRG method outlined above the left- and right-block bases are not optimized in the following sense: The DMRG estimate for the *target-state* energy, at the step when the length of the system is L, is not as close to the exact value of the target-state energy for this system size as it can be. It has been found that the FSDMRG method overcomes this problem [10]. In this method we first use the infinite-system DMRG iterations to build up the system to size L. The L-site superblock configuration is now given by $\mathbf{B}^\ell_{\frac{L}{2}-1}\bullet\ \bullet\ \mathbf{B}^r_{\frac{L}{2}-1}$. In the next step of the FSDMRG method, the superblock configuration $\mathbf{B}^\ell_{\frac{L}{2}}\ \bullet\ \bullet\ \mathbf{B}^r_{\frac{L}{2}-2}$, which clearly keeps the system size fixed at L, is used. This procedure is called *sweeping* in the right direction since it increases (decreases) the size of the left (right) block by one site. For this superblock the *system* is $\mathbf{B}^\ell_{\frac{L}{2}}\bullet$, the *universe* is $\bullet\mathbf{B}^r_{\frac{L}{2}-2}$, the associated density matrix can be found, and from its most significant states the new effective Hamiltonian for the left block, with $(\frac{L}{2}+1)$ sites, is obtained. We sweep again, in this way, to obtain a left block with $(\frac{L}{2}+2)$ sites and so on till the left block has $(L-3)$ sites and the right block has 1 site so that, along with the two sites in between these blocks, the system still has size L; or, if a preassigned convergence criterion for the target-state energy is satisfied, this sweeping can be terminated earlier. Note that, in these sweeping steps, for the right block we need $\mathbf{B}_1^r$ to $\mathbf{B}_{L-3}^r$, which we have already obtained in earlier steps of the infinite-system DMRG. Next we sweep leftward: the size of the left (right) block decreases (increases) by one site at each step. Furthermore, in each of the right- and left-sweeping steps, the energy of the target state decreases systematically till it converges (we use a six-figure convergence criterion in our calculations).

In our FSDMRG method in which we sweep, as described above, at *every step* of the DMRG scheme and not only in the one that corresponds to the largest value of L. This helps in obtaining 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 removed by using finite-size scaling as we show below. For this purpose, the energies and correlation functions, obtained from a DMRG calculation, should have converged properly 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.

Since the bases of left- and right-block Hamiltonians are truncated by neglecting the eigenstates of the density matrix corresponding to small eigenvalues, this leads to truncation

errors. If we retain M states, the density-matrix weight of the discarded states is $P_M = \sum_{\alpha=1}^{M}(1-\omega_\alpha)$, 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, correlation length in a phase. For a fixed M, we find very small truncation errors in the gapped phase and the truncation errors are largest in the SF phase. In our calculations we choose M such that the truncation error is always less than 5×10^{-5}; we find that $M = 128$ suffices.

3. 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.,

$$G_L = E_L(N_a+1, N_b) + E_L(N_a-1, N_b) - 2E_L(N_a, N_b) \tag{2}$$

and the on-site density correlation function

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

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 by the FSDMRG method discussed above. Defining the ratio of the inter and intra species interactions $\Delta = U^{ab}/U$, 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 dominate. 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 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 superfluid phase with a and b bosons spatially separated into different regions of the lattice. 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

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

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 $\langle n_i \rangle (= \langle (n_i^a + n_i^b) \rangle) = \rho$ continue to remain uniform across the lattice.

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 [4]. In the critical region, i.e., SF region, the gap

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

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.

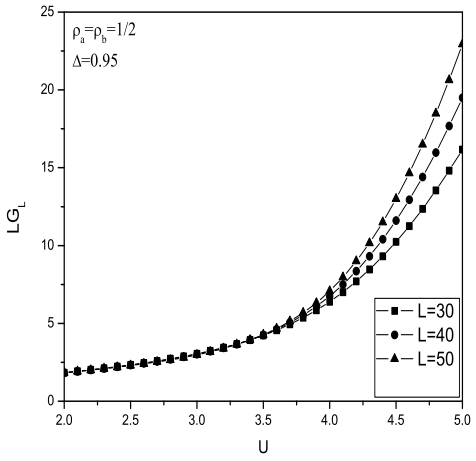

Figure 1. Scaling of gap LG_L is plotted as a function of U for different system sizes for $\Delta = 0.95$. The coalescence of different curve for $U \simeq 3.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

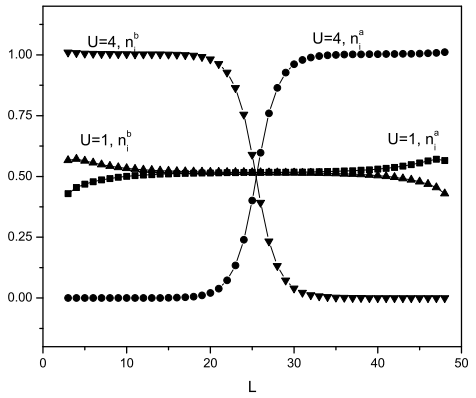

Figure 2. Plots of $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ versus i for $U = 1$ and $U = 4$ and $\Delta = 1.05$, for system size $L = 50$. The deviation in $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ near the boundaries for $U = 1$ is due to the open boundary condition used in our FSDMRG

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. 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 since $\rho_a = \rho_b = 1/2$, the MI phase is absent when $U^{ab} = 0$ and the model (1) will have only the 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 $U \leq U_c \simeq 3.4$ indicating a MI phase for $U > U_c$. The emergence of this phase is due to the intra-species as well as inter-species interaction strengths. The fact that $U_c \simeq 3.4$, indicates that the model (1) when $\Delta \approx 1$ behaves like a single species of bosons at unit density [4]. These results are along expected lines because, when $U^{ab} \approx U$, every boson in the system interacts with all the other bosons, irrespective of whether they are of type

a or b, with the same strength and therefore the 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 $\Delta = 1.05$. It is clear 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 (PS) 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. (3). It is evident that the transition to the MI phase happens 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 $\Delta = 1.05$, 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 $U > 3.4$.

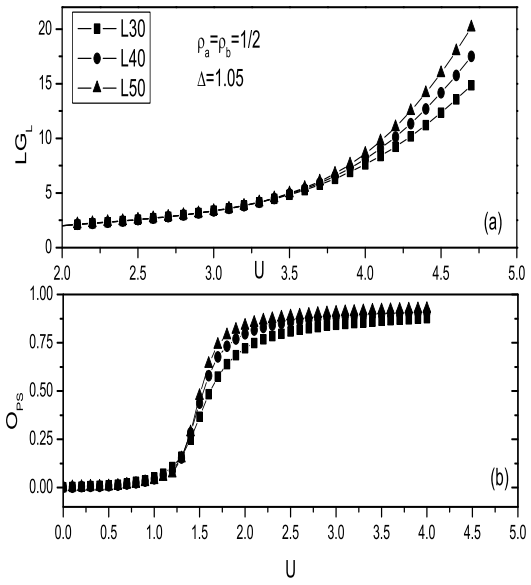

Figure 3. Plots of LG_L (a) and O_{PS} (b) versus U demonstrate various phases in the case $\Delta = 1.05$.

4. Conclusion

From the above discussion, the following conclusions can be drawn. For the values of the interaction strengths and the density considered here, we obtain several phases: 2SF, MI, PS-SF and PS-MI. For $U^{ab} \leq U$, the Mott Insulator phase is possible since 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 behaviour, however, occurs for $U^{ab} > U$, where we observe a phase separation. The Mott insulator phase is then phase separated. In this case, we observe a phase separated superfluid PS-SF sandwiched between 2SF and PS-MI.

Acknowledgments
One of us (TM) thanks K. V. P. Latha of Indian Institute of Astrophysics for useful suggestions.

References

[1] Greiner M, *et al*, Nature **415**, 39 (2002).
[2] Stöferle T, *et. al.* Phys. Rev. Lett. **92**, 130403 (2004).
[3] Batrouni G G, Höbert F, and Scalettar R T Phys. Rev. Lett. **97**,
[4] Pai R V, Pandit R, Krishnamurthy H R, and Ramasesha S, Phys. Rev. Lett. **76**, 2937 (1996); Pai R V and Pandit R, Phys. Rev. B **71**, 104508 (2005).
[5] Isacsson A, Min-Chul Cha, Sengupta K and Girvin S M, Phys. Rev. B **72**, 184507 (2005).
[6] Shi-Jian Gu, Rui Fan and Hai-Qing Lin, *Preprint* cond-mat/0601496.
[7] Albus A, Illuminati F and Eisert J, Phys. Rev. A, **68**, 023606 (2003).
[8] Lewenstein M, Santos L, Baranov M A and Fehtmann H, Phys. Rev. Lett. **92**, 050401 (2004).
[9] Jaksch D, *et al*, Phys. Rev. Lett. **81**, 3108 (1998).
[10] White S R, Phys. Rev. Lett. **69**, 2863 (1992).
[11] Schollwöck U, Rev. Mod. Phys. **77**, 259 (2005).