Induced supersolidity in a mixture of normal and hard-core bosons

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We present a scenario where a supersolid is induced in one of the components of a mixture of two species bosonic atoms where there are no long-range interactions. We study a system of normal and hard-core boson mixture with only the former possessing long-range interactions. We consider three cases: the first where the total density is commensurate and the other two where it is incommensurate to the lattice. By suitable choices of the densities of normal and hard-core bosons and the interaction strengths between them, we predict that the charge density wave and the supersolid orders can be induced in the hard-core species as a result of the competing interatomic interactions.

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I. INTRODUCTION

The hallmark of the supersolid (SS) phase is the coexistence of the superfluid and the charge density wave (CDW); i.e., solid orders.[1] This phase has not been observed unambiguously in experiments. However, in recent years several theoretical predictions of this phase have been made in different lattice systems.[2–5] Though the claim of the observation of this phase by Kim *et al.*[6] could not be verified,[7] the search for the supersolid phase has become an active area of research.

The pioneering observation of the superfluid (SF) to Mott insulator (MI) transition in an optical lattice using cold bosonic atoms,[8] which had been predicted by Jaksch *et al.*[9] based on an earlier work by Fisher *et al.*,[10] has opened up several directions in the field of ultracold atoms. The possibility of tuning the interatomic interactions in the optical lattice makes this system ideal for obtaining exotic phases of ultracold atoms with long-range interactions.[4,11] The observation of BEC in ^{52}Cr atoms which have large magnetic dipole moments[12] and recent experiments on two species Bose mixtures by the LENS group[13,14] provide hope for the realization of mixtures of dipolar atoms in optical lattices. These developments in combination with the advancing research in optical lattice systems could lead to the observation of the supersolid phase in the future.

Theoretical studies of the possible existence of the supersolid phase in a single species as well as mixtures of bosonic atoms and Bose-Fermi mixtures have attracted much attention.[2,5,15–17] Mixtures of ultracold atoms are of great interest because of the various competing interactions between the atoms that lead to many exotic phases. In this context, we have considered a mixture of two species bosonic atoms with one species consisting of normal and the other hard-core bosonic atoms. For the latter species, a single lattice site can be occupied by no more than one atom. This mixture can therefore be considered equivalent to a system of Bose-Fermi (spinless) atoms only in one dimension. We assume that the normal bosonic species exhibits long range interactions, but the interatomic interactions in the hard-core species are limited only to onsite interactions. The model Hamiltonian for such a system can be written as

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

Here a_i and b_i, respectively, are the bosonic annihilation operators for atoms of a (normal) and b (hard-core) bosons localized on-site i, $n_i^a = a_i^\dagger a_i$ and $n_i^b = b_i^\dagger b_i$ represent its number operators, and t^a and t^b are the hopping amplitudes between the nearest neighbors $\langle ij \rangle$. U^a and (V^a) are the on-site (nearest neighbor) intraspecies repulsive interactions for the normal atoms. We have taken only the nearest neighbor interactions because the dipole-dipole interaction potential varies as $1/r^3$, where r is the distance between the dipoles. The interspecies (between normal and hard-core bosons) interaction is given by U^{ab}. The hopping amplitudes (t^a, t^b) and interaction parameters (U^a, V^a, U^{ab}) are related to depth of the optical potential, recoil energy, and the scattering lengths.[9,18] The ratio U^{ab}/U^a as well as U^a/V^a can be varied over a wide range of values experimentally.[19,20] In this work we consider $t^a = t^b = t = 1$ which set all parameters dimensionless.

II. METHOD OF STUDY

We identify various ground states phases of the model (1), by calculating (i) the single particle excitation gap G_L^α for species $\alpha = a, b$ defined as the difference between the energies needed to add and remove one atom of species α; i.e.,

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

$$G_L^b = E_L(N_a, N_b + 1) + E_L(N_a, N_b - 1) - 2E_L(N_a, N_b), \quad (3)$$

and (ii) the on-site number density defined by

$$\langle n_i^\alpha \rangle = \langle \psi_{LN_aN_b} | n_i^\alpha | \psi_{LN_aN_b} \rangle. \quad (4)$$

Here N_a and N_b corresponds to total number of a and b bosons in the ground state $|\psi_{LN_aN_b}\rangle$ of a system of length L with the ground-state energy $E_L(N_a, N_b)$. The former is used to distinguish the gapless superfluid phase from the Mott insulator or the charge-density wave phase, both having finite gap in their energy spectrum. In the one-dimension systems the appearance of the SF phase is indicated by $G_L^\alpha \to 0$ for $L\to\infty$. However, for a finite system G_L^α is finite, and we must extrapolate to the $L\to\infty$ limit, which is best done by the finite size scaling of the gap.[21,22] In the critical region, $G_L^\alpha \equiv L^{-1} f(L/\xi^\alpha)$, where ξ^α is the correlation length for species α which diverges in the SF phase. Thus plots of LG_L^α versus the nearest-neighbor interaction for different values of L coalesce in the SF phase. On the other hand, when this trend does not follow, then the system is considered to be in the gapped, either a MI or a CDW phase, which is further distinguished from each other via the CDW order parameter defined as

$$O_{CDW}^\alpha(L) = \frac{1}{L}\sum_i \langle \psi_{LN_aN_b}|(|n_i^\alpha - \rho^\alpha|)|\psi_{LN_aN_b}\rangle. \qquad (5)$$

The existence of the solid order is verified from the finite value of $O_{CDW}^\alpha(L\to\infty)$ and also from the finite density structure factor,

$$S(k) = 1/L\sum_{i,j}^{N} e^{ik(i-j)}\langle n_i n_j\rangle, \qquad (6)$$

at $k=\pi$.

We have employed the finite size density matrix renormalization group (FS-DMRG) method with open-boundary conditions to determine the ground state. This method has proved to be one of the most powerful techniques for studying one-dimensional (1D) systems.[23,24] In addition to this method, the quantum Monte Carlo method with periodic boundary conditions has been successfully applied to such systems. Both these methods are capable of treating a large number of lattice sites in one-dimensional systems. For the normal species, we have taken the maximum occupation per site as 4 and the weights of the states neglected in the density matrix of the left and right blocks are less than 10^{-6}. The occupation cutoff is based on previous DMRG results.[21,25] It has been shown that the values of important physical quantities change very little when the occupation cutoff is increased beyond four.

III. RESULTS AND DISCUSSION

The charge-density wave phase in Bose systems is possible when the density of bosons are commensurate with the underlying lattice. For example, the earlier studies of the one-dimensional single species extended Bose-Hubbard model have shown the existence of the CDW phase for $\rho=1/2$ and 1.[21,25] Later this study was extended in the case of two species extended Bose-Hubbard model, where the solid order is achieved for $\rho^a=\rho^b=1/2$ by suitably varying the strengths of the nearest-neighbor interactions.[26] Supersolid phase is then possible only moving away from these commensurate densities.[2,5]

The recent study of a two species Bose mixture in a one-dimensional lattice shows that phase separation occurs if the ratio U^{ab}/U^a is larger than unity.[26] In order to avoid this condition, we consider $U^a=U^{ab}=U$ and study the effect of V^a

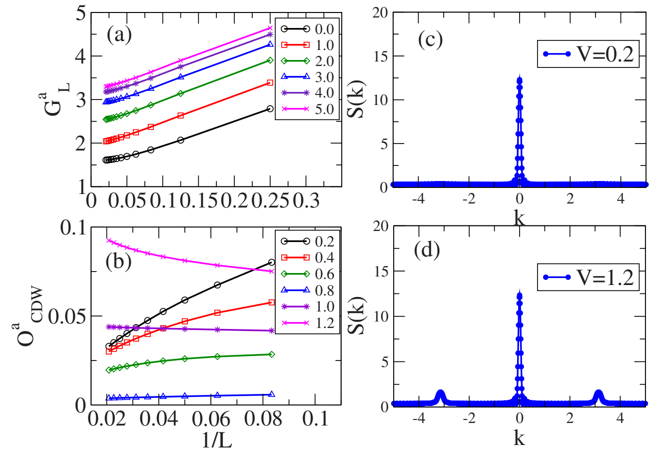

FIG. 1. (Color online) (a) Single particle energy gap G_L^a for normal bosons as a function of $1/L$ for different V^a showing finite gap in the thermodynamic limit. (b) $O_{CDW}^a(L)$ versus $1/L$ for different V^a showing the onset of CDW order for $V^a > V_C^a \approx 1.0$. (c) and (d) Structure function $S(k)$ for $V=0.2$ and 1.2 respectively.

on the ground state of model (1) for three possible combinations of densities; (i) $\rho^a=\rho^b=1/2$, (ii) $\rho^a=1/2$ and $\rho^b=1/4$, and (iii)$\rho^a=3/4$ and $\rho^b=1/2$. In the first case, the total density of the system, i.e., $\rho=\rho_a+\rho_b$, is commensurate, but in other two cases it is not. In all the above three cases we have taken $U=6$, which is very large compared to the nearest neighbor tunneling amplitude $t=1$.

A. $\rho^a=\rho^b=1/2$

In this case for $V^a=0$, the system is in the MI phase because the onsite intraspecies interactions, $U^a=6$, $U^b=\infty$, and the interspecies interaction, $U^{ab}=6$ are all greater than $U_C \approx 3.4$, the critical strength of the on-site interaction for the SF-MI transition in the one-dimensional Bose-Hubbard model for $\rho=1$.[21,25,26] The system continues to remain gapped as V^a increases. The gap corresponding to lattice size L for species a, G_L^a is plotted for different values of V^a in Fig. 1(a), which yields that $G_{L\to\infty}^a > 0$ for $V^a>0$. However, the gapped phase at higher V^a is not a MI but a CDW, since $O_{CDW}^a(L\to\infty)$ is finite for $V^a > V_C^a \sim 1.0$. In Fig. 1(b) we have plotted $O_{CDW}^a(L)$ versus $1/L$ for different values of V^a. The order parameter $O_{CDW}^a(L)$ goes to zero for small values of V^a and branches out for higher values indicating the onset of the CDW phase. This has been further verified by calculating the density structure factor $S(k)$. For small values of V, $S(k=\pi)$ vanishes. $S(k=\pi)$ becomes finite after some critical value of V which appears as a peak in the $S(k)$ vs k plot. The emergence of the peak is the signature of the CDW phase in the system. In Fig. 1(c), we have plotted $S(k)$ vs k for $V=0.2$ which does not show a peak at $k=\pi$, however, it peaks at $V=1.2$, as shown in Fig. 1(d). The appearance of the peak for large values of V indicates the emergence of the CDW phase. $O_{CDW}^b(L)$ also exhibits a similar behavior indicating that both the normal and the hard-core bosons undergo a MI to CDW transition. The dependence of this transition on V^a for the normal bosons is expected on the basis of an earlier work.[25] However, it was not obvious that the hard-core

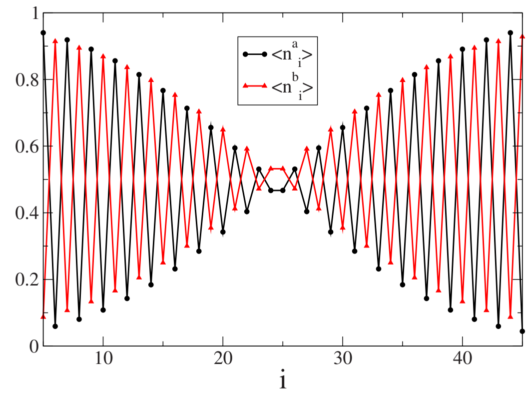

FIG. 2. (Color online) The onsite number density for a and b bosons are plotted against the site index i taking $V^a=5$ for $\rho^a=1/2$, $\rho^b=1/2$. The black curve corresponds to $\langle n_i^a \rangle$ and the red corresponds to $\langle n_i^b \rangle$. The node at the center is due to open boundary condition.

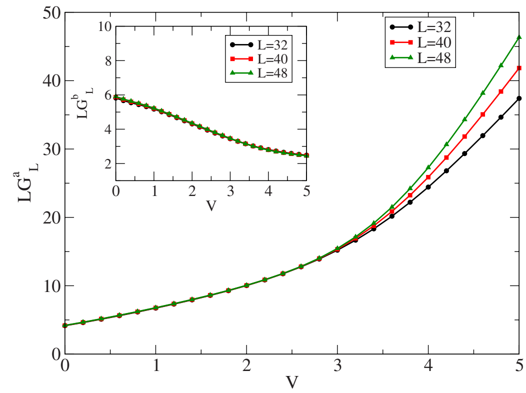

FIG. 3. (Color online) Finite size scaling of gap LG_L^α is plotted as a function of V^a for different system sizes for the case $\rho^a=1/2$ and $\rho^b=1/4$. The coalescence of the different curves for $V^a \leq 3.0$ for the normal species shows the transition from the gapless SF phase to a gapped phase. (Inset) The coalescence of the different curves for all the values of V^a for the hard-core species indicates the existence of the SF phase.

bosons would also undergo a similar MI to CDW transition as they lack long range interactions to exhibit density oscillations.

The physical scenario when $\rho^a=\rho^b=1/2$ is the following: when $V^a=0$, the system is in the MI phase due to the strong repulsion between the bosons. As V^a increases, there is competition between the interactions U^a and V^a and hence an atom of species a (normal bosons) cannot occupy the sites next to another atom of the same species, thereby forming a CDW phase. In addition, the atoms of the hard-core species b cannot occupy a site where there is either a hard-core boson or a normal boson because of the strong repulsive onsite interaction, U^{ab}. These physical conditions give rise to the intermingled CDW phase where the nearest-neighbor sites are occupied by atoms of different species as shown in Fig. 2. It is interesting to note that the presence of V^a is sufficient to induce the solid order in the hard-core species in spite of the absence of any long-range interaction between them. This type of induction of the solid order makes the other combinations of densities presented below very interesting.

B. $\rho^a=1/2$ and $\rho^b=1/4$

In this case the total boson density $\rho=3/4$, and it is not commensurate with the lattice. In the present problem, since we have not considered long-range interactions beyond the nearest neighbors, the commensurate densities are integers or half integers. In a normal two species bosonic mixture with incommensurate density (e.g., $\rho=3/4$), there is no transition from a SF to a gapped phase.[26] However, such a transition does occur, as shown below, in a normal—hard-core boson mixture described by model (1). The finite size scaling of the gap LG_L^α is given in Fig. 3 shows a transition from the gapless SF phase to a gapped phase for the normal bosonic species with critical value $V_C^a \sim 3.0$. The hard-core species, however, remains in the SF phase showing no gap in the excitation spectrum.

The calculation of the CDW order parameters given in Fig. 4 for both the normal and the hard-core bosons show a finite O_{CDW}^α in the limit $L \to \infty$ for $V^a > V_C^a \sim 3.0$. Thus the gapped phase of the normal bosonic species is identified to be the CDW phase while the gapless phase of hard-core bosons is a supersolid since both the superfluid and the CDW phases coexist. The CDW oscillations are similar to the case of $\rho_a=\rho_b=1/2$ as given in Fig. 2.

C. $\rho^a=3/4$ and $\rho^b=1/2$

The phase transitions that we have obtained for this case are in the reverse order compare to that of case (ii), i.e., the normal species shows a transition from the SF to the supersolid phase, its gap remain zero as shown in Fig. 5 and it shows a finite CDW order parameter for $V^a > V_c^a \sim 1.2$ and the hard-core species shows a transition from the SF to the gapped CDW phase at the same critical point $V_c^a \sim 1.2$. The normal bosons have incommensurate density (i.e., $\rho^a=3/4$) which results in the supersolid phase for $V^a > V_C^a$. However, the density of the hard-core bosons is half and is commensurate, yielding the gapped CDW phase. It is interesting to note that in the normal single species extended Bose-

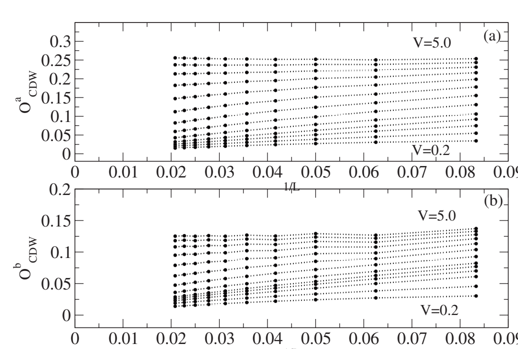

FIG. 4. $O_{CDW}(L)$ versus $1/L$ for (a) normal and (b) hard-core species for V^a ranging from 0.2 to 5.0 in steps of 0.4 is shown for $\rho^a=1/2$ and $\rho^b=1/4$. It is clear from the scaling that the O_{CDW}^α becomes finite for $V^a \gtrsim 3.0$ for both the species indicating the transition to the CDW phase.

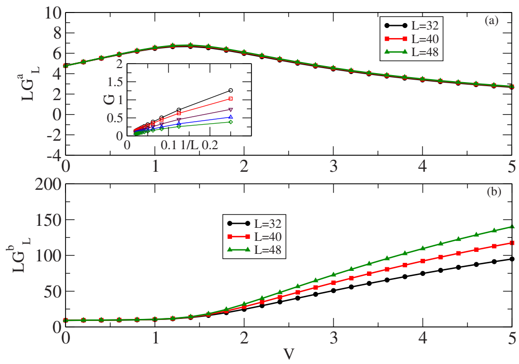

FIG. 5. (Color online) Scaling of gap LG_L is plotted as a function of V^a for different system sizes for $\rho^a=3/4$ and $\rho^b=1/2$. (a) The coalescence of the different curves for all the values of V^a for the normal species shows that the system remains in the gapless SF phase. (Inset) Shows the G_L^a plotted against $1/L$ for different V^a ranging from 1 to 5 in steps of 1 which shows that the gap vanishes as $L\to\infty$. (b) The coalescence of the different curves for $V^a \le 1.2$ for the hard-core species indicates the transition from the SF to the CDW phase.

Hubbard model (i.e., model 1 in the absence of hard-core bosons), the supersolid phase is stable only for large U^a and V^a.[5] However, in the present case, the presence of the hard-core bosons stabilizes the supersolid phase at much smaller values of V^a.

IV. CONCLUSION

We have considered a system of normal and hard-core bosonic mixture with the normal species possessing long range interactions. By taking three different sets of densities of both the species, we have investigated the conditions that give rise to the supersolid phase in either or both the species. The main findings of this work is that by suitably tuning the nearest-neighbor interaction strength V^a, the solid order can be stabilized in the normal bosonic species and it can also be induced in the hard-core species as a result of the competition between the U^a, U^{ab}, and V^a. This induction of the solid order can lead to both the species being in the CDW and more interestingly one species in the CDW phase and the other in the supersolid phase depending on the choice of densities. By keeping the onsite repulsion for the normal species $U^a=6$ and varying the nearest-neighbor interaction strength of the hard-core species V^a, we obtain different interesting quantum phases which are listed in Table I shown above.

TABLE I. Different phases.

ρ_a	ρ_b	Normal	Hard-core
1/2	1/2	MI-CDW	MI-CDW
1/2	1/4	SF-CDW	SF-SS
3/4	1/2	SF-SS	SF-CDW

In recent experiments on dipolar atoms, it has been demonstrated that the ratio between the on-site and the nearest-neighbor interactions can be controlled by Feshbach resonance.[20] In the present work, we take a fixed on-site interaction and vary the nearest-neighbor interaction, which is equivalent to the experimental situation where the ratio is varied. In the experiment by LENS group,[13,14] the interspecies interactions in a K-Rb mixture has been manipulated using Feshbach resonance. We are not certain whether there is an other Feshbach resonance in such system to control the intraspecies interaction. However, two separate Feshbach resonances exist in a mixture of ^{85}Rb-^{87}Rb.[27,28] Therefore, this mixture of bosonic atoms could be experimentally used to test the prediction we have made regarding induced supersolidity by varying U^a(intraspecies interaction) and U^{ab}(interspecies interaction). In addition, it is possible to vary U^a by changing the depth of the optical potential following Greiner *et al.*[8]

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