Induced supersolidity in a normal and hardcore boson mixture

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It is well known that the supersolid form of matter can arise in a single species of cold bosonic atoms in an optical lattice due to long range interactions. We present a scenario where a supersolid is induced in one of the components of a mixture of two species bosonic atoms where there is no long range interactions. We study a system of normal and hardcore 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 they are incommensurate. By suitable choices of the densities and the interaction strengths of the atoms, we predict that the charge density wave and the supersolid orders can be induced in the hardcore species as a result of the competing interatomic interactions.

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The hallmark of the supersolid(SS) phase is the coexistence of the superfluid and the charge density wave (CDW); i.e. solid orders [1, 2]. 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 [3, 4, 5, 6, 7]. The observation of BEC atomic interactions in optical lattice makes this system of ultracold atoms. The possibility of tuning the interatomic interactions for the normal atoms. The inter-species (between normal and hardcore bosons) interaction is given by calculating (i) the single particle excitation gap \( \langle i,j \rangle \), by calculating (ii) the single particle excitation gap \( \langle i,j \rangle \), by calculating (iii) the single particle excitation gap \( \langle i,j \rangle \) as well as \( \langle i,j \rangle \) 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 [12], which had been predicted by Jaksch et. al. [13], has opened up new directions in the field of ultracold atoms. The possibility of tuning the interatomic interactions in optical lattice makes this system ideal for obtaining exotic phases of ultra cold atoms with long range interactions. The observation of BEC in \(^{52}\text{Cr}\) atoms which have large magnetic dipole moments in a trap [16] in combination with the advancing research in optical lattice systems raises the hope of the observation of the supersolid phase in the future.

Theoretical studies of the possible existence of supersolids in mixtures of bosonic atoms and Bose-Fermi mixtures have attracted much attention [17, 18, 19]. Mixtures of ultracold atoms are very interesting because of the various competing interactions between the atoms leading to many exotic phases. It has been shown that for a single species ultracold atoms in a one dimensional lattice, the supersolid exists for large on-site as well as nearest neighbour interactions when the density of the system is not commensurate to the lattice and also larger than half filling \( \frac{3}{2}, \frac{2}{3} \). In this Letter, we have considered a mixture of two species bosonic atoms with one species consisting of normal and the other hardcore 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. We assume that the normal bosonic species exhibits long range interactions, but the inter atomic interactions in the hardcore species are limited only to onsite interactions. The model Hamiltonian for such a system can be written as:

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

Here \( a_i \) and \( b_i \), respectively, are the bosonic annihilation operator for atoms of a (normal) and b (hardcore) 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 neighbours \( \langle ij \rangle \). \( U^a \) (\( V^a \)) is the on-site (nearest neighbour) intra-species repulsive interactions for the normal atoms. The inter-species (between normal and hardcore bosons) interaction is given by \( U^{ab} \). The hopping amplitudes \( t^a \) and \( t^b \) and interaction parameters \( U^a, V^a, U^{ab} \) are related to depth of the optical potential, recoil energy and the scattering lengths [13, 21]. The ratio \( U^{ab}/U^a \) as well as \( U^a/V^a \) can be varied over a wide range of values experimentally [22, 23]. In this work we consider \( t^a = t^b = t \) and set our energy scale by taking \( t = 1 \).

We identify various ground states phases of the model [11], by calculating (i) the single particle excitation gap \( G^a_L \) for species \( \alpha = a, b \) defined as the difference between the energies needed to add and remove one atom of species \( \alpha \); i.e., \( G^a_L = E_L(N_a + 1, N_b) + E_L(N_a - 1, N_b) - E_L(N_a, N_b) = E_L(N_a + 1, N_b) - E_L(N_a, N_b) - t^a \sum_{<i,j>} (a_i^\dagger a_j + \text{H.c.}) - t^b \sum_{<i,j>} (b_i^\dagger b_j + \text{H.c.}) + \frac{U^a}{2} \sum_i n_i^a (n_i^a - 1) + U^{ab} \sum_i n_i^a n_i^b + V^a \sum_{<i,j>} n_i^a n_j^a\).
$2E_L(N_a, N_b), G^a_L = E_L(N_a, N_b + 1) + E_L(N_a, N_b - 1) - 2E_L(N_a, N_b)$ and (ii) the on-site number density defined by

$$\langle n^a_i \rangle = \langle \psi_{LN_a,N_b}|n^a_i|\psi_{LN_a,N_b}\rangle. \quad (2)$$

Here $\alpha$, as mentioned before, is an index representing normal $(a)$ or hardcore $(b)$ bosons, with $N_a \ (N_b)$ corresponds to total number of $a \ (b)$ bosons in the ground state $|\psi_{LN_a,N_b}\rangle$ 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 one dimension the appearance of the SF phase is indicated by $G^a_L \rightarrow 0$ for $L \rightarrow \infty$. However, for a finite system $G^a_L$ is finite, and we must extrapolate to the $L \rightarrow \infty$ limit, which is best done by the finite size scaling of the gap [24, 25]. In the critical region

$$G^a_L \equiv L^{-1} f(L/\xi^a) \quad (3)$$

where $\xi^a$ is the correlation length for species $a$ which diverges in the SF phase. Thus plots of $LG^a_L$ versus the nearest neighbour 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, MI or CDW phase which is further distinguished from each other via the CDW order parameter defined as

$$O^a_{CDW}(L) = \frac{1}{L} \sum_i \langle \psi_{LN_a,N_b}|(n^a_i - \rho^a)|\psi_{LN_a,N_b}\rangle. \quad (4)$$

The existence of the solid order in the thermodynamic limit is verified from the finite value of $O^a_{CDW}(L \rightarrow \infty)$.

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 1D systems [24, 25, 26, 27]. For the normal species, we have taken the maximum occupation per site 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 weights of the states neglected in the density matrix of the left and right blocks are less than $10^{-6}$.

The charge density wave phase in boson systems is possible when the density of bosons is 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 $\rho = 1/2, 1$ [3, 20, 24, 28]. 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 neighbour interactions [29]. Supersolid phase is then possible only moving away from these commensurate densities. In a recent study on a Bose-Fermi mixture with different hopping amplitudes, the supersolid phase has been predicted without the nearest neighbour interactions by doping the bosonic species [18]. In order to achieve the supersolid phase in these systems, the interatomic interactions have been carefully controlled such that the added bosons do not destroy the CDW phase by occupying sites that are already occupied.

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 [30]. In order to avoid this condition, we consider $U^a = U^{ab} = U$ and study the effect of $V^a$ 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 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 neighbour tunneling amplitude $t = 1$.

$$\rho^a = \rho^b = 1/2: \text{ In this case the total density of bosons } \rho = \rho^a + \rho^b = 1. \text{ For } V^a = 0, \text{ the system is in the MI phase because the onsite intra species interactions, } U^a = 6, U^b = \infty \text{ and the inter species interaction, } U^{ab} = 6 \text{ are all greater than } U_C \approx 3.4, \text{ the critical strength of the on-site interaction for the SF-MI transition in the one-dimensional Bose-Hubbard model [24, 25, 30]. The system continues to remain gapped as } V^a \text{ increases. The gap corresponding to lattice size } L \text{ for species } a, G^a_L \text{ is plotted for different values of } V^a \text{ in Fig.11. This figure clearly shows that } G^a_{L \rightarrow \infty} \text{ is finite for all the values of } V^a \text{ that we have considered. However, the gapped phase at higher } V^a \text{ is not a MI but a CDW, since } O^a_{CDW}(L \rightarrow \infty) \text{ is finite for } V^a > V^a_G \approx 1.0. \text{ In Fig.2 we have plotted } O^a_{CDW}(L) \text{ versus } 1/L \text{ for different values of } V^a. \text{ The order parameter } O^a_{CDW}(L) \text{ goes to zero for small values of } V^a \text{ and branches out for higher values indicating the onset of the CDW phase. } O^b_{CDW}(L) \text{ also exhibits a similar behaviour indicating that both the normal and hard-core bosons undergo a MI to CDW transition. The dependence of this transition on } V^a \text{ for the normal bosons is expected on the basis of an earlier work [28]. However, it was not obvious that the hard-core 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 \text{ is the following: when } V^a = 0, \text{ due to the strong repulsion between the bosons, the system is in the MI phase with both normal and hard-core bosons uniformly distributed through out the lattice giving the average density of the total number of bosons at every site equal to one. As } V^a \text{ increases, there is competition between the interactions, } U^{ab}, U^a \text{ and } V^a \text{ and hence an atom of species } a \text{ (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 hardcore species \( b \) cannot occupy a site where there is either a hardcore 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 neighbour sites are occupied by atoms of different species as shown in (Fig.3). It is interesting to note that the presence of \( V^a \) is sufficient to induce the solid order in the hardcore 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.

\[ \rho^a = 1/2 \text{ and } \rho^b = 1/4 \]  

In this case the total boson density \( \rho = 3/4 \), and it is not commensurate with the lattice. In the present problem, we have not considered long range interactions beyond the nearest neighbour, the commensurate densities are therefore 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 \[30\]. However, such a transition does occur in a normal - hardcore boson mixture described by the model \[10\]. The finite size scaling of the gap \( LG^L \) that is obtained from our FS-DMRG calculation shows, a transition from the gapless SF phase to a gapped phase for the normal bosonic species in Fig.4. The critical value of \( V^a \) is \( V_c^a \approx 3.0 \). However, the hardcore species remains in the SF phase showing no gap in the excitation spectrum. The calculation of the CDW order parameters given in Fig.5 for both the normal and the hardcore bosons show a finite \( O_{CDW}^a \) in the limit \( L \to \infty \) for \( V^a > V_c^a \approx 3.0 \). Thus the gapped phase of the normal bosonic species is identified to be the CDW phase while the gapless phase of hardcore bosons is a supersolid since both sperfluid and CDW coexist. The CDW oscillations are similar to the case of \( \rho_a = \rho_b = 1/2 \) as given in Fig.3.

\[ \rho^a = 3/4 \text{ and } \rho^b = 1/2 \]  

The phase transitions that we have obtained for this case for the two species are in the reverse order as that of case (ii). The normal species shows a transition from the SF to the supersolid phase not showing any gap in the excitation spectrum (see Fig.6) and a finite CDW order parameter at \( V_c^a \approx 1.2 \) (see Fig.7). However, the hardcore species makes a transition from the SF to the CDW phase at the same critical point \( V_c^a \approx 1.2 \).

In recent experiments on dipolar atoms, it has been shown that the the ratio between the on-site interaction and the nearest neighbour interaction can be controlled by Feshbach resonance \[23\]. In the present work, we take
Conclusion:- We have considered a system of normal and hardcore 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 neighbour interaction strength $V^a$, the solid order can be stabilized in the normal bosonic species and it can also be induced in the hardcore 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 neighbour interaction strength of the hardcore species $V^a$, we obtain different interesting quantum phases which are listed in the table shown below.

| $\rho_a$ | $\rho_b$ | softcore | hardcore |
|----------|----------|----------|----------|
| 1/2      | 1/2      | MI-CDW   | MI-CDW   |
| 1/2      | 1/4      | SF-CDW   | SF-SS    |
| 3/4      | 1/2      | SF-SS    | SF-CDW   |
FIG. 7: Finite size scaling of $O_{CDW}$ for (a) softcore and (b) hardcore species for $V^a$ ranging from 0.8 to 2.4 in steps of 0.2 is shown for $\rho^a = 3/4$ and $\rho^b = 1/2$. It is clear from the scaling that the $O_{CDW}$ becomes finite for $V_c^a \sim 1.2$ for both the species indicating the transition to CDW phase.

If the individual density of a species is commensurate then there exists a SF-CDW or MI-CDW transition whereas if it is incommensurate then the transition is from SF to SS. It is interesting to note that for incommensurate fillings the transition from the SF phase to the CDW or SS phases occur at the same critical value $V_c^a$ for both the species.

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[1] A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP 29, 1107 (1969).