Quantum phases of two coupled $XXZ$ spin chains: A DMRG study

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We consider hardcore bosons in two coupled chains of one dimensional lattices at half filling with repulsive intra-chain interaction and inter-chain attraction. This can be mapped on to a coupled chain of spin-$1/2$ $XXZ$ model with inter chain ferromagnetic coupling. We investigate various phases of this spin model at zero temperature by density matrix renormalization group method. Apart from the usual superfluid, supersolid and density wave phases, pairing of inter chain bosons leads to the formation of novel phases like pair-superfluid and pair-supersolid states. We discuss the possible experimental realization of such correlated phases in the context of cold dipolar gas.

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I. INTRODUCTION

After successful experimental realization of dipolar Bose-Einstein-condensation (BEC) of $^{52}Ca$, $^{164}Dy$, and Rydberg atoms, possibility of finding exotic phases like superfluid, pair-superfluid, supersolid, pair-supersolid and charge density wave and phases involving quantum magnetism have increased tremendously. Usually bosons can form superfluid by condensation of bosonic particles to a single ground state, whereas fermionic superfluidity in superconductors and in cold atoms occurs due to the formation of pairs. For sufficiently strong attractive interactions, bosons can also form pairs which leads to the formation of ‘pair-superfluidity’ of bosons. Pair-superfluidity can be realized in cold atom systems by interspecies-attractive interactions, bilayer dipolar systems, and through Feshbach resonance. Theoretically ‘pair-superfluidity’ has also been studied in models with correlated hopping. Supersolid phase is described by simultaneous existence of crystalline order and superfluid order in the system. Various experimental and theoretical studies have been carried out for finding supersolidity. Bilayer dipolar systems also provide existence of pair-supersolid (PSS) phase. Pair-supersolid is defined as a phase where one finds simultaneous existence of pair-superfluidity and modulation in density, with vanishing single-particle superfluidity. Interestingly, PSS phase has been studied theoretically by considering polarized dipolar particles in two decoupled 2D layers, and solving effective extended Bose-Hubbard Hamiltonian in the low-energy subspace of pairs, by means of a mean-field Gutzwiller approach and exact diagonalization methods. In fact, PSS phase has also been proposed in two-species Bose-Hubbard model in a two-dimensional square lattice by using quantum Monte-Carlo simulations. Recently, there has been studies, on extended Bose-Hubbard model with atom hopping and atom-pair hopping in a triangular lattice, by quantum Monte Carlo methods, where pair supersolid phase has also been obtained in its phase diagram.

Low dimensional quantum systems are quite unique, as in low dimension, a number of quantum fluctuations emerge, due to which these systems cease to show true long range order (LRO). Instead, the low dimensional systems quite often show quasi long range order (QLRO), if the correlation length is of the order of the system size. Incidentally, for the system to show QLRO, the equal-time correlation functions, $<\psi^\dagger(\mathbf{r})\psi(\mathbf{0})>$, would decay algebraically as $R(\mathbf{r})\sim |\mathbf{r}|^{-\alpha}$ with finite $\alpha$. However, if the correlation function decays exponentially, the system shows short range order (SRO). For bosonic low-dimensional systems, there have been studies where a number of phases, namely, superfluid, pair-superfluid, and supersolid phases have been reported.

In this work, we have studied a two-leg ladder system consisting of spin-half at every site of the ladder with two chains. We solve the Hamiltonian by using density matrix renormalization group (DMRG) method. DMRG is a very powerful and accurate method for finding ground state energy, equal time correlation functions of low dimensional strongly interacting systems. Since a spin-$1/2$ object is equivalent to a hard core boson, as a spin-half with two states (↑ and ↓) can be exactly mapped to a hardcore boson with two states (with 0 particle and 1 particle). Although, here we have worked on spin half model, at times, we specify the spin results in terms of hard core bosons. We have found homogeneous phase, where spins are ordered in the X-Y plane, which is equivalent to single particle superfluidity (SF) in terms of hard core bosons. When the spins are ordered in the X-Y plane as well as along the z-axis (the so called mixed phase) in bosonic terms, the system behaves as a supersolid. However, with sufficient increase in the attractive interactions along the rungs of the ladder, system has quasi pair-superfluid phase. However, if moderate repulsive interaction is present, there exists quasi-pair-supersolid phase, where the pairs of spins are ordered along the z-axis as well as in the X-Y plane. In the limit of large attractive and repulsive interactions, we found collinear anti-ferromagnetic phase (↑↑↓↓↑↑...). This phase corresponds to the density wave (↑↑↑↑↑↑...).
II. MODEL HAMILTONIAN AND METHODS

We start with hard core bosons with dipolar interaction in two leg ladder with an effective Hamiltonian taking only nearest-neighbour interactions.

\[
H = -t \sum_{\alpha,\langle i,j \rangle} \left( b_{\alpha,i}^+ b_{\alpha,j} + h.c. \right) + V \sum_{\alpha,\langle i,j \rangle} \hat{n}_{\alpha,i} \hat{n}_{\alpha,j} - U \sum_i \hat{n}_{1,i} \hat{n}_{2,i}
\]

where \( \alpha \) is the chain index, \( t \) is the hopping term within the chains, \( V \) is the strength of intra-chain nearest-neighbour repulsion, \( U \) is the strength of inter-chain attraction. As spin-1/2 operator and hard core boson operator obeys same commutation relation, we can transform hard core boson operator to the spin 1/2 operators \( b_{\alpha,i} \rightarrow s_{\alpha,i}^\pm \), \( s_{\alpha,i} \rightarrow b_i \) and \( s_{\alpha,i}^z \rightarrow n_i - 1/2 \). The final spin Hamiltonian turns out to be for two coupled XXZ chains

\[
H = -t \sum_{\alpha,\langle i,j \rangle} \left( s_{\alpha,i}^+ s_{\alpha,j}^- + h.c. \right) + V \sum_{\alpha,\langle i,j \rangle} s_{\alpha,i}^z s_{\alpha,j}^z - U \sum_i s_{1,i}^z s_{2,i}^z
\]

III. DISCUSSION OF NUMERICAL RESULTS

To characterize different phases, we have calculated spin-density, two points and four points correlation functions and the corresponding structure factors. We first discuss about on-site spin-density, \( < s_{\alpha,i}^z > \), for each chains. We found for lower values of \( U \) and \( V \), expectation value, \( < s_{\alpha,i}^z > \), turns out to be zero for all sites, \( i \), while for larger values of \( U \) and \( V \), \( < s_{\alpha,i}^z > \) has non-zero values and the quantity is same for the both chains. In Fig.2, we show the expectation value of \( < s_{\alpha,i}^z > \) with site index \( i \) for each chains. For \( U = 0.4 \) and \( V = 0.4 \), on-site spin-density, \( < s_{\alpha,i}^z > \), is zero, while for \( U = 2.4 \) and \( V = 2.4 \), \( < s_{\alpha,i}^z > \), takes nonzero values. In fact, since \( U \) term is negative, the rung spins make parallel pairs. With increase in \( V \) values the neighbouring rungs spins become anti-parallel to minimize repulsive interaction. As shown in the inset of the Fig.2, such a configuration with parallel spin within each rungs and anti-parallel spin within each chain of the ladder structure can be represented as \( \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \ldots \), a collinear state.

To solve the above Hamiltonian and to find various possible quantum phases in the parameter space, we have used Density-matrix renormalization group method (DMRG) considering spin-1/2 in every site. We have calculated properties of systems with size up to 256 sites, varying DMRG cut-off (max = \( m \)) from 200 to 400, with consistent results however, below we have given results with \( m = 200 \), unless other wise stated. We have used open boundary condition for both chains. We have compared our DMRG results, namely energy and properties with results from exact diagonalization, up to 28 lattice sites and the results compare fairly well. For all of our numerical simulation below, we have set \( t = 1 \) and express all the parameters in units of \( t \).

For calculating short or quasi-long-range order of spin along X-Y plane and along z-axis through correlation functions, we have first shown the results corresponding to these parameter values: \( U = 0.5 \), \( t = 1.0 \) and a number of \( V \) values varying from 0 to 2. The transverse spin-spin correlation function is defined as \( C_\alpha(r) = \langle S_{\alpha,i}^z S_{\alpha,r}^z \rangle \) where \( \alpha \) is the chain index of the ladder and \( r \) is the distance from middle part of the chain. To reduce finite size effect, we have calculated correlation function, \( C_1(r) \), of chain length 128, where total system size is 256. Algebraic decay of correlation function \( C_1(r) \), is fitted with straight line, as a function of \( r \) on a log-log scale and the exponent is termed as \( \gamma \). For the power law fitting of correlation function, \( C_1(r) \), we took only data from distance 10 to 46, so that effect of boundary and finite size are reduced. As shown in Fig.3, the transverse correlation function, \( C_1(r) \), decays algebraically, for \( U = 0.5 \) and \( V = 0.4, 0.9 \), with exponent \( \gamma \sim 0.74 \) and 0.98 respectively. In fact, the correlation function, \( C_1(r) \), decays algebraically up
to $V \sim 1.1$ for $U = 0.5$. We found exponent ($\gamma$) of the correlation function, $C_1(r)$, in the superfluid phase nearly equal to one. One can also obtain signature of superfluidity by calculating second moment of correlation function\textsuperscript{20} given as $\zeta = \sum_i r^2 C_1(r)/\sum_i C_1(r)$. As shown in the inset of the Fig.3, plot of correlation length, $L/\zeta$, versus attractive interaction $V$, by the coalescence of the curves, for different system sizes of length $L = 192, 224, 256$, give signature of transition from superfluid to density wave at $V \sim 1.1$. From these extensive calculations, we find that the system has quasi long range order in the X-Y plane up to $V \sim 1.1$ for $U = 0.5$. In terms of hard core boson language, this scenario corresponds to single particle superfluidity in the system. The structure factor defined as, $C_1(k) = \frac{1}{L} \sum_i \exp(ik \cdot r) \langle s_{1,0}^z s_{1,r}^z \rangle$, has peaks at $k = 0$ for lower values of $V$, while, the strength of the peak in $C_1(k)$ decreases with increase in $V$ and $U$ values.

For characterizing order along z-axis (density wave), we have calculated the correlation function $G_\alpha(r) = \langle S_{\alpha,0}^z S_{\alpha,r}^z \rangle$. In Fig.4, we have shown the correlation function $G_1(r) = \langle S_{1,0}^z S_{1,r}^z \rangle$, where $r$ is the distance between spin sites of the first chain for $V = 0.4, 0.9$ and 1.4. To find transition along z-axis more precisely, we took average of expectation values of correlation function $G_1(r)$ taking data from the bulk, $O_G = \langle \sum_r |G(r)| \rangle$ where average is over site index, and $r$ is taken after discarding quarter length from both sides of the length of the chain(of correlation function), so that effect of boundary and finite size will be small. For minimizing finite size effect, we have done finite size scaling of $O_G$ for system size lengths $L = 96, 128, 160, 192, 224$ and 256. Considering $G_1(r)$ for these six L values, we have fitted the curve with function $a0 + a1/L + a2/L^2$, as shown in the inset of Fig.4. As can be seen there is no order along z-axis for $V \sim 0.8$, while for $V > 0.8$, nonzero value of $O_G$ in thermodynamic limit gives signature of order along z-axis.

The mixed phase (quasi-supersolid) which is believed to be present in the system for finite values of attractive interaction $U$ and moderate values of $V$. In this phase system has order along z-axis as well as in the X-Y plane. From comparing Fig.3 and Fig.4, we can see that system has quasi-supersolidity for $U = 0.5$ and $V$ in the range of $V \sim 0.8$ to 1.1, as system has both diagonal (Density Wave) and quasi off-diagonal (superfluid) orders present in this range. For $V > 1.1$, the system has only order along z-axis which corresponds to density wave phase in the large V region of the phase space.

With increase in $U$, spins start making pairs along the rungs of the ladder and for sufficiently large $U$, spins get dimerized. The signature of the dimerization can be seen through pair-pair correlation function, density-density correlation function, and in terms of the number of pairs. To find the phase coherence between pairs, we have calculated pair-correlation functions, defined as, $P(r) = \langle S_{1,0}^z S_{2,0}^z S_{1,r}^z S_{2,r}^z \rangle - \langle S_{1,0}^z S_{1,r}^z \rangle \langle S_{2,0}^z S_{2,r}^z \rangle$, where 1 and 2 stand for chain indices of the ladder and $r$ is the site index on each ladder. We have calculated pair-correlation function with max $m = 400$. The algebraic decay of pair-correlation function, $P(r)$, is fitted with straight line, as a function of $r$ on a log-log scale and the exponent is termed as $\eta$. As shown in the Fig.5, pair correlation, $P(r)$, decays algebraically for $U = 1.8$, $V = 0.0$ and 0.3 with exponent $\eta \sim 0.81$ and 1.03 respectively. In terms of hardcore boson, this is the quasi pair-superfluidity phase, where single particle superfluidity cease to exist. To show the effect of repulsive interaction $V$, on the pair-superfluidity of the system, we have calculated $P_{uv} = \langle \sum_r P(r) \rangle$, where average is over the site index, for system size $L = 256$. We have discarded around one fourth of the data so that boundary effects are less. As shown in the inset of Fig.5,
we have plotted $P_{av}$ versus $U$ with different values of $V$, for system size of length $L = 256$. We found that pair superfluidity decrease, sharply with increase in $V$. The number of pairs in the system can be defined as, $N_{pair} = \sum_s <s_i^z s_{i+1}^z>/N$, where 1 and 2 are the chain indices and $i$ is the site index of the ladder. For small values of $U$, since the system has large fluctuation effects, the number of spin pairs is quite small, while the same increases with increase in the $U$ values. The details of this is shown in the inset of the Fig.5.

![FIG. 5. Plot of correlation functions $P(r)$, as a function of $r$ on a log-log scale, for $U = 1.8$ and with different value of $V$: $V = 0.0$ (star), $V = 0.3$ (cross). In the first inset, $N_{pair}$ is plotted against $U$ and in the second inset $P_{av}$ with $U$ for different values of $V$.](image)

The phase corresponding to parallel rung spins and anti-parallel neighbours spins (large $U$ and $V$ limits), can be characterized by, $G(l) = \langle s_i^z s_{i+1}^z \rangle$ where $l$ is the site index for total system. As shown in Fig.6, we found that the spins make pairs along the rungs of the ladder and get dimerized with increase in $U$ and $V$, in such a way that they dimerize giving rise to an alternating spin arrangements (collinear arrangements) in the system (see schematic in Fig.2). In the bosonic language, dimerization of spins along the rungs of the ladder is equivalent to density wave (DW) of strongly bound pairs. Structure factor, defined as, $G(k) = \frac{1}{N} \sum_l \exp(ik \cdot l) \langle s_i^z s_{i+1}^z \rangle$, has peaks at $-\pi/2$ and $\pi/2$ for higher values of $U$ and $V$.

The other interesting phase is quasi pair-supersolid phase (PSS), which occur for sufficiently high value of $U$ and moderate values of $V$. Pair-supersolid phase, which is defined as simultaneous existence of pair-superfluidity and density wave phases, with vanishing single-particle superfluidity. For example, as shown in the Fig.5, $P(r)$, decays algebraically and in Fig.6, there is also density wave order for $U = 1.8$ and $V = 0.3$. With increase in repulsive interaction, $V$, system loses phase coherence and make density-wave of tightly bound-pairs. This scenario is same like pseudo-gap phase in fermionic system where system have strong bound pairs although phase coherence (pair-superfluidity) is very small.

![FIG. 6. Plot of correlation functions $G(l)$, as a function of $l$, for $U = 1.8$ and with different value of $V$: $V = 0.0$ (star), $V = 0.3$ (circle) and $V = 0.7$ (square). In the inset, plot of structure factor $G(k)$, at $V = 0.7$ and $U = 1.8$.](image)

![FIG. 7. Two dimensional phase diagram in the phase space of two parameters, $U$ and $V$. The phase diagram is quite rich with many phases, namely, Single-particle superfluid (SF), supersolid (SS), pair-superfluid (PSF), pair-supersolid (PSS) and Density wave (DW) phases.](image)

To obtain complete phase diagram in the $U-V$ plane, we have calculated all the required quantities with varying $U$ and $V$ values from 0.0 to 2.5 and 0.0 to 2.5, respectively, all in units of $t = 1$. The phase diagram is shown in Fig 7. As can be seen, for the low values of $U$ and $V$, the system has quasi-long range order in the X-Y plane (single-particle superfluidity, SF phase). In this case, the effect of fluctuation is quite large and there is no order along the z-axis. With increase in $U$ and $V$ values, the system develops a phase where there is QLRO order in the X-Y plane as well as along the z-axis. This is the so called ‘mixed phase’. In fact, in terms of bosonic terms, it is supersolid phase (coexistence of density wave and single particle superfluid phases) and this appears for the intermediate values of $U$ and $V$ values. In fact, for sufficiently large attractive interaction, $U$, and small re-
pulsive, $V$ values, the spins along two chains make strong pairs, forming a dimerized phase. In such a phase, flipping of a single spin costs large energy, while it costs less to flip the pairs of spins (rung pairs). Therefore, in this limit, there is quasi-pair-superfluidity in the system without the trace of single particle superfluidity. With this limit, there is quasi-pair-superfluidity in the system less to flip the pairs of spins (rung pairs). Therefore, in flipping a single spin costs large energy, while it costs pairs, forming a dimerized phase. In such a phase, flip-

IV. CONCLUSION

In summary, we studied various phases of spin-half particles in two coupled chains, with inter chain attraction and intra chain nearest neighbor repulsion between the spins. Which is equivalent to hardcore bosons in two coupled one dimensional lattices at half filling. When two chains are completely decoupled, the bosons can undergo a transition from superfluid to density wave phase by increasing the nearest-neighbour repulsion. The attractive inter chain interaction leads to the formation of ‘supersolid’ phase and pairing of bosons in two different chains. In the atomic limit the ground state of the system is density wave of strongly bound pair of bosons. For sufficiently strong inter chain attraction and by increasing the hopping strength, the DW phase of pairs melts and forms ‘paired supersolid’ phase. In this novel phase the pairs of bosons have phase coherence as well as density ordering. Finally a homogeneous paired superfluid state is formed by increasing the hopping strength. When the inter chain attraction is sufficiently strong, the pairs of bosons hop to nearest neighbor sites in correlated manner and two coupled spin chains become similar to a single chain of spin-1 XXZ model.

The model discussed in this article is a simplified description of bilayer dipolar bosons with dipole moments perpendicular to the plane. Although we truncated the long range dipolar interaction to nearest neighbour repulsion, this model contains essential ingredients for the formation of ‘pair superfluid’ and ‘pair supersolid’ phases. Inclusion of longer range interaction can lead to the formation of various density wave phases and supersolid phases with different patterns. Similar to the BCS-BEC crossover of fermions, in this system bosons can undergo transition from weakly bound paired superfluid state to paired supersolid phase and finally to density wave of strongly bound pairs.

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