Anomalous pairing of bosons: Effect of multibody interactions in an optical lattice

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Abstract

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Anomalous pairing of bosons: Effect of multibody interactions in an optical lattice

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A first-order type phase transition between Mott lobes has been reported in Phys. Rev. Lett. 109, 135302 (2012) for a two-dimensional Bose-Hubbard model in the presence of an attractive three-body interaction. We revisit the scenario in systems of ultracold bosons both in one- and two-dimensional lattices using the density matrix renormalization group method and the self-consistent cluster mean-field theory approach, respectively. We show that an unconventional pairing of particles occurs due to the competing repulsive two-body and attractive three-body interactions. This leads to a pair superfluid phase sandwiched between the Mott insulator lobes corresponding to densities density one and three in the strongly interacting regime. This is in contrast to the direct first-order jump as predicted before. Interestingly, the Mott to pair superfluid phase transitions are found to be continuous in nature. We also show that the pair superfluid phase is robust with respect to the ratio between the two- and three-body interaction strengths. In the end, we establish a connection between the Bose-Hubbard model presented in Phys. Rev. Lett. 109, 135302 (2012) with a more general Bose-Hubbard model and analyze the fate of the pair superfluid phase in the presence of an external trapping potential.

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I. INTRODUCTION

Ultracold atoms in optical lattices offer an exquisite control over the system parameters such as the tunneling and interaction among atoms and have led to the observation of numerous interesting phenomena, such as the superfluid (SF)-Mott insulator (MI) transition for bosons following its theoretical prediction [1,2]. A strong on-site two-body repulsion which can be controlled by the technique of Feshbach resonance or by tuning the laser intensity freezes the particle motion in the lattice and drives the system from the SF phase to MI phase. In addition to the two-body interaction, ultracold atomic systems in optical lattices also possess on-site three- and higher-body interactions whose natural existence has been found in a recent experiment [3]. It is to be noted that a small attractive interaction in an optical lattice leads to the collapse of all the atoms onto a single site [4]. In such a scenario a tunable three- or higher-body interaction stabilizes the system against collapse, e.g., a very strong three-body repulsion could prevent more than two atoms per site and an ensemble of pairs of bosons can be created. Under proper conditions of density and two-body interactions, the system exhibits a pair superfluid (PSF) phase which can be characterized by the finite off-diagonal long-range order of composite particles or pairs. The infinitely strong three-body interaction can arise as a result of three-body loss process due to the elastic scattering of atoms [5]. Moreover, proposals have been made to engineer such three-body as well as higher-order interactions in bosonic lattice systems in a controlled manner [6–8].

The effect of three-body interaction on the SF-MI transition has been a topic of interest recently in the context of the Bose-Hubbard model. As mentioned before, a critical two-body attraction between atoms and three-body hardcore constraint may lead to the PSF-SF/ASF (atomic superfluid) transition [5,9–11]. On the contrary, for two-body repulsive interaction, the MI lobe for density $\rho > 1$ expands (shrinks) for repulsive (attractive) three-body interaction [10,12]. It is to be noted that the large three-body attraction will eventually lead to collapse. Hence, a strong four-body repulsion is required which can stabilize the system against such a collapse [12].

In this paper we study the Bose-Hubbard model with a tunable three-body interaction which has been introduced earlier in Ref. [13]. We rigorously analyze the ground-state properties both in one (1D) and two dimensions (2D) and obtain complete phase diagrams in both cases. Interestingly, we find that there exists a pairing phenomenon of bosons in the regime of strong interaction even though the two-particle interaction is repulsive in nature. As a result of this a PSF phase appears in the phase diagram which is sandwiched between the Mott lobes corresponding to $\rho = 1$ and $\rho = 3$. This contradicts the previous prediction of the direct first-order transition between the Mott lobes as presented in Ref. [13]. Moreover, we show that the MI-PSF-MI transitions are continuous phase transitions. A detailed analysis is presented in the following sections.

The rest of the paper is arranged as follows. In Sec. II we describe the model and methods we have used for our study. This is followed by Sec. III in which we present our results for 1D and 2D cases with detailed discussion on various order parameters used. In this section we also provide a comparison between the CMFT and QMC data in two dimension. Section IV gives a brief discussion of experimental feasibility of the PSF phase. Finally, we give a brief conclusion of our results in Sec. V.
II. MODEL AND METHOD

Recently, in a proposal, it was shown that the three-body interaction can be engineered in such a way that it affects only the triply occupied sites [13]. This special form of the three-body interaction which is different from the conventional three-body interaction modifies the Bose-Hubbard model as

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + H.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) + W \sum_i \delta_{n_i,3},$$

(1)

where $a_i^\dagger$ ($a_i$) is the bosonic creation (annihilation) operator, $n_i$ is the number operator for the $i$th site, and $i$, $j$ are site indices. $U$ and $W$ are the on-site two- and three-body interactions and $t$ is the hopping amplitude between the nearest neighbor sites ($i$, $j$). We scale all the physical quantities in our Hamiltonian by $t$ to make them dimensionless.

It was shown that model (1) exhibits shrinking of the MI ($\rho$) lobes for $\rho = 2$ and $\rho = 4$ as a function of repulsive $U$ and attractive $W$ in a two-dimensional (2D) Bose-Hubbard model eventually leading to a first-order transition from the MI(1) to MI(3) lobe [13]. This first-order transition was attributed to the suppression of double occupancy in favor of triply occupied sites in the limit of dominant three-body attraction. In this limit, the doping of particles (holes) in MI(1) [MI(3)] lobe plays a very important role. In such a scenario we first investigate this model in one dimension, wherein the correlation effects are maximum, and try to find out if such a phenomena can occur in lower dimensions. From our calculations we find that in the 1D case there exists an unconventional PSF phase sandwiched between the Mott lobes, in support of which we provide evidence in the form of density distribution, parity order parameter, correlation function, and momentum distribution calculations. Then we revisit the scenario given in the 2D case and find that the PSF in the 1D case is reproduced here as well. Once again we present density distribution and correlation function calculations to confirm our results. With the help of these results we therefore convincingly refute the claim of a direct first-order transition between the Mott lobes reported in Ref. [13]. Calculations in 1D and 2D were carried out using the density matrix renormalization group method (DMRG) and cluster mean-field theory (CMFT) approach, respectively. In the DMRG simulations we consider system sizes of up to 80 sites with 800 DMRG eigenstates and maximum number of bosons per site $n_{\text{max}} = 6$. We find that the ground state energy of our system converges and does not change for $n_{\text{max}} > 6$. In the CMFT calculations we consider cluster sizes up to six sites which is sufficient to capture the underlying physics as shown below.

III. RESULTS AND DISCUSSION

A. One-dimensional case

In this section we present our results for the 1D case by analyzing the Bose-Hubbard model given in (1) using the density matrix renormalization group (DMRG) method [14]. By considering repulsive $U$ and attractive $W$, we obtain the complete phase diagram for a fixed ratio of $W/U$. Interestingly, in this case, we see a counterintuitive situation where bosons pair up to form a PSF phase. This anomalous PSF phase is sandwiched between the MI(1) and MI(3) lobes for large values of interaction strengths as shown in the DMRG phase diagram in Fig. 1(a). We discuss the details of the phases and phase transitions shown in Fig. 1(a) in the following paragraphs.

The phase diagram of Fig. 1(a) shows different quantum phases, namely, the MI(1), MI(3), ASF, and the PSF phases. We fix the ratio $W/U = -1.5$ and vary $U$ to obtain the complete phase diagram. The gapped MI phases are identified by analyzing the density ($\rho$) as a function of chemical potential ($\mu$) [15]. The plateaus in the $\rho$-$\mu$ plots characterize the MI phases, whereas the superfluid phases appear around the Mott plateaus [15]. The areas bounded by the black lines are the MI lobes, the shaded region bounded by red dots between the two MI lobes is the PSF phase, and the remaining space is the ASF phase.

The existence of the PSF phase can be seen in the $\rho$-$\mu$ curve shown in Fig. 2(a) for a cut through the phase diagram in Fig. 1(a) at $t/U = 0.053$. In the region between the plateaus at $\rho = 1$ and 3, the density jumps in discrete steps with respect to the chemical potential which is a signature of the superfluid phase. Within the superfluid region, the PSF phase can be discerned by the characteristic finite system size behavior which exhibits a series of jumps of $\Delta N = 2$, whereas the jump of $\Delta N = 1$ particle indicates the ASF phase. Here $N$ is the total particle number of the system. The subplots Figs. 2(b) and 2(c) show a zoomed in section of PSF and ASF regions. The plateaus at $\rho = 1$ and 3 indicate the MI(1) and MI(3) phases, respectively. The formation of PSF phase between the Mott lobes can be represented by sketch given in Figs. 1(b), 1(c) and 1(d).

The emergence of the PSF phase in a model with repulsive two-body interaction can be understood from the analysis of
possible doping of particle (holes) from the MI(1) [MI(3)] phases in the regime of a strong coupling $t \ll U, W$. As a result, when the chemical potential increases gradually after the MI(1) region, the system accumulates two particles at a time to minimize the energy. Eventually the system enters into the MI(3) phase at $\rho = 3$ skipping the MI(2) phase. As the uniform MI(1) phase in the background provides a constant repulsive interaction, a pair of particles can always hop around the lattice without any cost of energy [Fig. 1(a)]. Within the limit of $t \ll U, W$, we may estimate this effective pair hopping amplitude as $\sim \frac{\delta t^2}{U+W}$. Hence, contrary to the mean-field analysis, for any $0 < t \ll U, W$ between the MI(1) and MI(3) lobes, an intermediate region of superfluid pairs may be found. For small $0 < t \ll U, W$ the distance between MI(1) and MI(3) boundaries increases with $\sim t^2/(U - W)$ as is clearly observed in Fig. 1(a).

In order to further understand this pairing phenomenon, we analyze the parity order which has been measured in the ultracold quantum gas experiments recently [16,17].

The parity order parameter is defined as

$$O^2_p(i, j) = \langle e^{i \sum_{k < l} \pi n_k} \rangle. \quad (2)$$

Here $n_k$ stands for the number operator at the $k$th site. In Fig. 3 we plot the parity order $O^2_p \equiv O^2_p(L/4, 3L/4)$ as a function of $(t/U)$ for different system sizes ($L$) at filling $\rho = 2$. The order parameter $O^2_p$ is finite in the PSF phase and gradually vanishes in the ASF phase as the system size increases and the point of vanishing parity order parameter approaches the critical value $(t/U)_c \approx 0.045$ for the PSF-ASF transition. To determine the order of PSF-ASF transition, we calculate fidelity susceptibility [18] at the critical point which is given by

$$\chi_{FS}(t) = \lim_{\delta t \to 0} \frac{-2 \ln |\langle \Psi_0(t) | \Psi_0(t + \delta t) \rangle|}{(\delta t)^2}. \quad (3)$$

with $|\Psi_0(t)\rangle$ being the ground-state wave function for a tunneling $t$ and $\delta t$ is a small parameter. In Fig. 4 we plot $\chi_{FS}(t)/L$ for different values of $t/U$ across the PSF-ASF phase transition at $\rho = 2$ for $L = 20, 40$, and 80 sites. As the system size increases, the $\chi_{FS}/L$ develops a distinct divergent single peak at $t/U \approx 0.045$ which is the critical point of the PSF-ASF transition at $\rho = 2$. The linear scaling of the peak-height ($\chi_{FS}^{\text{max}}/L$) with respect to its wings in the inset of Fig. 4 confirms the Ising character of this phase transition [19–21]. We also
correlation function \((G)\) for a broad range of parity order parameter it is clear that the PSF phase can exist for the entire parameter space. This is complemented by the \(\rho\) plot for different system sizes in Fig. 6(a). From the behavior of any finite jumps, even for larger system sizes, clearly signals a continuous phase transition.

Another evidence of the PSF phase can be found by looking at the long-distance scaling of pair-pair correlations in real space. We therefore plot single particle \((G)\) and pair \((G^p)\) correlation functions for a fixed value of \(t/U\) when \(\rho = 1.25\) the system is in the PSF phase and hence \(G(\text{black } \times)\) decays exponentially while \(G^p(\text{red } \circ)\) remains substantially large and decays algebraically. On the other hand, for the same value of \(t/U\) when \(\rho = 2.25\), the system is in the ASF phase and hence \(G(\text{green } +)\) shows clear algebraic form, whereas \(G^p(\text{blue } \square)\) decays at a faster rate. This behavior is consistent with the one reported in Ref. [5] for an ASF-PSF transition.

We continue our analysis further to find out the fate of this newly found PSF phase by moving away from the ratio \(W/U = 1.5\). To achieve this, we look into the parity order parameter \(O^2\) as defined before and plot it with respect to \(W/U\) for different system sizes in Fig. 5(a). It can be seen that the absence of any finite jumps, even for larger system sizes, clearly signals a continuous phase transition.

In Figs. 6(b)–6(d) we plot \(n(k)_{\text{single}}\) and \(n(k)_{\text{pair}}\) with respect to \(k/\pi\) for three different values of \(W/U\) ratios. At \(W/U = -2.0\) [Fig. 6(b)] the system is deep into the PSF phase, hence \(n(k)_{\text{pair}}\) (black dashed line) exhibits a sharp peak at \(k/\pi = 0\) while \(n(k)_{\text{single}}\) (red solid line) remains almost flat. Whereas at \(W/U = -1.0\) [Fig. 6(c)] this trend is reversed, indicating that the system is predominantly in the ASF phase. Finally, when \(W/U = -0.5\) [Fig. 6(d)], both \(n(k)_{\text{single}}\) and \(n(k)_{\text{pair}}\) peaks at \(k/\pi = 0\) disappear indicating that the ASF/PSF regions are replaced by gapped MI phase.

**B. Two-dimensional case**

With the insights into the emerging PSF phase in between the MI lobes for the 1D chain, one may ask why the above mentioned arguments of boson pairing will not hold for a two-dimensional optical lattice system? To this end we reinvestigate the two-dimensional Bose-Hubbard model, using a self-consistent cluster mean-field theory (CMFT) approach [22] in the grand canonical ensemble. The CMFT approach works very well for the simple models like Eq. (1) and matches fairly well with the quantum Monte Carlo results, as discussed in the subsection towards the end of this section. Within the CMFT approach, we decompose the model Hamiltonian (1) to clusters of connected sites \(C\) parqueting the lattice, with the effective Hamiltonian of a cluster being described by

\[
H_C = H_{\text{exact}} + H_{\text{mf}}
\]

Here \(H_{\text{exact}}\) is the exact Hamiltonian (1) of the cluster and \(H_{\text{mf}}\) describes the mean-field decoupled terms connecting the cluster to its neighbors and is given as

\[
H_{\text{mf}} = -t \sum_{i,j \neq 0,C} (a_i^\dagger \phi_j - \phi_i^\dagger \phi_j + \text{H.c.})
\]

The cluster Hamiltonian is then solved in a self-consistent way with respect to \(\phi_i\) \((= a_i)\). Within our CMFT approach considered for model (1), it is difficult to clearly determine the
order of the MI(1)-PSF-MI(3) and the PSF-ASF transitions as the PSF order parameter vanishes. Therefore, we include second-order terms in tunneling in the Hamiltonian (1) to understand the order of these transitions. In the strong coupling limit $t \ll U, W$ within second-order perturbation theory we find an effective two-particle hopping amplitude of $t_{\text{eff}} = t^2/(U - W)$. We may explicitly include such second-order tunneling terms in the mean-field Hamiltonian of the CMFT approach in order to obtain a better resolution of the PSF phase. In particular we employ

$$
\tilde{H}_{\text{mf}} = H_{\text{mf}} - t_{\text{eff}} \sum_{i,j \in \mathcal{C}} \left( \langle a_i \rangle \bar{\psi}_j - \bar{\psi}_i \psi_j + \text{H.c.} \right)
$$

with $\psi_j = \langle a_j^\dagger \rangle$. By using a four-site cluster and analyzing the ground state properties we obtain the complete phase diagram as shown in Fig. 7. Interestingly, in this case also, we obtain a finite region of PSF phase which survives between the MI(1) and MI(3) phases. This result is in contrast with the direct first-order MI(1)-MI(3) phase transition shown in Ref. [13]. The inset of Fig. 7 shows the zoomed in region depicting the PSF phase.

The phase diagram in Fig. 7 is obtained by the analysis of the behavior of density $\rho$ and the superfluid density $\rho_s = \phi^2$ (where $\phi$ is the superfluid order parameter) with respect to the chemical potential $\mu$. We plot $\rho$ and $\rho_s$ with respect to $\mu$ along a cut through the CMFT phase diagram of Fig. 7 for $zt/U = 0.05$ which passes through the MI(1), PSF, and MI(3) phases in Fig. 8(a). The discrete jumps in the $\rho-\mu$ plot (red circles) in steps of $\Delta N = 2$ indicate the PSF phase as shown in Fig. 8(a). The plateaus at $\rho = 1$ and $\rho = 3$ are due to the MI phases. The value of $\rho_s$ (blue diamonds) is zero throughout the cut. Furthermore, in Fig. 8(b) we plot two-site correlation functions for a single particle and a pair of particles of the form $C_{1p} = \langle a_i^\dagger a_j \rangle$ (red circles) and $C_{2p} = \langle a_i^\dagger a_j^2 \rangle$ (blue triangles) for $i = 1, j = 2$. It can be seen that $C_{2p}$ is significantly larger than $C_{1p}$ which confirms the existence of the PSF phase.

Although we have reported the above results for the case when the ratio $W/U = -1.5$, we further investigate the system using the CMFT method to establish the robustness of the PSF phase at other ratios as well, as done in the 1D case before. To this end, we analyze the behavior of $\rho$ as a function of $\mu$ for different ratios of $W/U$. The $W/U$ ratios considered are $-1.2$, $-1.4$, $-1.6$, and $-1.8$ for a fixed value of $zt/U = 0.02$. The density jumps in steps of two particles given in Fig. 9 show that the PSF phase exists for a wide range of $W/U$ and is robust with respect to change in the value of this ratio, which is an important feature from an experimental point of view.

We identify the order of the phase transitions across the MI-ASF boundaries from the behavior of $\rho-\mu$ and hysteresis curves. The first-order (continuous) phase boundary is marked as a solid (dashed) line in Fig. 7. The solid green circles correspond to the tricritical points. The MI-ASF transition boundaries constitute both first-order as well as continuous regions. This can be understood by observing the ground state.
FIG. 10. $E(\phi) - E(\phi = 0)$ vs $\phi$ around the critical chemical potential ($\mu_c = 18.2217$) across the MI-ASF phase boundary for $zt/U = 0.14$. The merging of three degenerate minima indicates a first-order transition which is further confirmed by the hysteresis curve (inset) behavior at this point.

FIG. 11. $E(\phi) - E(\phi = 0)$ vs $\phi$ around the critical chemical potential ($\mu_c = 12.7828$) across the MI-ASF phase boundary for $zt/U = 0.17$. The merging of two degenerate minima into one indicates a second-order transition.

FIG. 12. Density and order parameters with second-order tunneling terms for a cut along $\mu/U = 0.751$ in Fig. 7. Order parameters vary in a continuous manner across MI(3)-PSF and PSF-ASF phase boundaries indicating that these are second-order phase transitions.
are denoted as $\times$, whereas the $\square$ represent the corresponding QMC data. The figure shows a very good matching between both results obtained from both the method except in the region where the PSF phase occurs.

**IV. EFFECT OF EXTERNAL TRAPPING POTENTIAL**

In the following we discuss the fate of the PSF phase in the presence of an external confining potential. As the PSF phase is very narrow compared to the MI lobes, one can consider a suitable trapping potential to see the PSF region. In our calculation we consider $V_{\text{trap}} = 0.002$ and take a cut through the phase diagram corresponding to $zt/U = 0.05$. Keeping the trap center just inside the MI(3) phase by fixing $\mu/U = 0.753125$ we obtain the density profile as shown in Fig. 14. A clear wedding cake structure depicting the MI plateaus and the intermediate PSF phase is obtained which we map and show here in two dimensions for clarity. The black region is the MI(1) phase and the central bright spot is the MI(3) phase. The region in between these two MI phases is the PSF phase. This PSF phase can possibly be detected by using a very recently demonstrated sophisticated technique of single-atom and single-site imaging [25]. The detection scheme discussed therein is free from the problem of parity projection in quantum gas microscopes and can easily detect individual atoms (up to three) at a given site.

Note that the results discussed above for the model given in Eq. (1) can be achieved by starting from the conventional form of the three-body interaction $\frac{\hbar}{2} \sum_{i,j,k} n_i n_j n_k$ and including a four-body interaction $\frac{\hbar}{2} \sum_{i,j,k,l} n_i n_j n_k n_l$ in the most general Bose-Hubbard model which has been observed in the experiment [3]. It can be easily shown that in the limit $Q/W = -4$ and at $\rho = 3$, the system is equivalent to the one considered in Eq. (1). Hence, by suitably engineering the two-, three- and four-body interactions, i.e., by making $W/U = -1.5$ and $Q/W = -4$, one can achieve the PSF phase. As shown above, one can choose other ratios of $W/U$ as well and still the PSF phase can be achieved. In a recent proposal it was shown that it is possible to independently control these three interactions in an optical lattice [6]. The choice of multibody interactions, i.e., $W/U = -1.5$ and $Q/W = -4$, which translates the system into the one considered in Eq. (1) is one of many possible combinations shown in Ref. [7]. Therefore, it can be made possible to achieve the PSF phase in the optical lattice experiment with the tunable multibody interactions.

**V. CONCLUSIONS**

We investigate the Bose-Hubbard model in the presence of repulsive two-body ($U$) and attractive three-body ($W$) interactions. By analyzing the one- and two-dimensional systems using the DMRG and CMFT approach, respectively, we obtain the complete phase diagrams and show that there exists a PSF phase in between the MI(1) and MI(3) lobes. This result is in contrast to the previous study where a direct first-order phase transition from MI(1) to MI(3) has been reported in a two-dimensional system using the single site mean-field theory and the QMC methods [13]. By analyzing the finite-size scaling of important physical quantities, we show that the PSF-ASF transition in the 1D case is of Ising universality class at commensurate filling and the MI(1)-PSF, PSF-MI(3) transitions are continuous. In 2D, however, we predict that the MI-PSF and PSF-ASF phase transitions are continuous. Although there exists a tricritical point along the MI(1)-ASF and ASF-MI(3) boundaries in the 2D phase diagram, there is no such point in the 1D case. We also discuss the experimental proposal to achieve the model considered in our work.

The pairing of bosons obtained in our studies can be considered as repulsively bound pairs arising due to a novel phenomenon of interplay between multibody interactions in the system. It is contrary to the physics of repulsively bound pairs observed in an earlier experiment where it was induced because of the competition between the strength of on-site interaction and the bandwidth of the lattice dispersion [26]. The pair superfluid phase in this case is robust with respect to the ratio of two- and three-body interactions. Therefore, one can expect a longer lifetime of such pairs from the underlying
mechanism of pair formation which can be a topic of future interest. This finding can also lead to other interesting studies such as recently observed quantum random walk of pairs of particles [27] and can have potential implications in the field of quantum computers [28].

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[19] For incommensurate fillings we observe slight deviations from Ising scaling behavior in the order parameter and the fidelity susceptibility. This could hint a (weakly) first-order nature of the phase transition away from filling $\rho = 2$.