Detection of pair-superfluidity for bosonic mixtures in optical lattices

C. Menotti and S. Stringari
INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, I-38123 Povo (TN), Italy
(Received 22 December 2009; published 29 April 2010)

We consider a mixture of two bosonic species with tunable interspecies interaction in a periodic potential and discuss the advantages of low filling factors on the detection of the pair-superfluid phase. We show how the emergence of such a phase can be put dramatically into evidence by looking at the interference pictures and density correlations after expansion and by changing the interspecies interaction from attractive to repulsive.

DOI: 10.1103/PhysRevA.81.045604 PACS number(s): 67.85.Hj, 03.75.Mn

Ultracold atoms in optical lattices are presently one of the best environments for the study of exotic quantum phases [1,2]. The experimental demonstration of the superfluid-to-Mott transition [3] has opened the way to the study of strongly correlated phases in lattices. In the case of mixtures of different atomic species or different internal levels, new phenomena related to quantum magnetisms and spin physics arise (see, e.g., [4], and references therein).

The quantum phase that is central to this work is the pair-superfluid (PSF) phase for a mixture of two different bosonic species. This phase consists of the formation of a superfluid of pairs where atoms of different species preferentially hop together in the lattice. Single-species condensate is associated with the macroscopic occupation of the zero quasi-momentum state for each species, while a pair-superfluid requires the macroscopic occupation of the zero relative quasimomentum, without any constraint on the value that the single-species momenta can separately take. As a consequence, single-species condensation is destroyed. In this Brief Report, we will see how this picture is directly reflected into physical quantities accessible in experiments with optical lattices.

The question concerning the coexistence of single- and pair-superfluidity in free space has been previously discussed (see, e.g., [5]), and the existence of a pair-superfluid phase in lattices has been already pointed out in several papers [6–14]. In the lattice problem, the main emphasis has been put on the situation of equal density for the two species leading to total-integer and half-integer filling factors. For integer filling factors, PSF arises in the regime where the interspecies interaction almost completely compensates the repulsive intraspecies interaction. Unfortunately, the precision on the values of the interaction strengths and the very small values of the tunneling parameter required to get pair-superfluidity make this phase almost unaccessible experimentally. At half filling factor for each species (total integer filling), the PSF phase (analogous to the x-y ferromagnet), is predicted in a larger region of the phase space. At low tunneling and in the presence of asymmetries between the interaction and tunneling parameters of the two species, the PSF phase competes with the insulating-like antiferromagnetic ordering. Instead, for total incommensurate filling factor, no insulating-like phases (Mott or antiferromagnetic-like) exist. In this regime, easily accessible signatures for the experimental observation of pair-superfluidity are available. In this Brief Report, we would like to complement the predictions in [14], discussing the role played by the two-body momentum distribution and commenting on the effect of interactions in the expansion.

At total incommensurate filling factor and zero temperature, two important phases are naturally conceived[1]: (i) a double superfluid (2SF), where both species are independently superfluid and single-species coherence exists, and (ii) a PSF phase, characterized by pair-coherence. Assuming that interactions do not affect significantly the expansion of the atomic cloud after release, all required information needed to distinguish between the two phases is included in the pictures of the two species after expansion: First, the interference fringes, typical of single-species coherence, will appear for the 2SF phase and vanish in the case of PSF. Moreover, the density-density correlations between the two species after expansion carry information about the correlations in momentum space before expansion, which are dramatically different for the two phases.

We consider two bosonic atomic species in a lattice, described by the Bose-Hubbard Hamiltonian

$$H = -\sum_{\langle ij\rangle}[J_a a_i^\dagger a_j + J_b b_i^\dagger b_j] + \sum_{i,\sigma}\left[\frac{U_\sigma}{2} n_i^\sigma\left(n_i^\sigma - 1\right)\right] + \sum_i U_{ab} n_i^a n_i^b, \qquad (1)$$

where $\sigma = a,b$ indicates the two bosonic species and $a_i, b_i, a_i^\dagger, b_i^\dagger$, and n_i^σ are the annihilation, creation operators, and density of species a and b at site i, respectively. The notation $\langle ij\rangle$ represents nearest neighbors. The intraspecies on-site interactions U_σ and tunneling parameters J_σ depend in the standard way on the optical lattice potential and scattering lengths. Generally speaking, the most favorable conditions for PSF are given by a complete symmetry between the two species, as far as interaction, hopping, and density are concerned. This is the situation that we will assume in this Brief Report ($N_a = N_b = N$, $J_a = J_b = J$, $U_a = U_b = U$), focusing on the possibility of changing the interspecies interaction U_{ab} from negative to positive by tuning the interspecies scattering length via a Feshbach resonance over a wide range, as demonstrated in [15].

[1]In this Brief Report, we do not investigate the supersolid and pair-supersolid phases, which are instead discussed, e.g., in [13,14].

The solution of Hamiltonian (1) is a nontrivial many-body task. Quantum Monte Carlo (QMC) calculations provide the most accurate results [6,8,11]. Evidence of the PSF phase has been recently obtained also by matrix-product-state [9,13,14] and dynamical mean-field approaches [12]. Furthermore, a mean-field treatment of the effective Hamiltonian in the pair subspace applied to a bilayer system of 2-D dipolar lattice bosons has proven successful in describing the PSF and pair-supersolid (PSS) phases [16].

In order to capture the basic physics of the pair correlations underlying the emergence of the PSF, in this Brief Report, we employ a toy model based on the exact diagonalization of Hamiltonian (1) for a system of few atoms occupying few lattice wells in 1-D with periodic boundary conditions. Of course, sharp phase transitions are not accounted for by our treatment, but we believe that the main conclusions remain valid also for larger systems and higher dimensions.

The comparison between filling factors equal to and less than $1/2$ is useful. For filling factor exactly equal to $1/2$, there exists a particle-hole symmetry between positive and negative interspecies interaction in the almost hard-core limit $|U_{ab}| \ll U$, leading to the PSF for attractive interactions (pairing of two atoms of different species) and the so-called supercounterfluid phase (SCF) for repulsive interactions (pairing of one atom with a hole of the other species). Instead, for equal filling factors less than $1/2$ for each species, PSF still persists, but SCF pairing is suppressed. This different behavior for positive and negative interspecies interaction might help identify the formation of PSF, as discussed later.

In order to put into evidence the differences between filling factor $\nu = 1/2$ and $\nu < 1/2$, we will consider a system of four wells and two atoms of each species ($N_w = 4$, $N = 2$) and a system of six wells and two atoms of each species ($N_w = 6$, $N = 2$), which are the smallest cases including the possibility of having equal filling factors $\nu \leqslant 1/2$ and nontrivial on-site interactions. We look at the following quantities[2]:

$$\mathcal{V}_{\rm 2SF} = \langle a_i^\dagger a_{i+1}\rangle = \langle b_i^\dagger b_{i+1}\rangle, \tag{2}$$

$$\mathcal{V}_{\rm PSF} = \langle a_i^\dagger b_i^\dagger a_{i+1} b_{i+1}\rangle - \langle a_i^\dagger a_{i+1}\rangle\langle b_i^\dagger b_{i+1}\rangle, \tag{3}$$

$$\mathcal{V}_{\rm SCF} = \langle a_i^\dagger b_i a_{i+1} b_{i+1}^\dagger\rangle - \langle a_i^\dagger a_{i+1}\rangle\langle b_i b_{i+1}^\dagger\rangle. \tag{4}$$

The quantities $\mathcal{V}_{\rm 2SF}$, $\mathcal{V}_{\rm PSF}$, and $\mathcal{V}_{\rm CSF}$ characterize the 2SF, PSF, and SCF phases, respectively.[3] We also consider single-particle and two-particle momentum distributions in order to make a useful link to the experiments.

In Fig. 1, we show the phase diagram as a function of J and U_{ab}. One can clearly identify the PSF (or SCF) regions as the dark regions in Figs. 1(a) and 1(d), where single-species coherence vanishes, and at the same time pair-coherence (or counterpair-coherence) is different from zero, namely, the light regions in Figs. 1(b) and 1(e) [or Fig. 1(c) for SCF]. As explained earlier, for $\nu = 1/2$, PSF and SCF are found

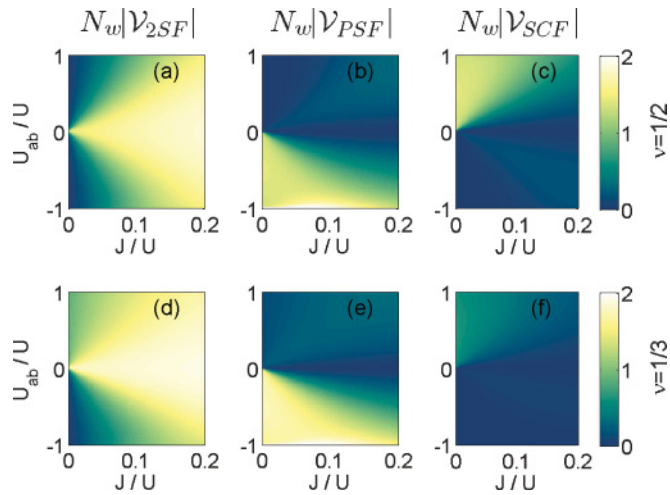

FIG. 1. (Color online) Phase diagram for (top) $N_w = 4$ and (bottom) $N_w = 6$ and $N = 2$. (a, d) Single-particle coherence $N_w|\mathcal{V}_{2SF}|$, as defined in Eq. (2); (b, e) pair-coherence $N_w|\mathcal{V}_{\rm PSF}|$, as defined in Eq. (3); (c, f) counterpair-coherence $N_w|\mathcal{V}_{\rm SCF}|$, as defined in Eq. (4). The factor N_w allows a better comparison between the two different lattice sizes. The region of parameters of strong attractive interaction $U_{ab} \lesssim -U$ corresponds to collapse in a large system.

for attractive and repulsive interaction, respectively. Instead, for $\nu < 1/2$, SCF is absent. For low filling, the crossover from 2SF to PSF is governed by the competition between the single-particle hopping J and the energy cost for breaking a pair, equal to $|U_{ab}|$. For that reason, PSF is found for attractive interspecies interactions at sufficiently low tunneling parameters $J \ll |U_{ab}|$.

An important quantity accessible in experiments that would provide an unquestionable proof of PSF is the measure of correlations in the momentum distribution, reflecting the fact that in the PSF and SCF phases, two atoms of different species form a pair and condense in the state of total quasi-momentum $q_a \pm q_b = 0$ (for atom-atom and atom-hole pairs, respectively), as shown in Figs. 2(a), 2(c), and 2(f). In the case of two noninteracting superfluids ($U_{ab} = 0$), the two species have completely uncorrelated momentum distributions, that is, $n^{(a,b)}(q_a,q_b) = n^{(a)}(q_a) \times n^{(b)}(q_b)$, where $n^{(a)}(q_a)$ and $n^{(b)}(q_b)$ separately present interference peaks at even multiples of the Bragg momentum q_B [see Figs. 2(b) and 2(e)], as happens for standard single-component condensates [3,17]. In the presence of interspecies interactions $U_{ab} \neq 0$, correlations build up in a very different way, depending on the filling factor and on whether the interactions are repulsive or attractive. For filling factors exactly equal to $1/2$, the situation is almost symmetric for positive and negative U_{ab} on particle-hole duality for the different species. The momentum correlations are opposite in the two cases, as shown in Figs. 2(a) and 2(c), indicating SCF and PSF, respectively. The 2SF phase is recovered in the vicinity of vanishing interspecies interactions [Fig. 2(b)]. For equal filling factors smaller than $1/2$, a 2SF is obtained both for vanishing and repulsive interactions [Figs. 2(d) and 2(e)] since the filling factor of one species does not match the filling factor of the holes of the other. Hence only negligible momentum correlations exist for $U_{ab} \geqslant 0$. On the contrary, attractive

[2] In the infinite system, the SF phase is defined by the conditions $\langle a\rangle, \langle b\rangle \neq 0$ and $\langle ab\rangle - \langle a\rangle\langle b\rangle = 0$, while the conditions for the PSF phase are $\langle a\rangle = \langle b\rangle = 0$ and $\langle ab\rangle - \langle a\rangle\langle b\rangle \neq 0$.

[3] We have checked that correlations at two lattice sites distance produce a similar phase diagram. Correlations at longer distances cannot be investigated within our model.

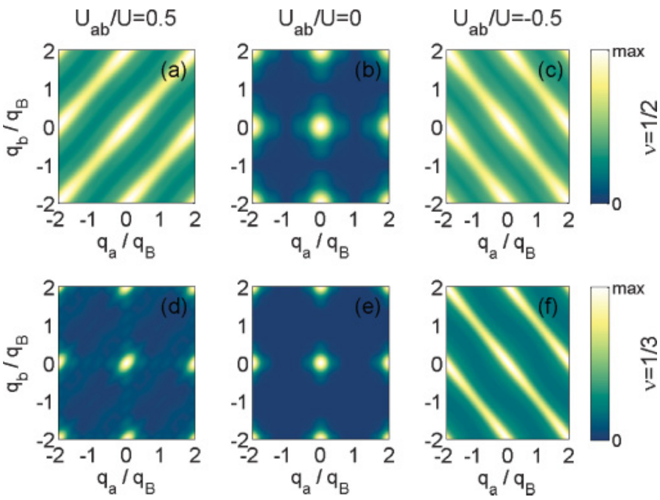

FIG. 2. (Color online) Two-body momentum distribution $n^{(a,b)}(q_a,q_b)$ for $N=2$ and $N_w=4,6$, i.e., filling factor (top) 1/2 and (bottom) 1/3. (a, d) Repulsive interparticle interaction $U_{ab}=0.5U$; (b, e) vanishing interparticle interaction $U_{ab}=0$; (c, f) attractive interparticle interaction $U_{ab}=-0.5U$. In all pictures, $J=0.01U$. Two Brillouin zones are shown for clarity.

interactions lead to PSF and very strongly correlate the two different species [$U_{ab}/U=-0.5$; Fig. 2(f)]. The existence of correlations is put even more into evidence by subtracting the uncorrelated part $n^{(a)}(q_a)\times n^{(b)}(q_b)$ of the momentum distribution.

The correlations in the two-body momentum distribution are strictly related to single-particle coherence and strongly affect the visibility of the single-particle momentum distribution, as shown in Fig. 3. The presence of momentum correlations in $n^{(a,b)}(q_a,q_b)$ leads to a reduced contrast in $n^{(\sigma)}(q_\sigma)$. Hence some signatures of the formations of the PSF/SCF phases are provided already by the interference in the single-particle expansion pictures, which is the most easily accessible experimental quantity [14]. For instance, at low enough tunneling, for $\nu<1/2$, interference is expected at $U_{ab}\geqslant 0$, while it disappears (under exactly the same conditions) by tuning U_{ab} to negative values.

Most important, the single-species expansion pictures carry information about the momentum correlations. In fact, as demonstrated in [18], the direct measurement of the momentum correlations can be performed by looking at the noise in the single-species expansion pictures [19,20]. Assuming first that interactions do not affect the expansion, the single-species densities after time of flight are given by $n^{\sigma}_{\rm TOF}(r_\sigma=q_\sigma t/m_\sigma)=n^{(\sigma)}(q_\sigma)$. Hence, in the case of PSF, where the correlations are of the type $q_a+q_b=0$, we expect the two expansion pictures to be correlated at correctly rescaled opposite positions and possibly at corresponding points in different Brillouin zones.

In usual experiments, interatomic interactions are not turned off during the expansion, and their effect is considered to be negligible because of the higher energy scales involved in the problem. In the present case, it would be a safe procedure to tune at least U_{ab} to zero just before releasing the cloud. However, this might not be so easily achievable in an experiment. For this reason, we have estimated the effect of the interspecies interactions on the expansion for two atoms released from a four-well lattice by integrating the full two-body Schrödinger equation. While with relatively weak attractive interactions [$|U_{ab}|/J\approx 20$; see Figs. 4(a) and 4(b)], the two-body momentum distribution is hardly modified during the expansion, we have seen that the two-body momentum distribution can be affected by attractive interspecies interaction U_{ab}, for interaction strengths leading to pairing [$|U_{ab}|/J\approx 60$; see Figs. 4(c) and 4(d)]. This effect tends to create also some correlations along the diagonal $q_a=q_b$ but does not destroy the correlations typical of the PSF phase (at $q_a=-q_b$). Hence, recovering the two-body density after expansion via noise correlation measurements, the distinction between PSF and 2SF phases still remains

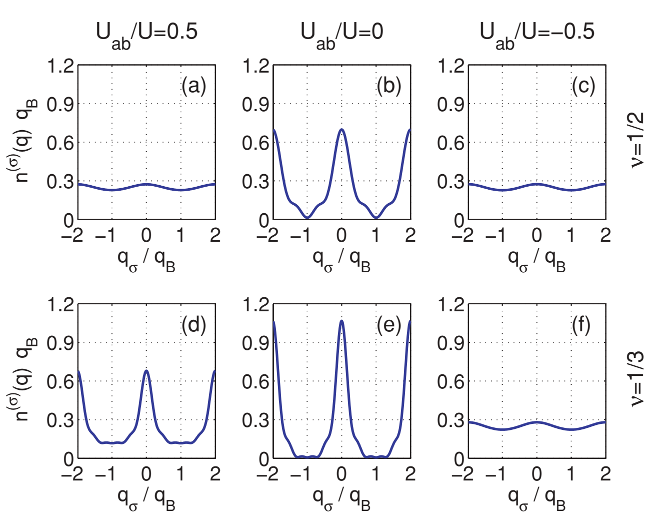

FIG. 3. (Color online) Single species momentum distribution $n^{(\sigma)}(q_\sigma)$ for $N=2$ and $N_w=4,6$, i.e., filling factor (top) 1/2 and (bottom) 1/3. (a, d) Repulsive interparticle interaction $U_{ab}=0.5U$; (b, e) vanishing interparticle interaction $U_{ab}=0$; (c, f) attractive interparticle interaction $U_{ab}=-0.5U$. In all pictures, $J=0.01U$. Two Brillouin zones are shown for clarity.

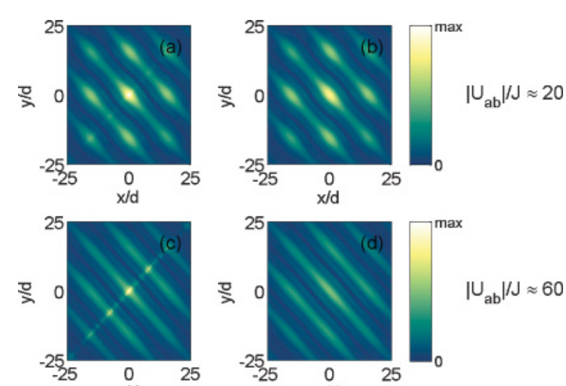

FIG. 4. (Color online) Effect of attractive interspecies interaction U_{ab} on the expansion. (a, c) Two-body density after expansion after a time of flight $E_r t_{\rm TOF}\approx 12$, where E_r is the recoil energy, in the presence of interspecies interaction U_{ab}; (b, d) free expansion at the same time of flight (shown for comparison). The strengths of interaction are $|U_{ab}|/J\approx 20$ in (a, b) and $|U_{ab}|/J\approx 60$ in (c, d), respectively.

very clear. More dramatic effects of the interactions during the expansion take place only for values of $|U_{ab}|/J$ which are much beyond the estimated onset of the PSF phase transition.

Small asymmetries in the Hamiltonian parameters of the two species do not destroy the PSF phase. Instead, an imbalance in the densities of atoms a and b hinders the formation of the pairs. Unfortunately, we are not able to quantify the realistic effect of the imbalance because of the small number of atoms considered. However, one can think of experimental procedures to create a sample with almost exactly equal populations of the two species. For instance, one could start with a Mott insulator at unit filling for both species and then tailor the optical potentials, introducing a second laser at half the wavelength such as to split each lattice well into two equal wells. Alternatively, one can create a unitary filled Mott region for both species in the trap center and then release the harmonic trap until the desired filling factor is reached. This method would favor the creation of the pairs in the Mott phase, which can then become superfluid once the filling factor is made incommensurate.

The physical ingredient on which pair-superfluidity relies is the second-order hopping of two atoms of the different species at once. This is closely related to the exchange interaction, whose observability has been recently demonstrated in [21]. The fact that pair hopping is a second-order process in J, where J is assumed to be small, might seem to be discouraging for the experimental observation of the PSF phase. However, exact 2-D QMC simulations of this problem [11] predict the transition between 2SF and PSF, at half-integer filling and symmetry between the two species, to happen at $J \approx 0.1|U_{ab}|$. Exploiting the possibility of having U_{ab} of the same order of U, this leads to relatively large values for the critical tunneling. On the other hand, careful analysis of the critical temperature and entropy for the formation of the PSF phase, as recently done in [22], is required.

Our model provides an oversimplified description of the system. We believe, however, that it includes correctly the fundamental ingredients of the physics involved. A more quantitative analysis based on exact numerical calculations, including the effects of two-species unbalance on the formation of the paired phases, will be the subject of future work.

We acknowledge financial support by MIUR PRIN 2007. The authors thank F. Becca, I. Bloch, J. Catani, F. Minardi, M. Modugno, B. Svistunov, and E. Taylor for interesting discussions.

[1] M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
[2] I. Bloch *et al.*, Rev. Mod. Phys. **80**, 885 (2008).
[3] M. Greiner *et al.*, Nature **415**, 39 (2002).
[4] M. Lewenstein and A. Sanpera, Science **319**, 292 (2008).
[5] P. Nozières and D. Saint James, J. Phys. **43**, 1133 (1982); C. A. R. Sá de Melo, Phys. Rev. B **44**, 11911 (1991); L. Radzihovsky, J. Park, and P. B. Weichman, Phys. Rev. Lett. **92**, 160402 (2004); M. W. J. Romans, R. A. Duine, S. Sachdev, and H. T. C. Stoof, *ibid.* **93**, 020405 (2004).
[6] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. **90**, 100401 (2003).
[7] E. Altman *et al.*, New J. Phys. **5**, 113 (2003).
[8] A. Kuklov, N. Prokofev, and B. Svistunov, Phys. Rev. Lett. **92**, 050402 (2004).
[9] A. Argüelles and L. Santos, Phys. Rev. A **75**, 053613 (2007).
[10] E. K. Dahl, E. Babaev, and A. Sudbo, Phys. Rev. Lett. **101**, 255301 (2008).
[11] S. G. Şöyler *et al.*, New J. Phys. **11**, 073036 (2009).
[12] A. Hubener, M. Snoek, and W. Hofstetter, Phys. Rev. B **80**, 245109 (2009).
[13] L. Mathey, I. Danshita, and C. W. Clark, Phys. Rev. A **79**, 011602(R) (2009).
[14] A. Hu *et al.*, Phys. Rev. A **80**, 023619 (2009).
[15] J. Catani, L. DeSarlo, G. Barontini, F. Minardi, and M Inguscio, Phys. Rev. A **77**, 011603(R) (2008).
[16] C. Trefzger, C. Menotti, and M. Lewenstein, Phys. Rev. Lett. **103**, 035304 (2009).
[17] P. Pedri *et al.*, Phys. Rev. Lett. **87**, 220401 (2001).
[18] M. Greiner, C. A. Regal, J. T. Stewart, and D. S. Jin, Phys. Rev. Lett. **94**, 110401 (2005).
[19] E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A **70**, 013603 (2004).
[20] A. Kuklov and H. Moritz, Phys. Rev. A **75**, 013616 (2007).
[21] S. Trotzky *et al.*, Science **319**, 295 (2008).
[22] B. Capogrosso-Sansone *et al.*, e-print arXiv:0912.1865 (2008).