Anisotropic pair superfluidity of trapped two-component Bose gases in an optical lattice

Yongqiang Li\textsuperscript{1,2,3}, Liang He\textsuperscript{1} and Walter Hofstetter\textsuperscript{1}

\textsuperscript{1} Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt am Main, Germany
\textsuperscript{2} Department of Physics, National University of Defense Technology, Changsha 410073, People’s Republic of China
E-mail: liyq@itp.uni-frankfurt.de

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Abstract. We theoretically investigate the pair-superfluid phase of two-component ultracold gases with attractive inter-species interactions in an optical lattice. We establish the phase diagram for filling $n=1$ at zero and finite temperatures, by applying bosonic dynamical mean-field theory, and observe stable pair-superfluid and charge-density wave quantum phases for asymmetric hopping of the two species. While the pair superfluid is found to be robust in the presence of a harmonic trap, we observe that it is destroyed already by a small population imbalance of the two species.
1. Introduction

Ultracold gases in optical lattices are promising and flexible quantum simulators for the study of quantum phases that are not easily accessible in condensed-matter physics [1]. Experimental realization of the superfluid-to-Mott transition has paved the way for studies of strongly interacting Bose or Fermi gases in optical lattices [2]. Recently, Bose–Bose mixtures of \(^{87}\)Rb and \(^{41}\)K have been produced and loaded into an optical lattice [3], which provide a new playground for investigating the interplay between kinetic energy, interaction and the spin degree of freedom. In a further line of investigation, a Bose–Bose mixture of two hyperfine states of \(^{87}\)Rb has been used as a spin-gradient thermometer for measuring the temperature of ultracold gases in an optical lattice [4, 5]. Moreover, the effect of a second species on bosonic superfluidity in an optical lattice has been studied [6]. In these mixtures of different species or different hyperfine states, the most fundamental physics associated with quantum magnetism and the spin degree of freedom can be explored [7].

One interesting ground state of bosonic gases is the pair-superfluid phase (PSF) for attractive interactions, which has been predicted and studied theoretically both in free space [8, 9] and in optical lattices [10–19]. However, it is widely believed that the stability of the bosonic many-body system is questionable when interactions between atoms are attractive. Recently, it was found that a three-body hard-core constraint can stabilize a system of bosons in an optical lattice with attractive two-body interactions [20], and numerical simulations have been performed to study the pair superfluidity of three-body-constrained bosons in an optical lattice [21–23]. For two-component bosons, stable heteronuclear \(^{87}\)Rb–\(^{41}\)K mixtures, with negative inter-species interactions tuned via Feshbach resonances [24], have been realized recently. Now the question is how to theoretically understand the PSF of two-component bosonic gases in an optical lattice. Qualitatively, the PSF can be viewed as a condensate of bosonic pairs of different species or hyperfine states due to a second-order hopping of the pairs, but with a strongly suppressed first-order tunneling of single atoms. For hard-core bosons with total filling \(n = 1\), the PSF for attractive interactions is equivalent to the \(XY\)-ferromagnetic phase (or super-counter-fluid state) for repulsive interactions, i.e. the PSF consists of particle–particle pairs of different species while the \(XY\)-ferromagnetic phase is composed of particle–hole pairs. It is apparent that the PSF can only exist at very low temperature compared to the critical temperature of quantum magnetic phases. The latter are also governed by second-order tunneling processes, leading to an effective spin-exchange coupling [25, 26], which has
already been observed for a double-well system [27, 28]. It is expected that these phases can be detected via momentum-space correlations observed in time-of-flight measurements [16, 29] or by optical microscopy with single-site resolution [30, 31].

Previous studies of the PSF in a two- or three-dimensional optical lattice mostly focus on symmetric parameters for the two species (for an exception, see [10, 18]), since this is the most favorable condition for the PSF [16]. However, there is still a lack of detailed quantitative investigations of the PSF for the homogeneous system with asymmetric hopping amplitudes of the two species, for the trapped system and for imbalanced mixtures of the two species. Here we investigate the properties of the PSF of two-component ultracold bosons with attractive interspecies interaction, both in a homogeneous and a trapped optical lattice. For sufficiently low filling, this system can be well described by a single-band Bose–Hubbard model with pure on-site interaction. We investigate the homogeneous system by means of bosonic dynamical mean field theory (BDMFT), which is a non-perturbative approach toward strongly correlated bosonic systems [32], and the trapped system by real-space bosonic dynamical mean field theory (RBDMFT) [33], which includes arbitrary inhomogeneity such as a harmonic trap. For the homogeneous system, we focus on the phase diagram with filling number \( n = 1 \). In particular, we also present the phase diagram for the experimentally realized heteronuclear \(^{87}\text{Rb}–^{41}\text{K} \) mixtures, where double-species Bose–Einstein condensates with negative interspecies interactions have been observed [24]. For the trapped Bose–Bose mixture we study the coexistence of Mott insulator, superfluid and PSF.

The paper is organized as follows. In section 2 we give a detailed description of the Bose–Hubbard model and the BDMFT approach. Section 3 covers our results on the homogeneous Bose–Bose mixture in an optical lattice and the effect of the trap. We conclude in section 4.

2. Model and method

We consider a two-component bosonic mixture loaded into a two-dimensional (2D) or three-dimensional (3D) optical lattice. In experiments this mixture could consist of two different species, e.g. \(^{87}\text{Rb} \) and \(^{41}\text{K} \) as in [3] or two different hyperfine states of a single isotope, e.g. \(^{87}\text{Rb} \) as in [4]. Besides the optical lattice, we also impose an external harmonic trapping potential which introduces inhomogeneity in the system. For sufficiently low filling, the whole system can be effectively described by a two-component inhomogeneous Bose–Hubbard model within the single-band approximation

\[
\mathcal{H} = - \sum_{\langle i, j \rangle, \nu} t_{\nu}(b_{i,\nu}^\dagger b_{j,\nu} + \text{h.c.}) + \frac{1}{2} \sum_{i,\lambda,\nu} U_{\lambda,\nu} \hat{n}_{i,\lambda}(\hat{n}_{i,\lambda} - \delta_{\lambda,\nu}) + \sum_{i,\nu = b, d} (V_i - \mu_\nu) \hat{n}_{i,\nu},
\]

where \( \langle i, j \rangle \) denotes summation over nearest-neighbor sites \( i, j \), and the two bosonic species are labeled by the index \( \lambda(\nu) = b, d \). \( \hat{b}_{i,\nu}^\dagger \) (\( \hat{b}_{i,\nu} \)) denotes the bosonic creation (annihilation) operator for species \( \nu \) at site \( i \) and \( \hat{n}_{i,\nu} = \hat{b}_{i,\nu}^\dagger \hat{b}_{i,\nu} \) the corresponding local density. Due to possibly different masses or a spin-dependent optical lattice, these two species generally hop with non-equal amplitudes \( t_b \) and \( t_d \). \( U_{\lambda,\nu} \) denotes the inter- and intra-species interactions, which can be tuned via Feshbach resonances or spin-dependent lattices [6, 34]. \( \mu_\nu \) is the global chemical potential for the two bosonic species, and \( V_i \equiv V_{\nu}^0 r_i^2 \) denotes the external harmonic trap, where \( V_{\nu}^0 \) is the strength of the harmonic trap for the \( \nu \) component and \( r_i \) is the distance from the trap center.

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order parameters are defined as \( \phi \) an initial set of the local Weiss Green functions and local bosonic superfluid order parameters (i.e. the rest of the lattice) and is obtained in a self-consistent manner. In practice, we start with the impurity site. where the index 0 indicates that the average is taken for the cavity system, i.e. excluding the finite potential is included via \( V \). Eventually, the self-consistency loop is closed by specifying the Weiss Green function via the local action in a homogeneous system [32]. The main difference to a homogeneous BDMFT calculation is that in the present case, the lattice Green function \( G_{\lambda \nu}(i \omega_n) \) is obtained via the real-space Dyson equation (3), which incorporates the effect of spatial inhomogeneity. We can now use standard

To obtain the ground state of this system, we apply BDMFT for a homogeneous lattice [32], and its real-space generalization (RBDMFT) for the trapped system [33]. Within RBDMFT, the Hamiltonian (1) is mapped onto a set of individual single-site problems where the physics of lattice site \( i \) is described by a local effective action

\[
S_{\text{eff}}^{(i)} = \int_0^\beta d\tau \sum_{\lambda, \nu = \{b, d\}} b^{(i)}_\lambda(\tau)G^{(i)}_{0,\lambda\nu}(\tau - \tau')^{-1}b^{(i)*}_\nu(\tau') + \int_0^\beta d\tau \left\{ \sum_{\lambda, \nu} \frac{1}{2} U_{\lambda, \nu} n^{(i)}_{\lambda}(\tau) \left( n^{(i)}_{\nu}(\tau) - \delta_{\lambda\nu} \right) - \sum_{\langle 0j \rangle, \nu} t_\nu \left( b^{(i)}_\nu(\tau) \phi_{j, \nu}(\tau) + b^{(i)*}_\nu(\tau) \phi_{j, \nu}^*(\tau) \right) \right\}.
\]

(2)

In this action \( \tau \) denotes imaginary time and the function \( G^{(i)}_{0,\lambda\nu}(\tau - \tau') \) is a local non-interacting propagator interpreted as a dynamical Weiss mean field which is determined in a self-consistent manner. We use the Nambu notation \( b^{(i)}_{\nu}(\tau) \equiv (b^{(i)}_{\nu}(\tau), b^{(i)*}_{\nu}(\tau)) \). Moreover, the superfluid order parameters are defined as

\[
\phi_{j, \nu}(\tau) = \langle b_{j, \nu} \rangle_0,
\]

where the index 0 indicates that the average is taken for the cavity system, i.e. excluding the impurity site.

Now, each of these local actions can be treated as an impurity in the presence of a bath (i.e. the rest of the lattice) and is obtained in a self-consistent manner. In practice, we start with an initial set of the local Weiss Green functions and local bosonic superfluid order parameters \( \phi_{j, \nu}(\tau) \). After solving the local effective action (2), we obtain a set of local self-energies for each species \( \Sigma^{(i)}_{\lambda\nu}(i \omega_n) \) with \( \omega_n \) being Matsubara frequencies. Then we employ the lattice Dyson equation in real-space representation in order to obtain the interacting lattice Green function

\[
G(i \omega_n)^{-1} = G_0(i \omega_n)^{-1} - \Sigma(i \omega_n).
\]

(3)

The site dependence of the Green functions is indicated by boldface quantities which denote a matrix form with site-indexed elements. Here \( G_0(i \omega_n)^{-1} \) is the inverse non-interacting Green function

\[
G_0(i \omega_n)^{-1} = (\mu + i \omega_n)1 - t - V.
\]

(4)

In this expression, the hopping amplitudes are given by matrix elements of \( t \) and the external potential is included via \( V_{ij} = \delta_{ij} V \). The diagonal elements of the lattice Green function are then identified with the interacting local Green functions, i.e. \( G^{(i)}(i \omega_n) = (G(i \omega_n))_{ii} \) where the spin dependence of the local Green functions is shown by boldface quantities which denote a matrix form. Eventually, the self-consistency loop is closed by specifying the Weiss Green function via the local Dyson equation

\[
G^{(i)}(i \omega_n)^{-1} = G_0(i \omega_n)^{-1} + \Sigma^{(i)}(i \omega_n).
\]

(5)

This self-consistency loop is repeated until the desired precision for the superfluid order parameter and the Weiss Green function is obtained.

In order to solve the local effective action, we map it onto a Hamiltonian described by an Anderson impurity model. This step is analogous to the solution of the local action in a homogeneous system [32].
techniques to solve the impurity problem. Here we adopt exact diagonalization as a solver [32, 35].

To include the effect of spatial inhomogeneity, we also employ an LDA approximation combined with single-site BDMFT. The advantage of this approach is the larger system size accessible. Within LDA+BDMFT, the local chemical potential for each species is set to $\mu_\nu(r) = \mu_\nu - V(r)$. In this work, we apply both RBDMFT and LDA+BDMFT to the 2D trapped square lattice, and only LDA+BDMFT to the 3D trapped cubic lattice.

3. Results

In this section, we will investigate properties of two-component bosonic mixtures with negative inter-species interactions in a homogeneous 3D optical lattice at zero and finite temperatures, and also in harmonically trapped, inhomogeneous systems, both in 2D and 3D. For the homogeneous system, we will study the stability of the PSF against asymmetric hopping and finite temperature. In the presence of an external harmonic trap, we will investigate finite-size effects of the PSF, both in 2D and 3D, within RBDMFT and LDA+BDMFT. We choose the absolute value of the inter-species interaction $|U_{bd}|$ as our unit of energy in the following. For simplicity, we denote $U_{bd}$ as $U$ in the following.

3.1. Bose–Bose mixture in a three-dimensional (3D) cubic lattice

We first investigate Bose–Bose mixtures with negative inter-species interaction $U < 0$ in a 3D cubic optical lattice. The system is unstable for $|U| > U_{b,d}$, since the strongly attractive inter-species interaction cannot be compensated by repulsive intra-species interactions, leading to a collapse of the system. In the following discussion, we choose $|U| < U_{b,d}$. We explore the

Figure 1. Zero-temperature phase diagram for two-component bosons with attractive inter-species interaction in a 3D cubic lattice. The interactions are set to $U_b = U_d = 12|U|$ and the total filling is $n = 1$ with $n_b = n_d = 0.5$. 

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Figure 2. Upper: finite-temperature phase diagram for two-component bosons in a 3D cubic lattice ($T = 0.001|U|$). The interactions are set to $U_b = U_d = 12|U|$ and the total filling is $n = 1$ with $n_b = n_d = 0.5$. Lower: local density–density correlator $g^{(2)}$ as a function of temperature for different hopping values $t_b = t_d$. Inset: zoom of main figure for $t_c = 0.04|U|$ ($v = b, d$), where the red dashed line indicates the disappearance of the PSF correlator $\phi_{bd}$.

zero-temperature phase diagram with asymmetric hopping parameters at total filling $n = 1$ (with $n_b = n_d = 0.5$), as shown in figure 1. We observe three different phases: the PSF with $\langle b \rangle = \langle d \rangle = 0$ but $\phi_{bd} \equiv \langle bd \rangle \neq 0$, the superfluid phase (SF) with $\langle b \rangle, \langle d \rangle > 0$ and a charge density wave (CDW) with $\Delta_{\text{CDW}} = |n_\alpha - n_\alpha'| > 0$ and $\langle b \rangle = \langle d \rangle = 0$, where $n$ denotes the filling and $\alpha$ the sublattice ($\alpha = -\alpha'$). In particular, we confirm the existence of a PSF for asymmetric hopping amplitudes $t_b \neq t_d$. In the regime of comparably weak hopping for both species, first-order tunneling is suppressed by the strong interactions. Formation of bosonic pairs between different species can thus be energetically favored and will typically compete with single-species condensation, since the bosonic pairs can hop via second-order tunneling. As a result, the PSF will have a non-vanishing order parameter $\phi_{bd}$ but vanishing superfluid order $\langle b \rangle$ and $\langle d \rangle$. On the other hand, when both species acquire comparably large hopping, a superfluid phase
Figure 3. Critical temperature of the PSF as a function of hopping amplitudes \( t_b = t_d \) on a 3D cubic lattice with total filling \( n = 1 \). Inset: melting of the PSF versus temperature along the vertical dashed line with hopping amplitudes \( t_b = t_d = 0.04 |U| \).

will appear with \( \langle b \rangle > 0 \) and \( \langle d \rangle > 0 \). For asymmetric hopping, we observe that CDW order develops, since the small hopping amplitude for one component localizes bosonic pairs of the two species and CDW order is favored by the system. We remark here that the transition from a PSF to a superfluid phase for symmetric hopping amplitudes occurs at the same value of \( t_{\nu}/U_{bd} \) as that from the \( XY \)-ferromagnetic to the superfluid phase in the corresponding system with repulsive \( U_{bd} > 0 \) of equal magnitude. In contrast to the \( XY \)-ferromagnetic phase, however, the PSF also exists for non-integer filling. Note that we have also investigated the influence of finite-size effects on the phase boundary due to a finite number of bath orbitals (4, 5 and 6 bath orbitals). We find that their effect is smaller than the symbol size.

The effect of finite temperature is shown in figure 2. Generally, the PSF is sensitive to temperature, since the pairs are formed in the weak hopping regime and their coherence can be easily destroyed by thermal fluctuations, due to their small effective pair tunneling of order \( O(t^2/U) \). At finite temperature, the PSF regime shrinks in the weak hopping regime in favor of developing a new unordered phase (UN) with vanishing values for \( \phi_{bd} \), \( \langle b \rangle \) and \( \langle d \rangle \). To further understand this unordered phase, we calculate the dependence of the local density–density correlator \( g^{(2)} \equiv \langle n_b n_d \rangle - \langle n_b \rangle \langle n_d \rangle \) on temperature, as shown in the lower panel of figure 2. We observe that \( g^{(2)} \) starts to decrease noticeably only above temperatures of the order of \( 10^{-1} |U| \), which indicates that local pairs still exist below this temperature. We therefore conclude that the unordered phase, shown in the upper panel of figure 2, consists of non-coherent pairs of different species. In sufficiently deep optical lattices, these pairs are localized, while for larger hopping the pairs delocalize over the whole lattice. As a result, the local density–density correlator decreases as a function of \( t_{b,d} \), as shown in the lower panel of figure 2. Another interesting feature of the temperature dependence of \( g^{(2)} \) is the increasing (non-monotonic) trend at low temperatures, since thermal fluctuations first localize and then break the pairs. We remark here that the temperature regime of non-condensed pairs (\( \approx 0.1 |U| \)) is experimentally accessible [36], and could be detected via radio frequency spectroscopy [37].
We also observe that the (single-particle) superfluid phase remains almost unchanged for the temperature considered here.

One crucial question regarding the observation of the PSF is how fragile it is against finite-temperature effects. To address this issue, figure 3 shows $T_c$ as a function of the hopping amplitudes $t_b = t_d$ at different interactions. We notice that $T_c$ rises as the hopping amplitudes increase, due to the growing second-order tunneling which stabilizes long-range order. The inset of figure 3 shows the temperature dependence of $\phi_{bd}$. It indicates a second-order phase transition from the PSF to the unordered phase. We also observe that the critical temperatures for the PSF shown here are comparable with those of the $XY$-ferromagnetic phase [33] and

**Figure 4.** Upper: comparison of the zero-temperature phase diagram for two-component hard-core bosons with the one obtained by a tensor-product-state approximation [17] for a square lattice with symmetric parameters: $t = t_b = t_d$, $\mu = \mu_b = \mu_d$. The red solid lines are phase boundaries obtained by BDMFT for $U_b = U_d = 200|U|$, while the blue dashed lines are the results of the tensor-product-state approximation. Lower: zero-temperature phase diagram for two-component soft-core bosons with $U_b = U_d = 2|U|$ obtained via BDMFT.
notably smaller than the coldest temperatures which have been measured in most experiments until now, with the exception of the MIT group where temperatures as low as 350 pK (≈ 0.01 \( U_{bd} \) with \( t_b/U_{bd} \approx 0.029 \)) have been achieved [5].

To verify the validity of the BDMFT results, comparison has been made with a hard-core boson model solved by a tensor-product-state approximation [17], as shown in figure 4. We find excellent agreement between the two methods. We also plot the phase diagram for soft-core bosons (\( U_b = U_d = 2|U| \)), and observe that in this case, the phase boundary, between the PSF and the superfluid phase is shifted to lower hopping values.

3.2. Rubidium–potassium mixture

Our investigations have so far focused on symmetric interactions \( U_b = U_d \), which is a good approximation for mixtures of hyperfine states of \(^{87}\text{Rb} \) [4]. However, this symmetry is not present for mixtures of \(^{87}\text{Rb} \) and \(^{40}\text{K} \), where a negative inter-species interaction has been achieved via a Feshbach resonance [24]. Here we consider a mixture of \(^{87}\text{Rb} \) and \(^{41}\text{K} \) loaded into a 3D cubic lattice with wavelength \( \lambda = 757 \text{ nm} \), which yields equal dimensionless lattice strength \( s \) for the two species. Due to different masses, the ratio of the intra-species interaction strengths is then fixed to \( U_{Rb}/U_K = m_K a_{Rb}/m_{Rb} a_K \approx 0.72 \) and the ratio of the hopping amplitudes to \( t_{Rb}/t_K \approx 0.47 \), where \( E_R \) is the recoil energy.

Now we explore the phase diagram of \(^{87}\text{Rb} \) and \(^{41}\text{K} \) mixtures in a 3D cubic lattice and make predictions for ongoing experiments. Since the depth \( s \) of the optical lattice and the inter-species scattering length \( a_{RbK} \) are tunable with high accuracy, we show in figure 5 the phase diagram in the \( a_{RbK} - s \) plane for total filling \( n = 1 \) (\( n_b = n_d = 0.5 \)) at zero temperatures. At zero temperature, three phases appear: superfluid, PSF and CDW. When the scattering length \( a_{RbK} \) is small, the system is in a superfluid phase for a shallow lattice. When the depth of the lattice is increased, the ratio of \( t_{Rb}/U_{Rb} \) decreases, resulting in a strong suppression of first-order tunneling. The dominant process will then be hopping of composite pairs, which energetically favors PSF. We also observe CDW phase in the intermediate regime, where it is surrounded by PSF.
Figure 6. Density distributions $n_b$ (black line), order parameters $\phi_b$ (green line) and PSF correlator $\phi_{bd}$ (red line) versus radial distance $r$ for different hopping amplitudes at zero temperature in a 2D square lattice, obtained by RBDMFT. The interactions are $U_b = U_d = 2|U|$, hopping amplitudes $t = t_b = t_d$ and harmonic trap $V_0 = 0.0002|U|$. 

It is expected that PSF and CDW shrink to a small region in parameter space at finite temperature due to thermal fluctuations, which is similar to results in [32].

3.3. Trapped Bose–Bose mixtures in two-dimensional and 3D lattices

In this section, we simulate the two-component bosonic system in both 2D and 3D in the presence of a harmonic trap, as is relevant for most experiments. In particular, we investigate the stability of the PSF in the trapped system. Here we choose a $41 \times 41$ square lattice for the 2D case and a $41 \times 41 \times 41$ cubic lattice for the 3D case. In 2D, in our simulations we apply both RBDMFT and BDMFT+LDA, while in 3D we only use BDMFT+LDA due to its lower computational effort. For simplicity, we investigate rubidium–rubidium mixtures with $V_0 = V_0$. 

3.3.1. Balanced mixture. Figure 6 shows the density distributions $n_b$, order parameter $\phi_b$ and correlator $\phi_{bd}$ for the PSF versus radius $r$ at different hopping amplitudes in a trapped 2D optical lattice. Since the PSF is stabilized only within a narrow region for the symmetric parameters (see figure 4), the harmonic trap should be very shallow and the hopping amplitudes need to be fine-tuned. Otherwise, the system will go through a phase transition directly from a Mott-insulating to a (single-component) superfluid phase. Here we choose completely symmetric parameters: $t = t_b = t_d$ and $U_b = U_d = 2|U|$ with balanced filling for the two components. Therefore only one value for $n_{b,d}$ and $\phi_{b,d}$ is shown in figure 6. We observe that a wedding-cake structure appears in the trapped system, and the coexistence of different phases sensitively depends on the hopping amplitudes. At lower hopping $t = 0.07|U|$, only two phases appear,
Figure 7. Comparison between results from RBDMFT (R) and those from BDMFT+LDA (L) for a 2D square lattice. Density distributions \( n_b \), order parameters \( \phi_b \) and PSF correlator \( \phi_{bd} \) versus radial distance \( r \) at zero temperature in a 2D square lattice. The interactions are \( U_b = U_d = 2|U| \) and the hopping amplitudes \( t_b = t_d = 0.09|U| \) with a harmonic trap \( V_0 = 0.0002|U| \).

Figure 8. Density distribution (black line), order parameter (green line) and PSF correlator \( \phi_{bd} \) (red line) versus radius \( r \) for different hopping amplitudes at zero temperature for a trapped 3D cubic lattice obtained within BDMFT+LDA. The interactions are \( U_b = U_d = 12|U| \), hopping amplitudes \( t = t_b = t_d \) and harmonic trap \( V_0 = 0.0002|U| \).
Figure 9. Temperature dependence of the PSF correlator as a function of radius $r$ for a 3D cubic lattice, obtained within BDMFT+LDA. The interactions are $U_b = U_d = 12|U|$, hopping amplitudes $t_b = t_d = 0.045|U|$ and harmonic trap $V_0 = 0.0002|U|$.

and the corresponding phase transition is from a Mott insulator with total filling $n = 2$ to a PSF with total filling $0 < n < 2$ indicated by the non-vanishing value of $\phi_{bd}$ while $\phi_b = 0$. If we increase the hopping amplitudes, the first-order tunneling of single atoms will increase, which induces large density fluctuations in the system, leading to a phase transition from the PSF to the superfluid phase. We clearly observe this effect from the middle panel of figure 6 where the superfluid phase starts to appear in the middle of the PSF. With further increase of the tunneling amplitudes the superfluid dominates, as shown in the lower panel of figure 6, where the PSF completely disappears at $t = 0.7|U|$.

Figure 7 shows a comparison between the results of RBDMFT and those of BDMFT+LDA for a 2D square lattice. We observe good agreement between the two methods except close to the phase transition. In spite of the artificially sharp phase transition feature of LDA, the results of BDMFT+LDA are still reliable with sufficient accuracy in the regime away from the transition. We will therefore apply BDMFT+LDA to tackle the 3D case due to its higher computational efficiency compared to RBDMFT.

Let us now investigate the stability of PSF in the 3D case in the presence of a harmonic trap. Results obtained within LDA are shown in figure 8. Here we choose completely symmetric parameters: $t = t_b = t_d$ and $U_b = U_d = 12|U|$ with balanced filling for the two components. Only one value for $n_{b,d}$ and $\phi_{b,d}$ is shown in figure 8, respectively. Compared to 2D, we observe a similar scenario of phase coexistence in the trapped 3D cubic lattice: at lower hopping amplitudes the Mott insulator and the PSF are coexisting, at intermediate hopping amplitudes, the superfluid phase appears due to increased density fluctuations, and at even larger hopping amplitudes, the PSF will disappear.

We are also interested in the effects of temperature on the PSF. Figure 9 shows the correlator $\phi_{bd}$ for different temperatures. We observe that the PSF is sensitive to thermal fluctuations. At finite $T$, the PSF is reduced in favor of developing an unordered phase
characterized by $\phi_{bd} = 0$. On the other hand, the density distribution is rather insensitive to small finite $T$.

3.3.2. Imbalanced mixture. As pointed out above, asymmetry in the hopping of the two species does not destroy the PSF. However, filling imbalance hinders the formation of the pairs [16, 38]. We will now study this effect in more detail. The imbalance, $N_b \neq N_d$, will be controlled by a non-zero chemical potential difference $\Delta \mu = \mu_b - \mu_d$ which can be viewed as an effective magnetic field. Results in 2D are shown in figure 10. Upon increasing $\Delta \mu$, the PSF will cease to exist and will be replaced by a superfluid phase, since the chemical potential difference eventually exceeds the pairing gap for the PSF, allowing unpaired excess atoms to enter the PSF region. We find that the density distribution is almost unchanged for small $\Delta \mu$, as shown in figure 10. When increasing the imbalance parameter $\Delta \mu$ further, the PSF will disappear already for a small population imbalance, since the particles form a conventional superfluid. Here we do not find any phase separation.

Figure 10. Density distributions $n_{b,d}$, order parameters $\langle b \rangle$, $\langle d \rangle$ and PSF correlator $\phi_{bd}$ versus radial distance $r$ for different $\Delta \mu$ at zero temperature in a trapped 2D cubic lattice, obtained within BDMFT+LDA. Panel (d) shows the filling difference $(n_b - n_d)$ versus radius $r$. The interactions are $U_b = U_d = 12|U|$, hopping amplitudes $t_b = t_d = 0.05|U|$, $(\mu_b + \mu_d)/2 = -0.48$ and harmonic trap $V_0 = 0.00015|U|$.
Figure 11. Density distributions $n_{b,d}$, order parameters $\langle b \rangle, \langle d \rangle$ and PSF correlator $\phi_{bd}$ versus radius $r$ for different $\Delta \mu$ at zero temperature in a trapped 3D cubic lattice, obtained within BDMFT+LDA. Panel (d) shows the filling imbalance $(n_b - n_d)$ versus radius $r$. The interactions are $U_b = U_d = 12|U|$, hopping amplitudes $t_b = t_d = 0.04|U|$, $(\mu_b + \mu_d)/2 = -0.47$ and harmonic trap $V_0 = 0.0003|U|$.

Finally, we discuss the influence of population imbalance on the PSF in a trapped 3D cubic lattice using BDMFT+LDA. From our results shown in figure 11 we conclude that here the physics is qualitatively similar to the 2D case.

4. Summary

We have investigated low-temperature properties of Bose–Bose mixtures with attractive interspecies interaction both in 2D and 3D optical lattices by means of BDMFT/RBDMFT. In particular, we found that the pair superfluid and charge density wave are stable for asymmetric hopping of the two species. We obtained the critical temperature of the PSF, which we found to be of the same order as that of the XY-ferromagnet in the corresponding system with repulsive interactions of equal magnitude. We have confirmed the stability of the PSF in a balanced Bose–Bose mixture in the presence of the harmonic trap both in 2D and 3D. On the other hand, we found that even a small population imbalance can destroy the PSF. This novel PSF
quantum phase can be detected in future experiments via the momentum distribution of pairs, which shows signatures of the pair condensate [16, 38].

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