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# Population-imbalanced fermions in harmonically trapped optical lattices

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The attractive Fermi-Hubbard Hamiltonian is solved via the Bogoliubov-de Gennes formalism to analyze the ground state phases of population imbalanced fermion mixtures in harmonically trapped two-dimensional optical lattices. In the low density limit the superfluid order parameter modulates in the radial direction towards the trap edges to accommodate the unpaired fermions that are pushed away from the trap center with a single peak in their density. However, in the high density limit while the order parameter modulates in the radial direction towards the trap center for low imbalance, it also modulates towards the trap edges with increasing imbalance until the superfluid to normal phase transition occurs beyond a critical imbalance. This leads to a single peak in the density of unpaired fermions for low and high imbalance, but leads to double peaks for intermediate imbalance.

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The phase diagram of dilute population-imbalanced fermion mixtures has been recently studied showing superfluid to normal phase transition with increasing imbalance as well as a phase separation between paired and unpaired fermions [1–4]. These recent works are extentions of the earlier works on dilute population balanced mixtures where a crossover from Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensation (BEC) type superfluidity is observed as a function of the attractive fermion-fermion interaction strength [5–9].

Arguably understanding the phase diagram of fermion mixtures in optical lattices is one of the next frontiers in cold atoms research because of their great tunability. In addition to the particle populations and the particle-particle interaction strengths, one can also precisely control the particle tunnelings, the lattice dimensionality, and the lattice geometry. For instance experimental evidence for the superfluid and the insulating phases of population balanced mixtures have been recently reported in trapped optical lattices [10], after overcoming some earlier difficulties [11–14]. This recent work has also opened the possibility of studying many-body properties of population imbalanced mixtures in optical lattices.

Earlier theoretical works on population imbalanced fermion mixtures in optical lattices were limited to homogenous systems [15,16], and they showed rich phase diagrams involving BCS type nonmodulating and Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) type spatially modulating superfluid phases in addition to insulating and normal phases. Furthermore the phase diagram of population-imbalanced mixtures in harmonically trapped optical lattices has been recently discussed within the semiclassical local density approximation (LDA) [17]. However it has been previously shown that the LDA type methods are not sufficient to describe even the dilute population imbalanced mixtures without an optical lattice [18,19]. In this Rapid Communication, we therefore analyze the ground state phases of fermion mixtures in harmonically trapped two-dimensional optical lattices via using the fully quantum mechanical Bogoliubov-de Gennes (BdG) method where the trapping potential is included exactly at the mean-field level.

Our main results are as follows. In the low density limit the superfluid order parameter modulates in the radial direction towards the trap edges to accommodate the unpaired fermions that are pushed away from the trap center with a single peak in their density. These findings are in good agreement with the recent theoretical [18–20] and experimental [1–4] findings on dilute population imbalanced mixtures without an optical lattice. However, in the high density limit while the order parameter modulates in the radial direction towards the trap center for low imbalance, it also modulates towards the trap edges with increasing imbalance until the superfluid to normal phase transition occurs beyond a critical imbalance. This leads to a single peak in the density of unpaired fermions for low and high imbalance but leads to double peaks for intermediate imbalance.

*BdG formalism.* To achieve these results we solve the Fermi-Hubbard Hamiltonian

$$H_{FH} = -\sum_{i,j,\sigma} t_{i,j,\sigma} a_{i,\sigma}^\dagger a_{j,\sigma} - \sum_{i,\sigma} (\mu_\sigma - V_{i,\sigma}) a_{i,\sigma}^\dagger a_{i,\sigma} - \sum_{i,j} U_{i,j} a_{j,\uparrow}^\dagger a_{j,\uparrow} a_{i,\downarrow}^\dagger a_{i,\downarrow}, \tag{1}$$

where $a_{i,\sigma}^\dagger$ ($a_{i,\sigma}$) creates (annihilates) a pseudospin $\sigma$ fermion at lattice site $i$, $t_{i,j,\sigma}$ and $U_{i,j} \geqslant 0$ are the particle-particle tunneling and the density-density interaction matrix elements, $\mu_\sigma$ is the chemical potential, and $V_{i,\sigma} = \alpha_\sigma |\mathbf{r_i}|^2/2$ is the trapping potential at position $\mathbf{r}_i$ with $\alpha_\sigma = m_\sigma \omega_\sigma^2$ such that the trapping potential is centered at the origin. Here the label $\sigma$ identifies $\uparrow$ or $\downarrow$ fermions and allows $\sigma$ fermions to have equal or unequal masses controlled by $t_{i,j,\sigma}$ and/or to have equal or unequal populations controlled by $\mu_\sigma$.

In the mean-field approximation for the superfluid phase, the Fermi-Hubbard Hamiltonian reduces to $H = -\Sigma_{i,j,\sigma} t_{i,j,\sigma} a_{i,\sigma}^\dagger a_{j,\sigma} - \Sigma_{i,\sigma}(\mu_\sigma - V_{i,\sigma}) a_{i,\sigma}^\dagger a_{i,\sigma} - \Sigma_{i,j}(\Delta_{i,j} a_{j,\downarrow}^\dagger a_{i,\uparrow}^\dagger + \Delta_{i,j}^* a_{i,\uparrow} a_{j,\downarrow} - |\Delta_{i,j}|^2/U_{i,j})$, where the self-consistent field $\Delta_{i,j} = U_{i,j} \langle a_{i,\uparrow} a_{j,\downarrow} \rangle$ is the superfluid order parameter and $\langle \cdots \rangle$ is a thermal average. The mean-field Hamiltonian can be diagonalized via the Bogoliubov-Valatin transformation $a_{i,\sigma} = \Sigma_n [u_{n,i,\sigma} \gamma_{n,\sigma} - s_\sigma v_{n,i,\sigma}^* \gamma_{n,-\sigma}^\dagger]$, where $\gamma_{n,\sigma}^\dagger$ ($\gamma_{n,\sigma}$) creates (annihilates) a pseudospin $\sigma$ quasiparticle with the wave function $u_{n,i,\sigma}$ ($v_{n,i,\sigma}$), and $s_\uparrow=+1$ and $s_\downarrow=-1$. This leads to the BdG equations

$$\sum_j \begin{pmatrix} T_{i,j,\uparrow} & \Delta_{i,j} \\ \Delta^*_{i,j} & -T^*_{i,j,\downarrow} \end{pmatrix} \varphi_{\mathbf{n},\mathbf{j},\sigma} = s_\sigma \epsilon_{n,\sigma} \varphi_{\mathbf{n},\mathbf{i},\sigma}, \tag{2}$$

where $T_{i,j,\sigma}=-t_{i,j,\sigma}-(\mu_\sigma-V_{i,\sigma})\delta_{i,j}$ is the diagonal element and $\delta_{i,j}$ is the Kronecker delta. Here $\epsilon_{n,\sigma}>0$ are the eigenvalues and $\varphi_{\mathbf{n},\mathbf{i},\sigma}$ are the eigenfunctions given by $\varphi_{\mathbf{n},\mathbf{i},\uparrow}^\dagger=(u^*_{n,i,\uparrow},v^*_{n,i,\downarrow})$ for the $\uparrow$ and $\varphi_{\mathbf{n},\mathbf{i},\downarrow}^\dagger=(v_{n,i,\uparrow},-u_{n,i,\downarrow})$ for the $\downarrow$ eigenvalues. Since solutions to the BdG equations are invariant under the transformation $v_{n,i,\uparrow}\to u^*_{n,i,\uparrow}$, $u_{n,i,\downarrow}\to -v^*_{n,i,\downarrow}$, and $\epsilon_{n,\downarrow}\to-\epsilon_{n,\uparrow}$, it is sufficient to solve only for $u_{n,i}\equiv u_{n,i,\uparrow}$, $v_{n,i}\equiv v_{n,i,\downarrow}$, and $\epsilon_n\equiv\epsilon_{n,\uparrow}$ as long as we keep all the solutions with positive and negative $\epsilon_n$.

In Eq. (2) the superfluid order parameter $\Delta_{i,j}$ is given by $\Delta_{i,j}=-\Sigma_n U_{i,j} u_{n,i} v^*_{n,j} f(\epsilon_n)$ where $f(x)=1/[\exp(x/T)+1]$ is the Fermi function and $T$ is the temperature. Notice that this equation is free from the ultraviolet divergence and therefore it does not explicitly involve any energy cutoff since the lattice spacing provides an implicit cutoff. Equation (2) and the order parameter equation have to be solved self-consistently with the number equations $0\leqslant n_{i,\sigma}=\langle a^\dagger_{i,\sigma}a_{i,\sigma}\rangle \leqslant 1$ for the $\sigma$ fermions, where $n_{i,\uparrow}=\Sigma_n|u_{n,i}|^2 f(\epsilon_n)$ and $n_{i,\downarrow}=\Sigma_n|v_{n,i}|^2 f(-\epsilon_n)$ such that $N_\sigma=\Sigma_i n_{i,\sigma}$ determines $\mu_\sigma$. In the following we consider only attractive and onsite $s$-wave interactions and set $U_{i,j}=U_0\delta_{i,j}$ with $U_0\geqslant 0$. Notice that this leads to $\Delta_{i,j}=\Delta_i\delta_{i,j}$. Furthermore fermions are allowed to tunnel only to the nearest neighbor sites and thus $t_{i,j,\sigma}=t_\sigma\delta_{i,j\pm 1}$.

*Ground state phases*. We now analyze the ground state phases of fermion mixtures with equal masses ($m_0=m_\uparrow=m_\downarrow$), equal tunnelings ($t_0=t_\uparrow=t_\downarrow$), and equal trapping potentials ($\alpha_0=\alpha_\uparrow=\alpha_\downarrow$), but with unequal chemical potentials. The theoretical parameters $t_0$ and $U_0$ can be expressed in terms of the experimental parameters of the two-dimensional optical lattice potential $V_L(x,y)=V_L[\sin^2(\pi x/a)+\sin^2(\pi y/a)]$ via the relations [21] $t_0=(4E_r/\sqrt{\pi})(V_L/E_r)^{3/4}\exp(-2\sqrt{V_L/E_r})$ and $U_0=-\sqrt{8\pi}a_F E_r (V_L/E_r)^{3/4}/a$. Here $a$ is half of the laser wavelength which corresponds to the lattice spacing, $V_L$ is the depth of the optical lattice potential, $E_r=\hbar^2\pi^2/(2m_0a^2)$ is the recoil energy, and $a_F$ is the two-body scattering length in vacuum. The experimental parameters $V_L$, $a$, and $a_F$ can be tuned by varying the laser intensity, the laser wavelength, and the externally applied magnetic field via using the Feshbach resonances, respectively, which makes optical lattices ideal systems to simulate the Fermi-Hubbard Hamiltonian.

For numerical purposes the superfluid order parameter is assumed to be real ($\Delta_i=\Delta_i^*$). This is sufficient to describe the nonmodulating and the spatially modulating superfluid phases in addition to the normal and the band insulator phases. We also take $U_0=3t_0$ and $V_0=\alpha_0 a^2/2=0.02t_0$ as the strength of the weak onsite interactions and the weak trapping potentials, respectively, and perform calculations on a two-dimensional square lattice with a length of $L=50a$ in both directions. The trap center is located at $\mathbf{r_c}\equiv(x=0a,y=0a)$. We want to emphasize that similar calculations also can be performed for three-dimensional optical lattices. However, they are computationally much more demanding and we do not expect any qualitative difference between our two-dimensional results and the three-dimensional ones.

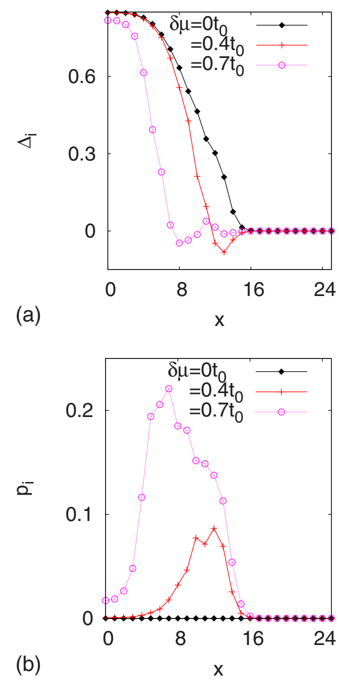


FIG. 1. (Color online) We show (a) the order parameter $\Delta_i$ (in units of $t_0$) and (b) the population difference $p_i=n_{i,\uparrow}-n_{i,\downarrow}$ (per lattice site) for the low density case as a function of distance $x$ (in units of $a$) from the trap center. Here $y=0a$.

We fix the total number of fermions $N=N_\uparrow+N_\downarrow$ to $N\approx 270$ (corresponding to $\mu\approx 0t_0$) in the low density and to $N\approx 1570$ (corresponding to $\mu\approx 5t_0$) in the high density case where $\mu=(\mu_\uparrow+\mu_\downarrow)/2$, while we vary the population imbalance $P=(N_\uparrow-N_\downarrow)/N$ or equivalently $\delta\mu=(\mu_\uparrow-\mu_\downarrow)/2$. For these parameters it is important to notice that the trapping potential provides a soft boundary leading to a finite system, and therefore it simplifies the numerical calculations considerably in comparison to infinite systems. Next we present self-consistent solutions of Eq. (2) with the order parameter and the number equations.

*(I) Low density mixtures*. In Fig. 1 we show the superfluid order parameter $\Delta_i$ and the population difference per lattice site $p_i=n_{i,\uparrow}-n_{i,\downarrow}$ for the low density case where $N\approx 270$. When $U_0=0$ and $N_\uparrow=N_\downarrow=N/2$, the maximum filling of this case corresponds to an almost half-filled band with $n_{i,\sigma}\approx 0.5$ at the trap center. For such low densities we expect that our results for the trapped mixtures with an optical lattice to recover the previously obtained results for the trapped dilute mixtures without an optical lattice [18–20]. This occurs when the interparticle separation becomes much longer than $a$ such that the particles do not feel the presence of a lattice potential. However to understand the ground state phases of population imbalanced mixtures, it is very illustrative to first discuss the population balanced case.

For a weakly attracting population balanced mixture with $U_0=3t_0$ and $\delta\mu=0$, the order parameter $\Delta_i$ is finite around the trap center for distances $|\mathbf{r_i}|\lesssim 15a$, and therefore the ground state corresponds to a BCS type superfluid. For longer distances $|\mathbf{r_i}| \gtrsim 16a$ away from the trap center, $\Delta_i$ gradually decreases until it eventually vanishes when the densities become very low $n_{i,\uparrow}=n_{i,\downarrow}\approx 0$. These features can be seen in Fig. 1(a), and they are in good agreement with the earlier experiments involving population balanced mixtures without an optical lattice [5–9].

In the case of population imbalanced mixtures, we find that $\Delta_i$ modulates in the radial direction towards the trap edges to accommodate the unpaired fermions. However, $\Delta_i$ decreases with increasing population imbalance as shown in Fig. 1(a), and it vanishes entirely beyond a critical imbalance signaling a transition from the superfluid to the normal phase. These features can be seen in Fig. 1(a) where $\delta\mu=0.4t_0$ and $\delta\mu=0.7t_0$ corresponding to $P\approx 0.12$ and $P\approx 0.34$, respectively. Similar spatial modulations have been recently found also in dilute population imbalanced mixtures without an optical lattice [18–20], however they have not yet been observed in the current experiments [1–4]. In contrast to our BdG results, the LDA type methods exclude the possibility of order parameter modulations and therefore they fail to produce such a spatially modulated superfluid phase which is one of the possible candidates for the ground state.

In the recent theoretical works on dilute population imbalanced mixtures without an optical lattice, such spatial modulations have been suggested as signatures for the FFLO type superfluidity by some authors [18,19] and as finite size effects by some others [20]. Here we remind the reader that the FFLO type superfluidity is characterized by the formation of Cooper pairs with nonzero center-of-mass momentum, in contrast with the BCS type superfluidity where Cooper pairs have zero center-of-mass momentum [22]. Therefore in two- and three-dimensional systems it is an open question whether these spatial modulations are related to the FFLO superfluidity or are simply finite size effects. However, we also remind the reader that the exact ground state phase diagram of one-dimensional systems have been recently calculated [23–26] showing that the superfluid phase has FFLO structure in trapped as well as infinite systems.

In Fig. 1(b) we show that the unpaired fermions are pushed away from the trap center towards the trap edges and they have a maximum at the position where $\Delta_i$ changes sign. This is because spatially bound Andreev type states form around the nodes of $\Delta_i$, and the occupation of these bound states is different for $\uparrow$ and $\downarrow$ fermions [18]. Since $\mu_\uparrow > \mu_\downarrow$ when $N_\uparrow > N_\downarrow$, the $\uparrow$ fermions mostly occupy these states leading to the single peak structure. This feature is in good agreement with the recent experiments on dilute population imbalanced mixtures without an optical lattice [1–4]. However, in contrast with the trapped mixtures without an optical lattice, both $\Delta_i$ and $p_i$ have $C_4$ symmetry which is consistent with the underlying symmetry of the square lattice. Here we notice that the LDA type methods always produce results with rotational symmetry and therefore they are not strictly applicable to optical lattices. Having shown that the ground state phases of low density mixtures in optical lattices are qualitatively similar to those of the dilute mixtures without an optical lattice, next we discuss the high density mixtures.

*(II) High density mixtures*. In Figs. 2 and 3 we show the superfluid order parameter $\Delta_i$ and the population difference per lattice site $p_i$ for the high density case where $N\approx 1570$.

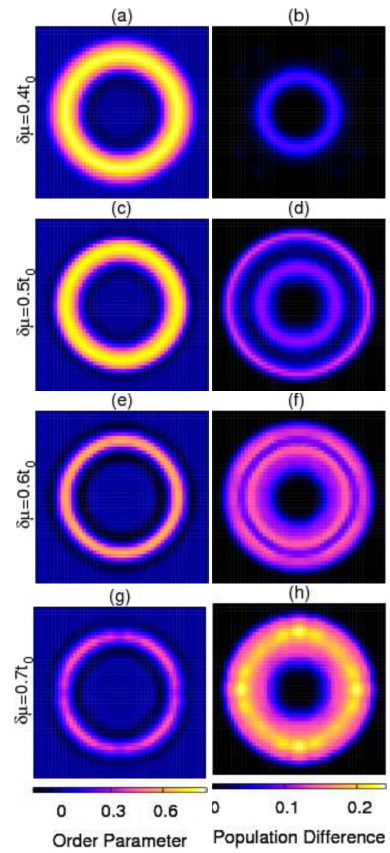


FIG. 2. (Color online) We show the order parameter $\Delta_i$ (on the left, in units of $t_0$) and population difference $p_i=n_{i,\uparrow}-n_{i,\downarrow}$ (on the right, per lattice site) for the high density case on a two-dimensional square lattice with $50a\times 50a$ sites. Here the chemical potentials are such that (a), (b) $\delta\mu=0.4t_0$; (c), (d) $\delta\mu=0.5t_0$; (e), (f) $\delta\mu=0.6t_0$; and (g), (h) $\delta\mu=0.7t_0$.

When $U_0=0$ and $N_\uparrow=N_\downarrow=N/2$, the maximum filling of this case corresponds to a fully filled band with $n_{i,\sigma}=1$ near the trap center. For such high densities the ground state phases are very different from those of the low density systems as can be seen in Figs. 2 and 3. To understand these ground state phases of population imbalanced mixtures, it is again very illustrative to first discuss the population balanced case.

For a weakly attracting population balanced mixture with $U_0=3t_0$ and $\delta\mu=0$, we find that $\Delta_i=0$ around the trap center for distances $|\mathbf{r_i}|\lesssim 4a$. This signals the band insulator phase characterized by a fully filled band where $n_{i,\uparrow}=n_{i,\downarrow}=1$. However since $n_{i,\uparrow}=n_{i,\downarrow}<1$ away from the trap center, $\Delta_i$ becomes finite signaling a transition from the band insulator to the superfluid phase. The maximum $\Delta_i$ occurs around $|\mathbf{r_i}|\approx 16a$ where $n_{i,\uparrow}=n_{i,\downarrow}=0.5$ corresponding to a half-filled band. This is purely a density of states $(D_i)$ effect since $\Delta_i \propto t_0 e^{-1/(U_0 D_i)}$ and $D_i$ has a maximum exactly at half-filling due to particle-hole symmetry of the Fermi-Hubbard Hamiltonian. For longer distances $|\mathbf{r_i}|\gtrsim 16a$ away from the trap center, $\Delta_i$ gradually decreases until it eventually vanishes for $|\mathbf{r_i}|\gtrsim 22a$ where $n_{i,\uparrow}=n_{i,\downarrow}\approx 0$. These features can be seen in Fig. 3(a) and they are very different from those of the low density case shown in Fig. 1(a). In contrast to our BdG results, the LDA type methods fail to describe the band insu-

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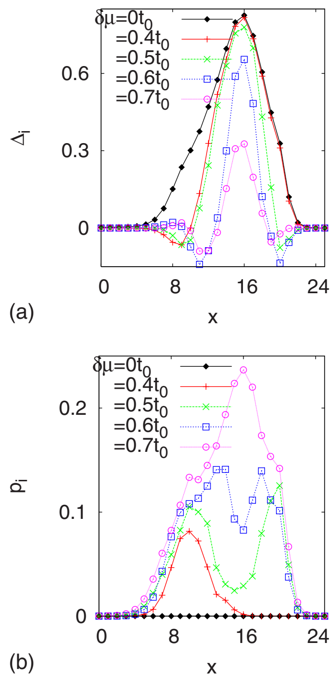


FIG. 3. (Color online) We show (a) the order parameter $\Delta_i$ (in units of $t_0$) and (b) the population difference $p_i = n_{i,\uparrow} - n_{i,\downarrow}$ (per lattice site) for the high density case as a function of distance $x$ (in units of $a$) from the trap center. Here $y=0a$.

lator region with unit filling because the density profiles do not vary smoothly as a function of $|\mathbf{r_i}|$.

In the case of population imbalanced mixtures, we find that $\Delta_i$ modulates in the radial direction towards the trap center for low imbalance as shown in Fig. 2(a) because $\Delta_i$ is a more slowly decreasing function of $|\mathbf{r_i}|$ towards the trap center than towards the trap edges when $\delta\mu=0$. However, $\Delta_i$ also modulates towards the trap edges with increasing imbalance as shown in Figs. 2(c)–2(e). Characteristic features of these spatial modulations are similar to those of the low density systems and they can be seen in Fig. 3(a) where $\delta\mu=0.4t_0$, $\delta\mu=0.5t_0$, $\delta\mu=0.6t_0$, and $\delta\mu=0.7t_0$ corresponding to $P\approx 0.017$, $P\approx 0.058$, $P\approx 0.090$, and $P\approx 0.12$, respectively. Therefore high density mixtures in trapped optical lattices are also good candidates for observation of such exotic superfluid modulations. Further increasing the population imbalance gradually decreases $\Delta_i$ as shown in Fig. 3(a), until it vanishes entirely beyond a critical imbalance signaling a transition from the superfluid to the normal phase.

In Figs. 2(b) and 3(b) we show for low imbalanced mixtures that the density of unpaired fermions has a single peak at the position where $\Delta_i$ changes sign. However since $\Delta_i$ also modulates towards the trap edges for intermediate imbalance, the unpaired fermions have double peaks in their density as shown in Figs. 2(d), 2(f), and 3(b). Furthermore, since $\Delta_i$ vanishes with further increase in imbalance, these two peaks merge leading to a single peak which is shown in Figs. 2(h) and 3(b). Notice that similar to the low density case both $\Delta_i$ and $p_i$ have $C_4$ symmetry which is consistent with the underlying symmetry of the square lattice.

To conclude we used the BdG method to analyze the ground state phases of population imbalanced fermion mixtures in harmonically trapped optical lattices. First we showed that the phase structure of low density mixtures in optical lattices are qualitatively similar to those of the dilute mixtures without an optical lattice. Then we discussed high density mixtures and found qualitatively different results. In both cases we found that the superfluid order parameter modulates spatially but it is an open question whether these modulations are related to the FFLO superfluidity or are simply finite size effects. Lastly we compared our BdG results with the LDA ones and argued that the LDA type methods are not sufficient to describe especially the high density mixtures in harmonically trapped optical lattices.

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