Exploring Exotic Superfluidity of Polarized Ultracold Fermions in Optical Lattices

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Enormous interest has been paid to ultracold Fermi gases due to the interplay between Cooper pairing and strong correlations [1, 2, 3]. Beautiful experiments on the superfluidity have been performed in these systems with unequal spin populations [4, 5, 6, 7, 8, 9]. Arrestingly, it was found that the superfluid paired core is surrounded by a shell of normal unpaired fermions while the density distribution of the difference of the two components becomes bimodal. Here we explore theoretically the novel superfluidity of harmonically-trapped polarized ultracold fermionic atoms in a two-dimensional (2D) optical lattice by solving the Bogoliubov-de Gennes equations. The pairing amplitude is found to oscillate along the radial direction at low particle density and along the angular direction at high density. The former is consistent with the existing experiments and the latter is a newly predicted Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, which can be tested in experiments.

Experimentally, optical lattices artificially created by standing-wave laser fields [10, 11, 12] provide unprecedented experimental tunability, such as a precise control of model Hamiltonian parameters including the interaction strength, lattice geometry and number of atoms. This versatile tool opens a door to explore rich and novel physical phenomena in various strongly correlated systems. Experimental exploration of the novel superfluid phase of imbalanced fermions in optical lattices is expected to be conducted in the near future, while in the theoretical aspect, there exists a long-standing debate on the nature of the exotic pairing state for the imbalanced systems. The inhomogeneous superconducting state, known as the FFLO state, was predicted about forty years ago, which contains nonzero momentum Cooper pairs with the superconducting gap exhibiting a periodic real-space modulations [13]. There have been suggestions for the possible FFLO phase for some of the high-Tc, layered organic, and heavy fermion superconductors at very low temperatures and high magnetic fields [14, 15]. This subject has also been studied in nuclear and high-energy physics [16]. Despite of many previous literatures in this field [17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28], it is still awaited to explore theoretically and unambiguously the exotic FFLO state with imbalanced ultracold fermions in optical lattices.

In this letter, we present an unrestricted Hartree-Fock study of a two-component fermionic atoms in a harmonically-confined 2D optical lattice. Due to the competition between the ferromagnetic and s-wave superfluid phases in the presence of harmonically trapped potential, the compromised ground state may exhibit rich patterns of order parameter configurations. Our main findings are as follows. (i) In the low fermionic filling regime, the superfluid-pairing gap modulates its sign along the radial direction, indicating an FFLO state. The calculated density profiles of the two components of the fermions show a striking resemblance to the experimental observations. (ii) In the high filling regime, a superfluid-pairing ring appears. As the imbalance increases, the pairing gap oscillates along the angular direction, signaling a novel FFLO state. (iii) A variety of intriguing distributions of the order parameter, such as square lattice FFLO state, emerges in the intermediate filling regime. In addition, we also observe that, as the imbalance increases, the superfluidity is suppressed and vanishes at a critical imbalance amplitude, implying the existence of the Clogston limit [29].

To simulate the neutral fermionic atoms in a 2D optical lattice, we begin with an effective tight-binding Hamiltonian, which captures the basic interplay between ferromagnetism and s-wave fermion-pairing in the presence of a confining potential,

\[
\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{\sigma} (\epsilon_i - \mu_\sigma) \hat{n}_{i\sigma} + \sum_{\langle ij \rangle} \left( \Delta_s \hat{c}_{i\sigma}^\dagger \hat{c}_{j\bar{\sigma}} + h.c. \right),
\]

where \(\hat{c}_{i\sigma}\) is an annihilation operator for an atom at site \(i\) (at position \(r_i\)) with spin \(\sigma\) and \(\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\) is the number operator. \(t\) is the effective nearest-neighbor hopping integral. The spin-dependent chemical potential due to the Zeeman splitting is defined as \(\mu_\sigma = \mu - \sigma \hbar \epsilon_i\). \(\epsilon_i = \frac{1}{2} m \omega^2 |r_i - r_0|^2\) is the harmonic confining potential at site \(i\), and \(r_0\) is the position of the trap center.

At the mean-field level, the model Hamiltonian can be diagonalized by solving the resulting Bogoliubov-de
respectively, where \( T \) is the temperature.

The atom density and the s-wave pairing order parameter satisfy the self-consistency conditions,

\[
\bar{n}_i \equiv \sum_{\sigma} n_{i\sigma}^n f(E_n) \quad \text{and} \quad \Delta_i = \sum_{\sigma} n_{i\sigma}^n \bar{n}_{i\sigma}^n \tanh(E_n/2k_BT),
\]
where \( n_{i\sigma}^n \) is the condensate density at the site \( i \). The pairing gap of the ground state of Hamiltonian (1) oscillates in space with a stripe-like pattern for the s-wave (BdG) equations self-consistently [30, 31],

\[
\sum_j \left( H_{ij,\sigma} \delta_{ij} - H_{ij,\bar{\sigma}}^* \right) \left( \begin{array}{c} u_{ij}^n \\ v_{ij}^n \end{array} \right) = E_n \left( \begin{array}{c} u_{i\bar{\sigma}}^n \\ v_{i\bar{\sigma}}^n \end{array} \right),
\]

where \( H_{ij,\sigma} = -t_{ij} - (\epsilon_i + \mu_\sigma)\delta_{ii} \) is the single particle Hamiltonian, \( \Delta_{ij} = \Delta \delta_{ii} \) is the pairing order parameter, and \( \left( u_{ij}^n, v_{ij}^n \right) \) are the Bogoliubov quasiparticle amplitudes at the site \( i \). The atom density and the s-wave pairing order parameter satisfy the self-consistency conditions,

\[
n_i = \sum_n |n_{i\sigma}|^2 f(E_n), \quad n_i = \sum_n |v_{i\sigma}|^2 \left[ 1 - f(E_n) \right]
\]

where \( \Delta_i \) is the pairing gap, \( V \) is the confinement energy, \( m \) is the mass, and \( T \) is the temperature. The local magnetization is defined as \( m_i = n_{i\uparrow} - n_{i\downarrow} \), which can be tuned by changing the magnetic field in the present model.

In a laboratory optical lattice, \( m_i \) can be tuned directly although there is no real magnetic field. In our calculations below, we set \( t = 1 \) as the energy unit and lattice spacing \( a = 1 \) as the length unit. We consider a very low temperature \( T = 0.001 \), and the amplitude of confining potential \( \frac{1}{2} m \omega^2 a^2 / t \sim (0.016 - 0.025) \). The dimension of lattice is \( 42 \times 42 \) with open boundary conditions and the trap center is located at \((21,21)\). All the order parameters or mean fields are calculated self-consistently by solving the BdG equations iteratively, with their initial values randomly distributed on the lattice. In the case of multi-solutions, we compare their corresponding free energies to determine the most energetically favored state.

The applied magnetic field may cause the density imbalance of the two species of fermions (spin-up and spin-down). The induced ferromagnetism competes with the superfluid pairing state, resulting in the emergence of exotic FFLO phases. In the special case \( \epsilon_i = 0 \) and in 2D, the pairing gap of the ground state of Hamiltonian (1) oscillates in space with a stripe-like pattern for the s-wave and a square lattice pattern for the d-wave [32]. In the crossing region of the positive and negative pairing amplitudes, there exist nodal lines where the ferromagnetism appears. The presence of the trapped potential may add up to the new complications.

In the widely used local density approximation (LDA), the spatial dependence of observable must follow contours of constant trapping potential in the same way that a spatially uniform system does. Our approach provides a consistent way to explore novel states beyond LDA. In particular, our results show that the compromising ground state depends crucially on the \( n_c \) (fermion density at the trap center). The features presented below can be classified into three regimes accordingly.

Low-filling regime \((n_c < 1)\). In Fig. 1, we plot typically three spatial profiles of the pairing order parameter \( \Delta_i \) together with local magnetization \( m_i \) as functions of magnetic field \( h \). At \( h = 0 \), there is no ferromagnetic order and the trapping potential may result in the accumulation of electron density around the center. As shown in Fig. 1(a)-(b), \( \Delta_i \) reaches its maximum value at the trap center and decreases to zero far away from the center. These results are consistent with those obtained by LDA, where no competing orders show up. As \( h \) increases, the ferromagnetic order may emerge and frustrate the conventional pairing state. In Fig. 1(c), our calculations show the appearance of superfluid pairing gap modulations along the radial direction, indicating an FFLO state. At the edge of the modulation, a continuous sign change of the pairing gap corresponds to a nodal line \((\Delta_i = 0)\).

Meanwhile the magnetic order parameter \( m_i \) is most remarkable around the ring-like nodal line so that its density profile exhibits a bimodal structure, as shown in Fig. 1(d). In other words, the minority fermions are squeezed into the inner core due to the pair condensation in the superfluid phase, while the unpaired majority fermions are repelled to the outside of the core. When the imbalance increases, the minority fermions contribute more effectively to the pairing states. This result is in good agreement with the experiments, and also with the previous theoretical studies on the FFLO state in a continuous model [18,19]. As \( h \) progressively increases, the pairing order may further be suppressed and the weak modulation of the pairing gap appears away from the trap center while the ferromagnetic order shows a plateau-like feature nearby the trap center. Furthermore, the superfluidity vanishes at a critical magnetic field \((h_c \sim 1.6)\), which corresponds to the Clogston limit. Note that the existing experimental realization [4,4,6,8,8] may correspond to the present low-filling case. The density profiles obtained in our theory exhibit remarkable resemblance to the experimental
measurements.

To show the bimodal structure more transparently, we display the density profiles along the lattice diagonal through the trap center. The density distribution has a four-fold symmetry, consistent with the underlying lattice structure. As shown in Fig. 2, the bimodal distribution of magnetization clearly shows up at finite $h$. There are three regions: a superfluid core with equal densities, a partially polarized shell, and a fully polarized region. By increasing $h$, these bimodal structures evolve to have more pronounced amplitude while the separation between peaks becomes narrower. As $h$ exceeds a critical value, the equal density core disappears and the condensation fraction also vanishes. In such a case, the ferromagnetic order reaches its maximum at the trap center and its density profile displays a plateau-like structure.

High-filling regime ($\rho_c$ close to 2). In this regime, the band is almost fully occupied, corresponding to an insulating state in a conventional solid state system, around the trap center. The pairing order can not survive far way from the center because of the low fermion density. In the intermediate distance from the center, one may naturally expect the formation of ring like fermion pairing state at the intermediate range. In Fig. 3(a)-3(b), the profile of $\Delta_1$ does show such a topological structure at $h = 0$. Upon increasing $h$, the ferromagnetic order may emerge and result in the frustration of the competing pairing state. It is well known that the lower angular momentum state has always the lower energy in the infinite system. However, in the present case, due to the highly nontrivial interplays among trapping potential, magnetization and pairing correlations, it is possible that the exotic pairing state with higher angular momentum state becomes energetically favorable. As depicted in Fig. 3(c), the pairing gap oscillates along the angular (ring) direction with alternating positive and negative signs. In Fig. 3(d), it shows clearly four regions with abrupt sign change where magnetization shows up. This special configuration lowers the free energy and allows oscillating fermion pairing state to remain stable. By further increasing $h$, there will be more oscillations along the angular direction as well as more appreciable magnetization, as displayed in Fig. 3(e)-3(f). When $h = 1.5$, the superconducting order is almost fully suppressed while the ferromagnetic order forms a shell pattern [Fig. 3(g)-3(h)].

An intuitive physical understanding of angular FFLO state can be given as follows: the main effect of the high filling at the trap center is the formation of superconducting shell structure as shown in Fig. 3(a). As is known, the FFLO is rather robust in 1D [33, 34]. If the superconducting shell is sufficiently thin like a 1D ring, then FFLO tends to emerge. That is to say, the spin imbalance will lead to the pairing oscillation along the angular direction rather than in the radial direction since the former state costs less kinetic energy. This novel angular FFLO state can be observed in 2D optical lattices where high filling regime can be easily achieved. We have checked our results for the $d$-wave pairing interaction, and the similar conclusions have also been reached. It is worth to mention that the simple LDA fails to get such a novel pairing state. Here we need to stress the critical role played by trapping potential in the formation of the FFLO states along radial or angular direction. The appearance of the FFLO state minimizes the relevant free energy, which is a direct manifestation of the competition between ferromagnetism and superconductivity. The trapping potential provides a confined and inhomogeneous background, which complicates the competition, but reveals some of the novel physics associated with the FFLO states.
Medium-filling regime ($n_c \in (1,2)$). In this regime, rich patterns of order parameter distribution show up. In the absence of the magnetic field, the pairing order parameter shows a small concaved structure around the trap center, as seen in Fig. 4(a). By tuning the magnetic field to $h = 0.4$, the pairing gap modulation along the radial direction shows up and the situation is analogous to the low filling case [Fig. 1(d)-1(f)]. When $h = 0.6$, the pairing order parameter modulates not only along the radial direction but also around the trap center, exhibiting a square lattice pattern as illustrated in Fig. 4(e).

Meanwhile, its ferromagnetic order exhibits a rich structure where there are many local maxima around the trap center which correspond to nodal lines in Fig. 4(f). As we further increases the magnetic field to $h = 0.9$, the square lattice pattern of FFLO state becomes more pronounced and the associated ferromagnetism exhibits itself as well [Fig. 4(g)-4(h)]. Note that the square lattice FFLO state appears in the infinite 2D system with the d-wave pairing [32]. When $h$ becomes quite large, the BCS pairing order is fully suppressed and the magnetization displays a plateau like structure around the trap center, as depicted in Fig. 4(i)-4(j).

So far, there has been no direct evidence of FFLO states in recent experiments since the probe of pairing gap distribution is very challenging. We now address an important issue on how to detect the peculiar real space patterns illustrated in Figs. 3 and 4 experimentally. First we propose a 2D optical lattice experiment with the fermionic atoms in the high filling regime. By increasing the imbalance progressively, we expect the emergence of angular dependent magnetization distribution, indicating the existence of angular FFLO state. Very recently, the MIT group produced preliminary experimental evidence for superfluidity of ultracold $^9$Li atoms in optical lattice [12]. We expect that a future experiment for imbalanced fermions will be conducted to examine our prediction. An alternative scenario to detect such an exotic state is to carry out the experiment in a thin superconducting ring of heavy fermion materials. By applying strong magnetic field parallel to the plane, the angular-dependent FFLO state may show up due to the special topology of the ring structure. Probe of the real space modulation of the pairing gap as well as magnetization can be achieved by using SQUID or STM techniques. The third proposal is to generate a Mexican hat trapping potential in 3D so that the distribution of the confined fermionic atoms may form a donut-like structure. In such a case, the angular dependent distribution of magnetization profile can be directly measured by using the time-of-flight imaging techniques.

In summary, we have explored theoretically the novel superfluidity and ferromagnetism in ultracold fermionic atoms on a 2D lattice combined with a harmonic trap. Due to the interplay between the confined ferromagnetic and superfluid orders, exotic FFLO phases have been revealed. At low density, our theory shows a bimodal distribution of the magnetization profile and a fermion pairing gap oscillating along the radial direction, reproducing the main features observed in recent experiments. We predict a more exotic angular FFLO state at high densities and square lattice like FFLO state at the intermediate densities.

References

[1] Jochim, S. et al. Bose-Einstein condensation of molecules, Science 302, 2101 (2003);
[2] Regal, C., Greiner, M. & Jin, D. Emergence of a molecular Bose-Einstein condensate from a Fermi gas, Nature 426, 537 (2003).
[3] Chin, C. et al. Observation of the pairing gap in a strongly interacting Fermi gas, Science 305, 1128-1130 (2004).
[4] Partridge, G.B., Li, W., Kamar, R.L., Liao, Y. & Hulet, R. Pairing and phase separation in a polarized Fermi gas, Science 311, 503-505 (2006);
[5] Partridge, G.B. et al. Deformation of a trapped Fermi gas with unequal spin populations, Phys. Rev. Lett. 97, 190407 (2006).
[6] Zwierlein, M.W., Schirotzek, A., Schunck, C.H. & Ketterle, W. Fermionic superfluidity with imbalanced spin populations, Science 311, 492-496 (2006).
[7] Zwierlein, M.W., Schunck, C.H., Schirotzek, A. & Ket-
terle, W. Direct observation of the superfluid phase transition in ultracold Fermi gases, Nature 442, 54-58 (2006).

[8] Shin, Y., Zwierlein, M.W., Schunck, C.H., Schirotzek, A. & Ketterle, W. Observation of phase separation in a strongly interacting imbalanced Fermi gas, Phys. Rev. Lett. 97, 030401 (2006);

[9] Schunck, C.H., Shin, Y., Schirotzek, A., Zwierlein, M.W. & Ketterle, W. Pairing without superfluidity: the ground state of an imbalanced Fermi mixture, Science 316, 867-870 (2007).

[10] Greiner M., Mandel O., Esslinger T., Hansch T.W., & Bloch I. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms, Nature 415, 39-44 (2002);

[11] Kohl, M., Moritz, H., Stoferle, T., Gunter, K. & Esslinger, T. Fermionic atoms in a three dimensional optical lattice: observing Fermi surfaces, dynamics, and interactions, Phys. Rev. Lett. 94, 080403 (2005).

[12] Chin, J. K. et al. Evidence for superfluidity of ultracold fermions in an optical lattice, Nature 443, 961-964 (2006).

[13] Fulde P. & Ferrell, R. A. Superconductivity in a strong spin-exchange field, Phys. Rev. 135, A550-A563 (1964);

[14] Balicas, L. et al. Superconductivity in an organic insulator at very high magnetic fields, Phys. Rev. Lett. 87, 067002 (2001);

[15] Bianchi, A., Movshovich, R., Capan, C., Pagliuso, P. G. & Sarrao, J. L. Possible Fulde-Ferrell-Larkin-Ovchinnikov superconducting state in CeCoIn5, Phys. Rev. Lett. 91, 187004 (2003);

[16] See, for example, Casalbuoni, R. & Nardulli, G. Inhomogeneous superconductivity in condensed matter and QCD, Rev. Mod. Phys. 76, 263 (2004).

[17] Liu, W.V. & Wilczek, F. Interior gap superfluidity, Phys. Rev. Lett. 90, 047002 (2003).

[18] Machida, K., Mizushima, T. & Ichioka, M. Generic phase diagram of fermion superfluids with population imbalance, Phys. Rev. Lett. 97, 120407 (2006).

[19] Kinnunen, J., Jensen, L.M. & Torma, P. Strongly interacting Fermi gases with density imbalance, Phys. Rev. Lett. 96, 110403 (2006).

[20] Sheehy, D.E. & Radzihovsky, L. BEC-BCS crossover in "magnetized" Feshbach-resonantly paired superfluids, Phys. Rev. Lett. 96, 060401 (2006).

[21] Pieri, P. & Strinati, G. C. Trapped fermions with density imbalance in the Bose-Einstein condensate limit, Phys. Rev. Lett. 96, 150404 (2006).

[22] Bulgac, A., Forbes, M.M. & Schwenk, A. Induced p-Wave superfluidity in asymmetric Fermi gases, Phys. Rev. Lett. 97, 020402 (2006).

[23] Iskin, M. & Sa de Melo, C.A.R. Two-species fermion mixtures with population imbalance, Phys. Rev. Lett. 97, 100404 (2006).

[24] Gubbels, K.B., Romans, M.W.J. & Stoof, H.T.C. Sarma phase in trapped unbalanced Fermi gases, Phys. Rev. Lett. 97, 210402 (2006).

[25] De Silva, T.N. & Mueller, E.J. Surface tension in unitary Fermi gases with population imbalance, Phys. Rev. Lett. 97, 070402 (2006).

[26] Pao, C.-H., Wu, S.-T. & Yip, S.-K. Superfluid stability in the BEC-BCS crossover, Phys. Rev. B 73, 132506 (2006).

[27] Yi, W. & Duan, L.-M. Phase diagram of a polarized Fermi gas across a Feshbach resonance in a potential trap, Phys. Rev. A 74, 013610 (2006).

[28] Chien, C.-C., Chen, Q., He, Y. & Levin, K. Superfluid phase diagrams of trapped Fermi gases with population imbalance, Phys. Rev. Lett. 98, 110404 (2007).

[29] Clogston, A. M. Upper limit for the critical field in hard superconductors. Phys. Rev. Lett. 9, 266–267 (1962).

[30] Chen, Y., Wang, Z. D., Zhu, J.-X. & Ting, C. S. Vortex charges in high-temperature superconductors, Phys. Rev. Lett. 89, 217001 (2002);

[31] Andersen, B.M. & Bruun, G.M. Magnetic and superfluid phases of confined fermions in two-dimensional optical lattices, cond-mat/0706.3611 (unpublished).

[32] Wang, Q., Chen, H.-Y., Hu, C.-R. & Ting, C.S. Local tunneling spectroscopy as a signature of the Fulde-Ferrell-Larkin-Ovchinnikov state in s- and d-wave superconductors, Phys. Rev. Lett. 96, 117006 (2006).

[33] Orso, G. Attractive Fermi gases with unequal spin populations in highly elongated traps, Phys. Rev. Lett. 98, 070402 (2007);

[34] Hu, H., Liu, X.-J. & Drummond, P.D. Phase diagram of a strongly interacting polarized Fermi gas in one dimension, Phys. Rev. Lett. 98, 070403 (2007).

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