Exploring exotic superfluidity of polarized ultracold fermions in optical lattices

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Superfluidity with imbalanced populations of harmonically trapped ultracold fermions in a two-dimensional optical lattice is investigated by solving the Bogoliubov-de Gennes equations. The intriguing richness of patterns between competing ferromagnetic and superfluid phases for different filling densities has been revealed. At low density, the main experimental features could be reproduced, especially the bimodal distribution of ferromagnetism. The superfluid-pairing gap oscillates radially, demonstrating the realization of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. In the high-density regime, another type of FFLO state with gap oscillation along the angular direction shows up and the accompanying ferromagnetic order modulates accordingly. The square lattice like FFLO state may appear at the intermediate densities. Moreover, we suggest other experimental proposals of observing the unique FFLO features straightforwardly.

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Enormous interest has been focused on the field of ultracold Fermi gases due to the interplay between Cooper pairing and strong correlations.[1–3] The use of optical lattices created by standing-wave laser fields[4,5] provides unprecedented experimental tunability such as precise control of model Hamiltonian parameters, e.g., interaction strength, lattice geometry, and number of atoms. This versatile tool opens up the possibility to study various strongly correlated systems. Beautiful experiments on the superfluidity have been performed in these systems with unequal spin populations.[6,7] 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. Experimental exploration of the unique superfluid phase of imbalanced fermions in optical lattices is expected to be conducted in the near future.

There is long-standing debate on the nature of the exotic pairing state for the imbalanced systems. The inhomogeneous superfluid state, known as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, was predicted 40 years ago, which contains nonzero momentum Cooper pairs with the superfluid-pairing gap exhibiting periodic real-space modulations.[8] There have been suggestions for the possible FFLO phase for some of the high-T_c, layered organic, and heavy-fermion superconductors at very low temperatures and high magnetic fields.[9] This subject has also been studied in nuclear and high-energy physics.[10] Despite much of the previous literature reported in this field,[11–21] it is still awaited to explore theoretically and unambiguously the exotic FFLO state with imbalanced ultracold fermions in optical lattices.

In this paper, we present an unrestricted Hartree-Fock study of two-component fermionic atoms in a harmonically confined two-dimensional (2D) optical lattice. Due to the competition between the ferromagnetic and s-wave superfluid phases in the presence of the trapping potential, the 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 a 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 spin imbalance increases, the pairing gap oscillates along the angular direction, signaling a unique FFLO state. (iii) A variety of intriguing distributions of the order parameter, such as the square lattice FFLO state, emerge in the intermediate-filling regime.

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,

$$\hat{H} = -t\sum_{\langle ij\rangle,\sigma}\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma} + \sum_{i\sigma}(\epsilon_i-\mu_\sigma)\hat{n}_{i\sigma} + \sum_i[\Delta_i\hat{c}_{i\uparrow}^{\dagger}\hat{c}_{i\downarrow}^{\dagger} + \text{H.c.}], \tag{1}$$

where $\hat{c}_{i\sigma}$ is an annihilation operator for an atom at site i (at position $\mathbf{r}_i$) with spin σ and $\hat{n}_{i\sigma}=\hat{c}_{i\sigma}^{\dagger}\hat{c}_{i\sigma}$ is the number operator. t is the effective nearest-neighboring hopping integral. The spin-dependent chemical potential due to the Zeeman splitting is defined as $\mu_\sigma=\mu-\sigma h$. $\epsilon_i=\frac{1}{2}m\omega^2|\mathbf{r}_i-\mathbf{r}_0|^2$ is the harmonic confining potential at site i and $\mathbf{r}_0$ is the position of the trap center.

The above mean-field Hamiltonian can be diagonalized by solving the resulting Bogoliubov-de Gennes (BdG) equations self-consistently,[22]

$$\sum_j\begin{pmatrix} H_{ij,\sigma} & \Delta_{ij}^* \\ \Delta_{ij} & -H_{ij,\bar{\sigma}}^* \end{pmatrix}\begin{pmatrix} u_{j\sigma}^n \\ v_{j\bar{\sigma}}^n \end{pmatrix} = E_n\begin{pmatrix} u_{i\sigma}^n \\ v_{i\bar{\sigma}}^n \end{pmatrix}, \tag{2}$$

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

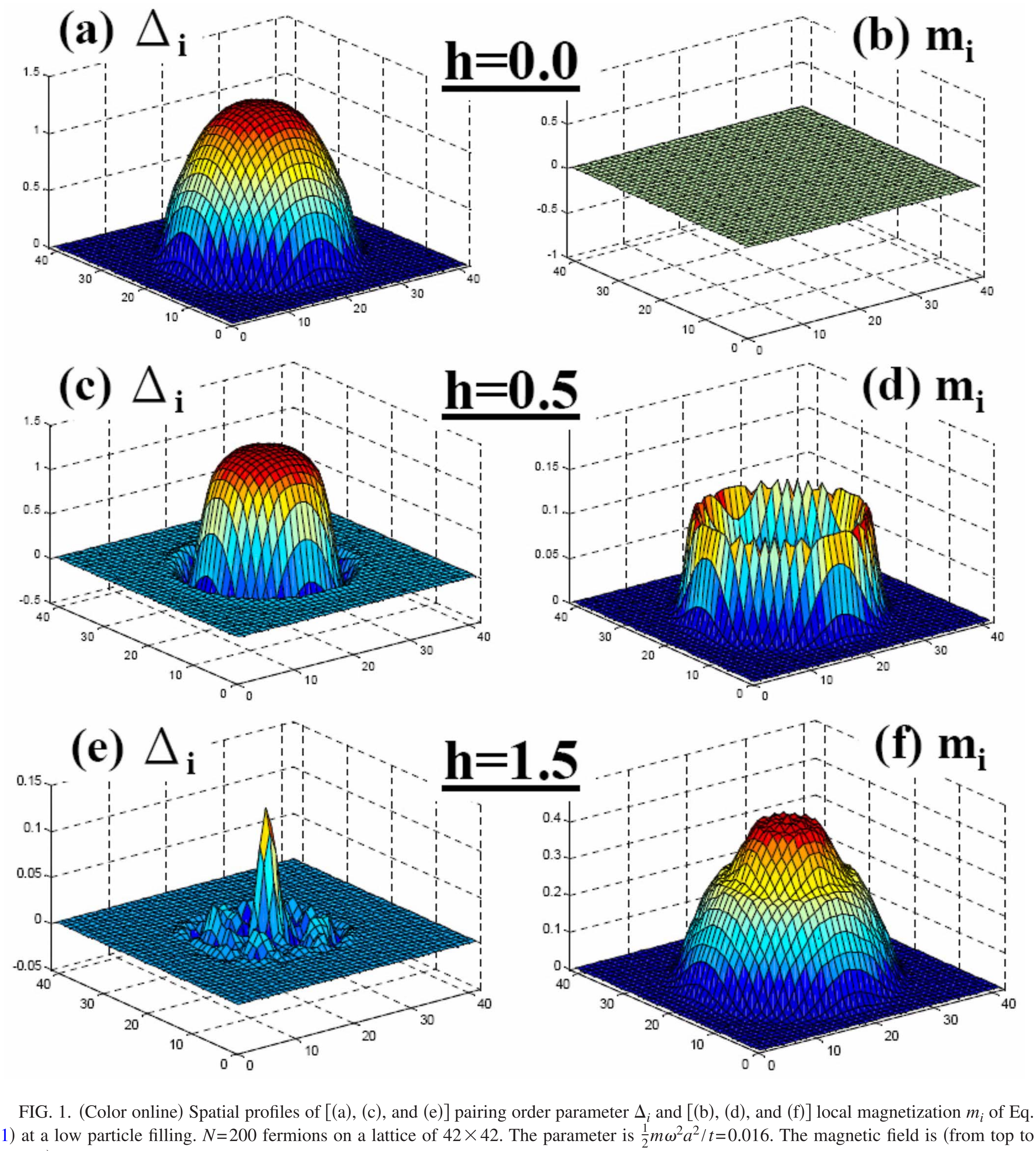

FIG. 1. (Color online) Spatial profiles of [(a), (c), and (e)] pairing order parameter Δ_i and [(b), (d), and (f)] local magnetization m_i of Eq. (1) at a low particle filling. $N=200$ fermions on a lattice of 42×42. The parameter is $\frac{1}{2}m\omega^2 a^2/t=0.016$. The magnetic field is (from top to bottom) $h=0$, 0.5, and 1.5, respectively.

order parameter satisfy the self-consistency conditions $n_{i\uparrow}=\Sigma_n |u_{i\uparrow}^n|^2 f(E_n)$, $n_{i\downarrow}=\Sigma_n |v_{i\downarrow}^n|^2[1-f(E_n)]$, and $\Delta_i = V\Sigma_n (u_{i\uparrow}^n v_{i\downarrow}^{n*} + v_{i\downarrow}^{n*} u_{i\uparrow}^n)\tanh(E_n/2k_B T)$, respectively, where V denotes the pairing interaction 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, we set t as the energy unit and lattice spacing a as the length unit. We consider a very low temperature $T=0.001$, pairing interaction $V=4.0$, and the amplitude of the confining potential $\frac{1}{2}m\omega^2 a^2/t \sim (0.016-0.025)$. The dimension of the lattice is 42×42 with open boundary conditions and the trap center is located at (21,21). All the fields of interest become vanishingly small at the boundary. The order parameters are determined by solving the BdG equations iteratively, with their initial values randomly distributed on the lattice. In the case of multisolutions, we compare their cor-

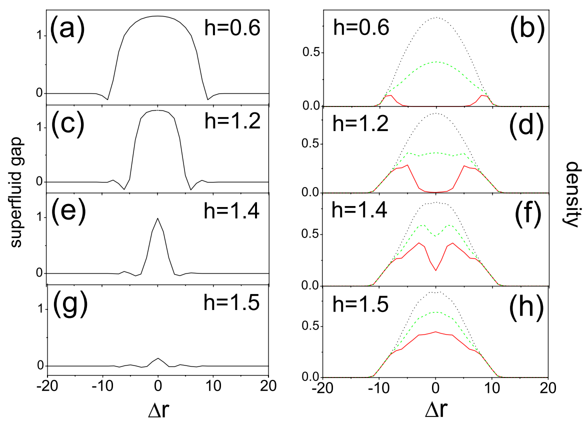

FIG. 2. (Color online) Plots of [(a), (c), (e), and (g)] Δ_i and [(b), (d), (f), and (h)] density along the diagonal of the lattice. Δr is the distance from the trap center. Red solid line denotes the magnetization while the black dotted and green dashed lines represent the spin-up and spin-down densities, respectively. All the parameters are the same as in Fig. 1.

responding free energies to obtain 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 $\epsilon_i=0$, the pairing gap of the ground state oscillates in space with a stripelike pattern for the s wave and a square lattice pattern for the d wave.[23] Ferromagnetism appears in the crossing region of the positive and negative pairing amplitudes. The presence of a trapping potential may add new complications. In the widely used local-density approximation (LDA), the spatial dependence of observables must follow the contours of the trapping potential in the same way that a spatially uniform system does. Our approach provides a consistent way to explore unique states beyond LDA. In particular, our results show that the ground state depends crucially on n_c (fermion density at the trap center) as described in the following.

Low-filling regime ($n_c<1$). In Fig. 1, we plot three typically spatial profiles of the order parameters as functions of magnetic field h. At $h=0$, there is no ferromagnetic order and the trapping potential may result in the accumulation of fermion density around the center. As shown in Fig. 1(a), Δ_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), Δ_i modulates along the radial direction, indicating an FFLO state. At the edge of the modulation, a continuous sign change in the pairing gap corresponds to a nodal line ($\Delta_i=0$). Meanwhile the magnetic order parameter m_i is most remarkable around the ringlike 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 while the unpaired majority fermions are repelled to the outside of the core. This result is in good agreement with the experiments and also with the previous theoretical studies on the FFLO state in a continuous model.[13,14] As h progressively increases, the pairing order may be further suppressed and the weak modulation of the pairing gap appears away from the trap center while the ferromagnetic order shows a plateaulike 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.[24] Note that the existing experimental realization[6,7] may correspond to the present low-filling case. The density profiles we obtained 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 fourfold 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 plateaulike structure.

High-filling regime (n_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 cannot survive far away from the center because of the low fermion density. One may naturally expect the formation of a ringlike fermion-pairing state at the intermediate range. In Figs. 3(a) and 3(b), the profile of Δ_i does show such a topological structure at $h=0$. Upon increasing h, the magnetization 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 the 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 Figs. 3(e) and 3(f). The precise number of the angular oscillations depends on the related parameters such as the pairing interaction, filling factor, and magnetic field. When $h=1.5$, the pairing order is almost fully suppressed while the ferromagnetic order forms a shell pattern [Figs. 3(g) and 3(h)].

An intuitive physical understanding of the angular FFLO state can be given as follows: the main effect of the high filling at the trap center is the formation of superfluid shell structure as shown in Fig. 3(a). As what is known, the FFLO is rather robust in one dimension (1D).[25] If the superfluid

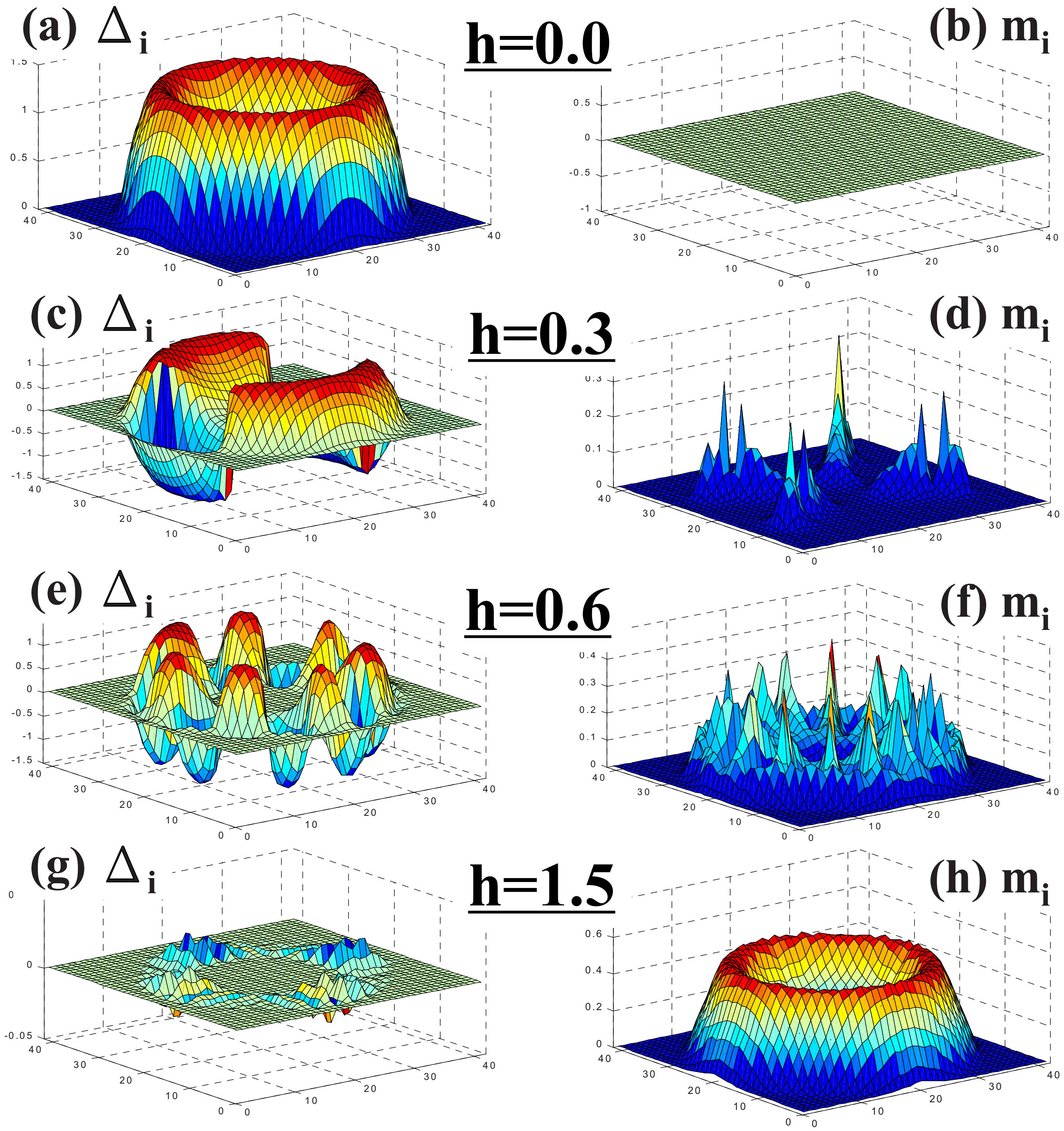

FIG. 3. (Color online) Spatial variations of [(a), (c), (e), and (g)] Δ_i and [(b), (d), (f), and (h)] local ferromagnetic order m_i at a high filling: $N=1200$ fermions.

shell is sufficiently thin like a 1D ring, then the 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. We have checked our results for the *d*-wave pairing and similar conclusions have also been reached. Here we need to stress the critical role played by the trapping potential in the formation of the FFLO states along the radial or angular direction. The appearance of the FFLO state minimizes the relevant free energy, which manifests the competition between magnetization and superfluidity. The trapping potential provides a confined and inhomogeneous background, which complicates the competition, but reveals some physics associated with the FFLO states.

Medium-filling regime [$n_c \in (1,2)$]. In this regime, rich patterns of the order-parameter distribution show up. At $h=0$, 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

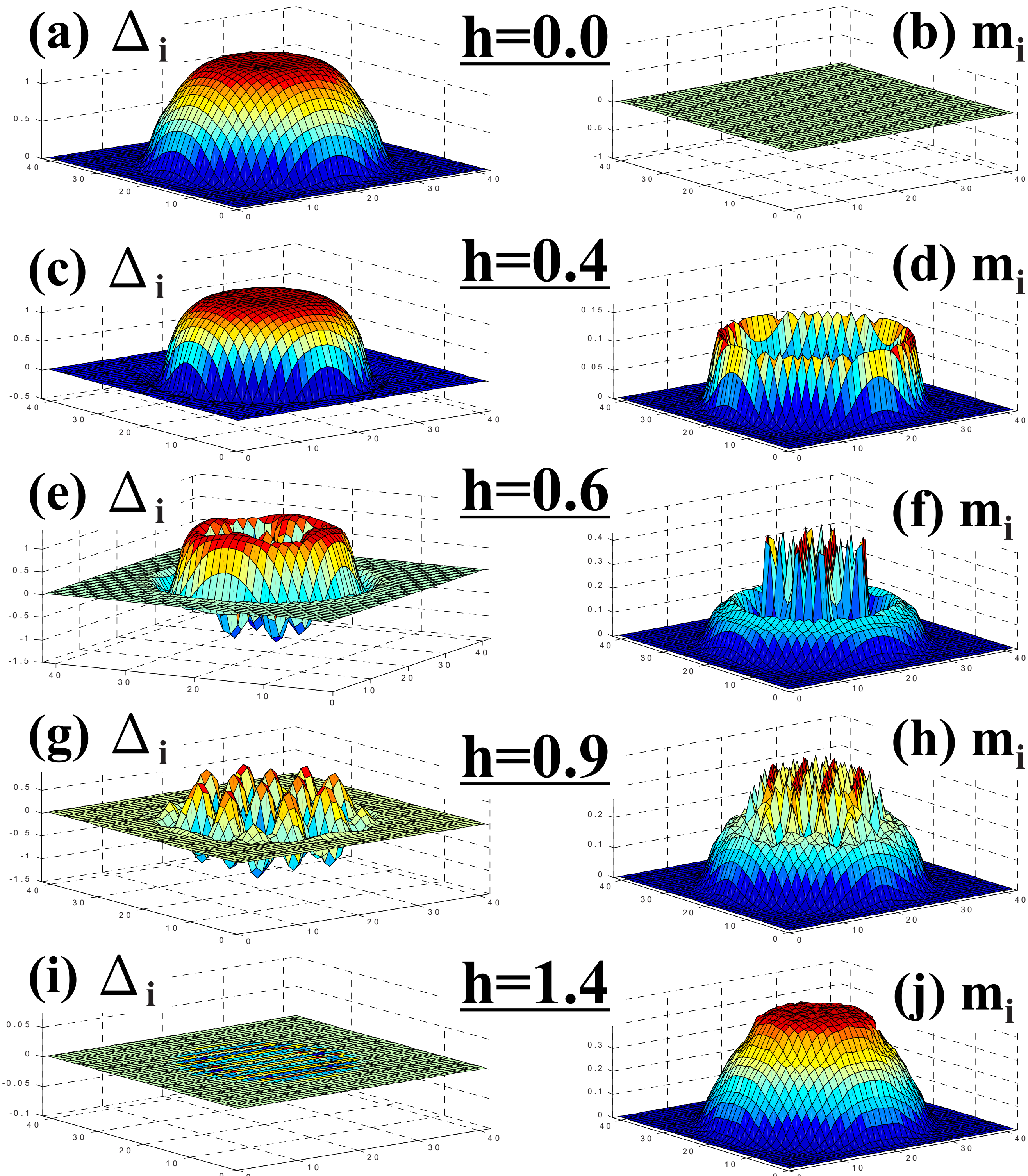

FIG. 4. (Color online) Spatial profile of (a) pairing order parameter and (b) magnetization m_i at an intermediate filling: $N=400$ fermions. The confining potential parameter is $\frac{1}{2}m\omega^2 a^2/t=0.025$.

analogous to the low-filling case [Figs. 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 increase the magnetic field to $h=0.9$, the square lattice pattern of the FFLO state becomes more pronounced and the associated ferromagnetism exhibits itself as well [Figs. 4(g) and 4(h)]. Note that the square lattice FFLO state appears in the infinite 2D system with the d-wave pairing.[23] When h becomes quite large, the BCS pairing order is fully suppressed and the magnetization displays a plateaulike structure around the trap center, as depicted in Figs. 4(i) and 4(j). It is worthwhile to note here that the value of critical magnetic field h_c is determined by the system parameters such as the confining potential, filling factor, and pairing interaction. It is worthwhile to note here that the predictions of our results survive at more realistic temperature regimes (e.g., $0.2T_F$).

So far, there has been no direct evidence of FFLO states in recent experiments since probing the 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 ^{6}Li atoms in the optical lattice.[5] 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 the strong magnetic field parallel to the plane, the angular-dependent FFLO state may show up due to the special topology of the ring structure. A probe of the real-space modulation of the pairing gap as well as magnetization can be achieved by using superconducting quantum interference device (SQUID) or scanning tunneling microscopy (STM) techniques. The third proposal is to generate a Mexican hat trapping potential in three dimensions (3D), so that the distribution of the confined fermionic atoms may form a donutlike structure. In such a case, the angular-dependent distribution of the magnetization profile can be directly measured by using time-of-flight imaging techniques.

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