F-wave pairing of cold atoms in optical lattices

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The tremendous development of cold atom physics has opened up a whole new opportunity to study novel states of matter which are not easily accessible in solid state systems. Here we propose to realize the f-wave pairing superfluidity of spinless fermions in the px,py-orbital bands of the two dimensional honeycomb optical lattices. The non-trivial orbital band structure rather than strong correlation effects gives rise to the unconventional pairing with the nodal lines of the f-wave symmetry. With a confining harmonic trap, zero energy Andreev bound states appear around the circular boundary with a six-fold symmetry. The experimental realization and detection of this novel pairing state are feasible.

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The study of unconventional Cooper pairing states has been a major subject in condensed matter physics for decades. In addition to the isotropic s-wave pairing, many unconventional pairing states have been identified. For example, different types of p-wave pairing states were found in the superfluid 3He systems including the anisotropic chiral A-phase and the isotropic B-phase. Evidence of the p-wave pairing was also found in the ruthenate compound of SrRuO3. The d-wave pairing states are most convincingly proved in the high-Tc cuprates with phase sensitive measurements including Josephson tunneling junctions and zero energy Andreev bound states. Many heavy fermion compounds exhibit evidence of unconventional Cooper pairing such as UPt3, UBe13, and CeCoIn5 with nodal points or lines. However, phase sensitive measurements are still lacking. These unconventional pairing states are driven by strong correlation effects, which brings significant difficulties for theoretical analysis and prediction. It would be great to find novel unconventional pairing mechanisms easier to handle.

On the other hand, cold atom physics has recently become an emerging frontier for condensed matter physics. In particular, the s-wave pairing superfluidity of fermions through the Feshbach resonances has become a major research focus. The Bose-Einstein condensation (BEC) and Bardeen-Cooper-Schrieffer (BCS) crossover has been extensively investigated. Naturally, searching for unconventional Cooper pairing states in cold atomic systems is expected to stimulate more exciting physics. For example, the p-wave pairing states have been proposed by using the p-wave Feshbach resonances, which, however, suffer from a drawback of heavy particle loss. The unconventional Cooper pairing states with cold atoms have not been realized yet.

In this article, we propose a novel f-wave pairing state of spinless fermions in the cold atom optical lattices. This unconventional pairing arises from the non-trivial band structure of the px,py-orbital bands in the honeycomb optical lattices combined with a conventional attractive interaction. The internal orbital configurations of the Bloch wave band eigenstates vary with the crystal momenta, resulting in an f-wave pairing order parameter. Along three high symmetry lines in the Brillouin zone whose directions differ by 120° from each other, the intra-band pairing order parameters are exactly suppressed to zero. The unconventional nature of this pairing exhibits in the appearance of the zero-energy Andreev bound states at the circular boundary with imposing a confining trap. Since no strong correlation effects are involved, our analysis below is well-controllable. This is a novel state of matter, which to our knowledge has not been unambiguously identified before neither in condensed matter nor in cold atom systems, thus this result will greatly enrich the study of unconventional pairing states.

The honeycomb optical lattice was experimentally constructed quite some years ago by using three coplanar blue detuned laser beams whose wavevectors \( \vec{k}_i \) (\( i = 1, 2, 3 \)) differ by 120° from each other. After the lowest s-orbital band is fulfilled, the next active ones are px,py-orbital bands lying in the hexagonal plane. Different from the situation in graphene whose px,py-orbital bands strongly hybridize with the s-orbital bands and are pushed away from the Fermi surface, the hybridization between the px,py and s-orbitals in the optical honeycomb lattice is negligible. The px-orbital band can be pushed to higher energies and thus unoccupied by imposing strong confinement along the z-axis. The px,py-orbital bands exhibit the characteristic features of orbital physics, i.e., spatial anisotropy and orbital degeneracy. This provides a new perspective of the honeycomb lattice, and is complementary to the research focusing on the px-band system of graphene which is not orbitally active. The novel physics which does not appear in graphene includes the flat band structure, the consequential non-perturbative strong correlation effects (e.g., Wigner crystals and ferromagnetism), frustrations in orbital exchange, and the quantum anomalous Hall effect.

We employ the px,py-orbital band Hamiltonian studied...
in Ref. \cite{30,31,33,34} as

\[ H_0 = t_{||} \sum_{\mathbf{r} \in A, i=1,2,3} \{ \hat{p}_{\mathbf{r},i} \hat{p}_{\mathbf{r}+\mathbf{e}_i} + \text{h.c.} \} - \mu \sum_{\mathbf{r} \in A \oplus B} n_\mathbf{r}, \]  

(1)

where \( \mathbf{e}_1,2,3 \) are unit vectors from one site in sublattice \( A \) to its three neighboring sites in sublattice \( B \) defined as \( \mathbf{e}_1 = -\frac{\sqrt{3}}{2} \mathbf{e}_x + \frac{1}{2} \mathbf{e}_y, \mathbf{e}_2 = -\mathbf{e}_x, \mathbf{e}_3 = (p_x \mathbf{e}_x + p_y \mathbf{e}_y) \cdot \mathbf{e}_i \) is the \( p \)-orbital projected onto the bond along the direction of \( \mathbf{e}_i \) and only two of them are linearly independent; \( n_\mathbf{r} = n_{\mathbf{r},x} + n_{\mathbf{r},y} \) is the particle number at site \( \mathbf{r} \); the \( \sigma \)-bonding \( t_\perp \) describes the hopping between \( p \)-orbitals on neighboring sites parallel to the bond direction and is rescaled to 1 below; \( a \) is the nearest neighbor distance. \( t_{||} \) is positive due to the odd parity of \( p \)-orbitals. Eq. (1) neglects the \( \pi \)-bonding \( t_\perp \) hopping between \( p \)-orbitals perpendicular to the bond direction. To confirm this, we have fitted \( t_{||} \) and \( t_\perp \) from a realistic band structure calculation for the sinusoidal optical potential \( V(\mathbf{r}) = V_0 \sum_{1 \leq i < j \leq 3} \cos ((\mathbf{K}_i - \mathbf{K}_j) \cdot \mathbf{r}) \). With a moderate potential depth of \( V_0/E_R = 12 \), \( t_{||}/t_\perp \) is already driven to 1% with \( t_{||} \approx 0.375E_R \). \( E_R = \frac{\hbar^2}{2m} \cdot \mathbf{r} \) is the recoil energy and \( M \) is the atom mass. Further increasing \( V_0/E_R \) decreases \( t_{||}/t_\perp \) even more.

Eq. (1) has a chiral symmetry, i.e., under the transformation of \( \hat{p}_{A,x(y)} \rightarrow -\hat{p}_{A,x(y)} \) only for sites in sublattice \( A \) but not for sites in sublattice \( B \), \( H_0 \rightarrow -H_0 \). Thus its four bands have a symmetric spectra respect to the zero energy as

\[ E_{1,4} = \pm \frac{3}{2} t_{||}, \quad E_{2,3} = \mp \frac{1}{2} \sqrt{3 + 2 \sum_{i<j} \cos \mathbf{r} \cdot (\mathbf{e}_i - \mathbf{e}_j)} \]  

(2)

The Brillouin zone (BZ) is a regular hexagon with the edge length \( \frac{2\pi}{3\sqrt{3}a} \). Two middle dispersive bands 2 and 3 have two non-equivalent Dirac points \( K(K') = (\pm \frac{\pi}{3\sqrt{3}a},0) \) with a band width of \( \frac{\pi}{3\sqrt{3}a} \). The bottom and top bands are flat. We define the four component annihilation operators in momentum space as \( \hat{\phi}(\mathbf{k}) = [\hat{p}_{A,x}(\mathbf{k}), \hat{p}_{A,y}(\mathbf{k}), \hat{p}_{B,x}(\mathbf{k}), \hat{p}_{B,y}(\mathbf{k})] \). In this basis, the eigen-operator \( \hat{\psi}_m(\mathbf{k}) \) for band \( m \) can be diagonalized as \( \hat{\psi}_m(\mathbf{k}) = \hat{\phi}_m(\mathbf{k}) U_{nm}(\mathbf{k}) \) where \( U(\mathbf{k}) \) is a \( 4 \times 4 \) unitary matrix. The phase convention for band eigenvectors, i.e., each column of \( U(\mathbf{k}) \), is conveniently chosen as \( R_x \hat{\psi}_m(\mathbf{k}) R_x^{-1} = \text{sgn}(m) \hat{\psi}_m(\mathbf{k}) \) with \( \text{sgn}(m) = -1 \) for \( m = 1,2 \) and \( \text{sgn}(m) = +1 \) for \( m = 3,4 \), where the symmetry operation \( R_x \) is the 60° rotation around a center of the hexagonal plaqette and \( \mathbf{k}' = R_x \mathbf{k} \). The analytical form of \( U_{nm}(\mathbf{k}) \) is given in the Appendix A.

The orbital configurations of band eigenvectors have interesting patterns as depicted in Fig. 1 which arise from the lattice \( D_{6h} \) symmetry. Only the lowest dispersive band (\( n = 2 \)) is plotted as an example. The lowest flat band (\( n = 1 \)) has the same symmetry structure except having different orbital polarization directions. The remaining two can be obtained by performing the operation of the chiral symmetry. Six lines in the BZ are with the reflection symmetry, i.e., three passing the middle points of the opposite edges and three passing the opposite vertices of \( K \) and \( K' \). The eigenvectors of each band along these lines should be either even or odd respect to the corresponding reflection. For example, for the reflection respect to the \( y \)-axis, the orbitals transform as \( \hat{p}_{A,B,x} \rightarrow -\hat{p}_{A,B,x} \). The eigenoperators \( \hat{\psi}_m(\mathbf{k}) \) with \( \mathbf{k} \parallel \mathbf{y} \) must be either purely \( \hat{p}_y \) (even) or \( \hat{p}_x \) (odd). For the other two middle lines, the corresponding eigenvectors are obtained by performing the \( \pm 120^\circ \) rotation. For the time-reversal partners \( \hat{\psi}_m(\mathbf{k}) \) and \( \hat{\psi}_m(-\mathbf{k}) \) along these lines, they only take the same real polar orbitals. On the other hand, the reflection respect to the \( x \)-axis gives rise to the transformation \( \hat{p}_{A,B,y} \rightarrow -\hat{p}_{A,B,y} \) and \( \hat{p}_{A,B,x} \rightarrow \hat{p}_{A,B,x} \). Furthermore, \( K \) and \( K' \) have three-fold rotational symmetry. Combining two facts together, \( \hat{\psi}_m(\mathbf{k}) \) should be of \( p_x + ip_y \) for sites in one of the sublattices and \( p_x - ip_y \) for sites in the other sublattice. Its time-reversal partner \( \hat{\psi}_m(K') \) has the opposite chiralties in both sublattices respect to those at \( K \). In other words, the orbital configurations of \( \hat{\psi}_m(\mathbf{k}) \) are linear-polarized at the middle points of the BZ edge, changes to circularly-polarized at the vertices, and elliptically polarized in between.

Next we introduce the on-site attractive interaction term between spinless fermions as

\[ H_{\text{int}} = -U \sum_{\mathbf{r}} n_{\mathbf{r},x} n_{\mathbf{r},y}, \]  

(3)

where \( U \) is positive. We perform the mean-field decom-
where the pairing order parameters in the A and B-sublattices are self-consistently defined as \( \Delta_{A(B)} = \langle G|p^\dagger_{A(B)}e^{i\Delta\theta}p_{A(B)}|G\rangle \). The means the average over the pairing ground state; the summation of \( \vec{k} \) only covers half of the BZ; the multi-band pairing order parameters in momentum space has a \( 4 \times 4 \) matrix structure as \( \Delta_{nm}(\vec{k}) = \langle G|e^{i\Delta\theta} \psi_n(\vec{k}) \psi_m(-\vec{k})|G\rangle \). Under the rotation of \( R_\varphi \), it transforms as \( R_\varphi \Delta_{nm}(\vec{k}) R^{-1}_\varphi = \text{sgn}(n) \text{sgn}(m) \Delta_{nm}(\vec{k}) \).

The intra-band gap functions \( \Delta_{nn} \) can be calculated analytically as \( \Delta_{nn}(\vec{k}) = i(-)^n \frac{3}{2}(\Delta_A - \Delta_B) F(\vec{k}) \) with the \( f \)-wave form factor of

\[
F(\vec{k}) = \frac{16}{\sqrt{3}N_0(\vec{k})} \sin \frac{\sqrt{3}}{2} k_x \left[ \cos \frac{\sqrt{3}}{2} k_x - \cos \frac{3}{2} k_y \right],
\]

where \( N_0(\vec{k}) = \frac{8}{3} \left\{ 3 - \sum_{1 \leq i < j \leq 4} \cos \vec{k} \cdot (\vec{e}_i - \vec{e}_j) \right\} \). \( \Delta_A \) can be fixed positive, and \( \Delta_B = |\Delta_B|e^{i\Delta\theta} \) with a relative phase \( \Delta\theta \). The optimal \( \Delta\theta \) takes the value of \( \pi \), i.e., \( \Delta_A = -\Delta_B \), to maximize the intra-band pairings. We have confirmed this in the explicit self-consistent mean-field solution for Eq. 1 and Eq. 4. Furthermore, the non-vanishing \( \pi \)-bonding \( t_4 \) term can further stabilize this solution as a result of the odd parity of \( \pi \)-orbitals.

The configuration of \( \Delta_A = -\Delta_B = \Delta \) exhibits the \( f \)-wave symmetry, i.e., the rotation of \( R_\varphi \) is equivalent to flipping the sign of \( \Delta \) as depicted in Fig. 2 A. In particular, the diagonal terms satisfy \( R_\varphi \Delta_{nm}(\vec{k}) R^{-1}_\varphi = -\Delta_{nm}(\vec{k}) \) as exhibit in \( F(\vec{k}) \) with three nodal lines of \( k_x = 0, k_y = \pm k_x/\sqrt{3} \). These are the same middle lines marked in Fig. 4 along which the time reversal partners \( \psi_n(\pm) \) have the same polar orbital configurations. The pairing amplitude vanishes along these lines because interaction only exists between two orthogonal orbitals. On the other hand, maximal pairings occur between \( \vec{K} \) and \( \vec{K}' \) with opposite signs whose orbital configurations are orthogonal to each other. Unlike other examples of unconventional pairing in condensed matter systems, this \( f \)-wave pairing structure mainly arises from the non-trivial orbital configuration of band structures but with conventional interactions.

We next study the pairing strength \( \Delta_A = -\Delta_B = \Delta \) in the weak coupling regime with \( U/t_\parallel = 3 \) in which the validity of the self-consistent mean-field theory is justified. The lattice chiral symmetry ensures that these results are symmetric respect to the filling \( n = 1 \). The case of \( 0 < n < 0.5 \) corresponds to the filling in the bottom flat band in which each band eigenstate can be constructed as localized within a single hexagon plaquette presented (see Refs. 30,33). The attractive interaction drives all the plaquette states to touch each other leading to phase separation until the flat band is fulfilled. which will be discussed in a later publication. In Fig. 3 A, we plot \( \Delta \) for \( 0.5 < n < 1.5 \) which corresponds to fill in the dispersive bands. The maximal \( \Delta \) appears at \( n = 0.5 \) because all the particles in the flat band participate pairing. As \( n \) increases, \( \Delta \) drops because pairing is less efficient in the dispersive bands. \( \Delta \) reaches the minimum at \( n = 1 \) where the Fermi energy touches the Dirac cones.

Due to the multi-band structure, this \( f \)-wave pairing state remains fully gapped for general values of \( U/t_\parallel \) and \( n \). We plot the branch of the lowest energy Bogoliubov excitations for \( U/t_\parallel = 3 \) and the filling \( 0.5 < n < 1 \) where the Fermi energy lies in band 2. For \( n \) close to 1 in Fig. 3 B (\( n = 0.96 \)), the Fermi surfaces form two disconnected pockets around the \( \vec{K} \) and \( \vec{K}' \) away from
the superfluidity develops below the Kosterlitz-Thouless transition. We performed a real space Bogoliubov-Andreev bound states. On the other hand, if the bound states are perpendicular to the nodal lines, no phase changes are possible. The behavior of $\Delta_{22}(k)$ depends on the orientation of the density of states, and then drops as close to zero as possible. As lowering $n$ in Fig. 2 C ($n = 0.79$), the Fermi surface becomes connected and intersects with the nodal lines of $\Delta_{22}$. At these intersections, the system in general remains gapped because of the non-zero inter-band pairing $\Delta_{12}(k)$.

The zero energy LDOS in real space with the maximal values at $\theta = n\pi/3$ is a signature of the $f$-wave pairing symmetry.

The superfluid density $\rho_s$ is plotted in Fig. 2 D for $0.5 < n < 1.5$ and $U/t_0 = 3$, which is defined as

$$\rho_s = \frac{\hbar^2}{2m^*} n_s = \lim_{\delta\theta \to 0} \frac{1}{2} \frac{\partial^2 E_{MF}}{\partial \delta\theta^2}$$

where $\delta\theta$ is the phase twist across the system boundaries. The behavior of $\rho_s$ is very different from that of the pairing gap, which is mostly determined by the states in the dispersive band. Close to $n = 0.5$, $\rho_s$ is small in spite of the large value of $\Delta$ because of the immobility of the flat band states. $\rho_s$ reaches the maximal value about $0.02t_0$ because the filling is close to the van Hove singularity of the density of states, and then drops as close to the Dirac points at $n = 1$. In two dimensional systems, the superfluidity develops below the Kosterlitz-Thouless (K-T) transition temperature $T_{KT} \approx 2\rho_s$.

One of the most convincing proofs of the unconventional pairing is the existence of the zero energy Andreev bound states at boundaries because of their phase sensitivity. Fig. 4 A depicts the situation of the boundary perpendicular to the antinodal lines of the intra-band pairing. The scattering of the Bogoliubov quasi-particles changes momentum from $k_{in}$ to $k_{ref}$ along which the pairing parameters switch the sign as $\Delta_{nn}(k_{in}) = -\Delta_{nn}(k_{ref})$, which gives rise to zero energy Andreev bound states. On the other hand, if the boundary is perpendicular to the nodal lines, no phase changes occur and thus Andreev bound states vanish.

Naturally in the experimental systems with an overall confining trap, the circular edge boundary samples all the orientations. We performed a real space Bogoliubov-de-Gennes calculation as

$$\begin{pmatrix} \hat{H} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{H} \end{pmatrix} \begin{pmatrix} u_n(i) \\ v_n(i) \end{pmatrix} = E_n \begin{pmatrix} u_n(i) \\ v_n(i) \end{pmatrix},$$

where $\hat{H} = H_0 + V_{ex}$; $V_{ex} = \frac{4}{\Omega} \Omega r^2$ is the harmonic confining potential with parameters $h\Omega = 0.02t_0$ and $l_\Omega = \sqrt{\frac{\hbar}{m\Omega}} = 4.5a$. The local density of states (LDOS) at energy $E$ is defined as $LD(\vec{r}, E) = \frac{1}{N} \sum_n |u_n(\vec{r})|^2 \delta(E - E_n) + |v_n(\vec{r})|^2 \delta(E + E_n)$, where $N$ is the total number of lattice sites. The numerical result of the zero energy LDOS $LD(\vec{r}, 0)$ is depicted in real space in Fig. 4 B with the parameter values of $U/t_0 = 3$ and $\mu = -0.18$ which corresponds to the filling in the center of the trap $n_c = 0.97$. Fig. 4 B shows that the $LD(\vec{r}, 0)$ is non-zero only at sites near the boundary, signaling the existence of the zero energy Andreev bound states with six-fold symmetry. The LDOS maxima occur at angles $\theta = n \frac{\pi}{5} (n = 1 \sim 6)$ which are perpendicular to the antinodal directions shown in Fig. 4 A, and the minima are located at $\theta = (n + \frac{1}{2}) \frac{\pi}{5}$.

The experimental realization of this novel $f$-wave state is feasible. To enhance the attractive interaction between spinless fermions, we propose to use atoms with large magnetic moments, such as $^{167}$Er, with $m = 7\mu_B$ on which laser cooling has been performed. Compared to another possibility to use the $p$-wave Feshbach resonance, this method has the advantage to maintain the system stability. The interaction between two fermions in $p_{x,y}$ orbitals reads

$$-U = \int d^3\vec{r}_1 d^3\vec{r}_2 V(\vec{r}_1 - \vec{r}_2) \left\{ |\psi_{p_x}(\vec{r}_1)| \psi_{p_y}(\vec{r}_2) |^2 ight\},$$

where $\psi_{p_x,p_y}$ are Wannier wavefunctions. The overall dipole interaction can be made attractive by polarizing the magnetic moments parallel to the hexagonal plane, which gives rise to $V(\vec{r}_1 - \vec{r}_2) = m^2 (1 - 3 \cos^2 \theta)/r^3$ where $r = |\vec{r}_1 - \vec{r}_2|$ and $\theta$ is the angle between $\vec{n}$ and $\vec{r}_1 - \vec{r}_2$. We take the laser wavelength $\lambda \approx 600nm$, and then the recoil energy $E_R = 157nK$. As shown in Appendix B, by choosing $V_0/E_R = 30$, the estimation shows that $U \approx 96nK$ and $t_\perp \approx 0.2E_H = 31nK$, and thus $U/t_\perp \approx 3$ as chosen above. As shown in Fig. 4 D, the maximal $T_{KT} \approx 2(0.02t_0) \approx 1 \sim 2nK$, which is within the experimentally accessible regime.

A successful detection of the zero energy Andreev bound states will be a convincing proof to the $f$-wave pairing state. The radio-frequency ($rf$) spectroscopy has been an established tool to determine the pairing gap in cold atom systems. It also has a good spatial resolution, which makes the direct imaging of the spatial distribution of the zero energy Andreev bound states feasible. The unique symmetry pattern of the zero energy Andreev bound states localized at the trap boundary can be revealed by identifying the locations of the zero energy spectrum determined from the spatially resolved $rf$ spectroscopy.
In summary, we have proposed the realization of a novel f-wave pairing state with spinless fermions which has not been identified in solid state and cold atom systems before. The key reason is the non-trivial p-orbital band structure of the honeycomb lattice rather than the strong correlation physics, which renders the above analysis controllable. The $T_{K_T}$ is estimated to reach the order of $\ln K$ within experimental accessibility. The rf spectroscopy detection of the six-fold symmetry pattern of the zero energy Andreev bound states along the circular boundary will provide a phase sensitive test of the $f$-wave symmetry.

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APPENDIX A: EIGENVECTORS OF THE BAND HAMILTONIAN AND THE PAIRING MATRIX

In this section, we present the spectra of the band Hamiltonian Eq. [1] and the pairing matrix $\Delta_{mn}$. With the four-component spinor operator defined as

$$\hat{\phi}(\vec{k}) = (p_{A\eta}(\vec{k}), p_{A\bar{\eta}}(\vec{k}), p_{B\eta}(\vec{k}), p_{B\bar{\eta}}(\vec{k}))^T,$$  \hspace{1cm} (A1)

Eq. [1] becomes

$$H_0 = \sum_{\vec{k}} \hat{\phi}^\dagger_{\eta}(\vec{k}) H_{0,\eta\eta}(\vec{k}) \hat{\phi}_{\eta}(\vec{k}),$$  \hspace{1cm} (A2)

where the matrix kernel $H_{0,\eta\eta}(\vec{k})$ takes the structure as

$$\begin{pmatrix} 0 & 0 & \Delta & 0 \\ 0 & 0 & 0 & \Delta \\ \Delta & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 \end{pmatrix}.$$

For each momentum $\vec{k}$, $H_0(\vec{k})$ is diagonalized as

$$H_{0,\eta\eta}(\vec{k}) U_{\eta\eta} = E_\eta U_{\eta\eta}.$$  \hspace{1cm} (A3)

The band eigen-operators are expressed as

$$\hat{\psi}_\eta(\vec{k}) = \hat{\phi}_{\eta}(\vec{k}) U_{\eta\eta}(\vec{k}).$$  \hspace{1cm} (A4)

The unitary matrix $U(\vec{k})$ reads

$$U(\vec{k}) = \begin{pmatrix} a(\vec{k}) & e^{-\frac{i\pi}{2}} b(\vec{k}) & e^{-\frac{2i\pi}{3}} b(\vec{k}) & a^*(\vec{k}) \\ -b^*(\vec{k}) & e^{-\frac{i\pi}{2}} a(\vec{k}) & e^{-\frac{2i\pi}{3}} a(\vec{k}) & -b(\vec{k}) \\ a(\vec{k}) & e^{-\frac{i\pi}{2}} b^*(\vec{k}) & e^{-\frac{2i\pi}{3}} b^*(\vec{k}) & -a(\vec{k}) \\ -b(\vec{k}) & e^{-\frac{i\pi}{2}} a^*(\vec{k}) & e^{-\frac{2i\pi}{3}} a^*(\vec{k}) & b(\vec{k}) \end{pmatrix},$$  \hspace{1cm} (A5)

where

$$a(\vec{k}) = \frac{f_{23}(\vec{k}) - f_{31}(\vec{k})}{\sqrt{3N_0(\vec{k})}}; \quad b(\vec{k}) = \frac{f_{12}(\vec{k})}{\sqrt{N_0(\vec{k})}}.$$  \hspace{1cm} (A6)

Using the eigenvector matrix $U(\vec{k})$, the pairing matrix $\Delta_{mn}$ can be spelled out straightforwardly as

$$\Delta_{mn}(\vec{k}) = \Delta_A \left[ \hat{U}_{2m}(-\vec{k}) \hat{U}_{1n}(\vec{k}) - \hat{U}_{1m}(-\vec{k}) \hat{U}_{2n}(\vec{k}) \right] + \Delta_B \left[ \hat{U}_{4m}(-\vec{k}) \hat{U}_{3n}(\vec{k}) - \hat{U}_{3m}(-\vec{k}) \hat{U}_{4n}(\vec{k}) \right].$$  \hspace{1cm} (A7)

For the solution of $\Delta_A = -\Delta_B = \Delta$, we have the pairing matrix as

$$\Delta(\vec{k}) = \begin{pmatrix} \Delta_1(\vec{k}) & \Delta_2(\vec{k}) & \Delta_3(\vec{k}) & 0 \\ \Delta_2(\vec{k}) & -\Delta_1(\vec{k}) & 0 & -\Delta_3(\vec{k}) \\ -\Delta_3(\vec{k}) & 0 & -\Delta_1(\vec{k}) & \Delta_2(\vec{k}) \\ 0 & -\Delta_3(\vec{k}) & \Delta_2(\vec{k}) & \Delta_1(\vec{k}) \end{pmatrix},$$  \hspace{1cm} (A8)

where the matrix elements read

$$\Delta_1(\vec{k}) = i \frac{16\Delta}{\sqrt{3N_0(\vec{k})}} \sin \frac{3}{2} k_x \left[ \begin{array}{c} \cos \frac{3}{2} k_x - \cos \frac{3}{2} k_y \\ -\cos \frac{3}{2} k_x - \cos \frac{3}{2} k_y \end{array} \right]$$  \hspace{1cm} (A9)

and

$$K_1(\vec{k}) = \begin{pmatrix} 4 \cos^4 \frac{k_y}{2} & + \left( 4 \cos^2 \frac{\sqrt{3}}{2} k_x - 7 \right) \cos^2 \frac{k_y}{2} \\ -\cos \frac{k_y}{2} \cos \frac{\sqrt{3}}{2} k_x + 2 \sin^2 \frac{\sqrt{3}}{2} k_x \end{pmatrix} \begin{pmatrix} \sin \frac{k_y}{2} \cos \frac{\sqrt{3}}{2} k_x - \cos \frac{k_y}{2} \\ \sin \frac{k_y}{2} \cos \frac{\sqrt{3}}{2} k_x + \cos \frac{k_y}{2} \end{pmatrix}.$$  \hspace{1cm} (A10)

Both the band Hamiltonian Eq. [1] and the interaction Eq. [3] are invariant under the rotation $R_{\pi}$. Applying $R_{\pi}$ to the band Hamiltonian matrix in momentum space $H_0(\vec{k})$, it transforms as

$$H_0(\vec{k}) = R_{\pi} H_0(\vec{k}) R_{\pi}^{-1}.$$  \hspace{1cm} (A11)
where $R_\omega$ is defined as

$$ R_\omega = \begin{pmatrix} 0 & r_\omega \\ r_\omega & 0 \end{pmatrix}, $$

and

$$ r_\omega = \begin{pmatrix} \cos \frac{\omega}{2} & -\sin \frac{\omega}{2} \\ \sin \frac{\omega}{2} & \cos \frac{\omega}{2} \end{pmatrix}. $$

(12)

Correspondingly, it can be shown directly that

$$ R_\omega \psi_m(\vec{k}) = \text{sgn}(m) \psi_m(\vec{k}') $$

(14)

with $\text{sgn}(m) = -1$ for $m = 1, 2$ and $+1$ for $m = 3, 4$, and $R_\omega \Delta_{mn}(\vec{k}) R_\omega^{-1} = \text{sgn}(n) \text{sgn}(m) \Delta_{mn}(\vec{k}')$.

**APPENDIX B: CALCULATION OF THE ON-SITE HUBBARD INTERACTION WITH MAGNETIC DIPOLAR INTERACTION**

The optical potential around the center of each optical site can be approximated as

$$ V(\vec{r}) = \frac{m}{2} \omega^2 (r_x^2 + r_y^2) + \frac{m}{2} \omega_z^2 r_z^2, $$

(1)

where we assume that the confinement in the $z$-axis is stronger so that $\omega_z > \omega$. The wavefunctions for the $p_x$ and $p_y$ orbitals in this harmonic potential are

$$ \psi_{p_x}(\vec{r}) = C \frac{1}{2} r_x \exp \left\{ -\frac{r_x^2 + r_y^2 - r_z^2}{2l^2} \right\}, $$

and

$$ \psi_{p_y}(\vec{r}) = C \frac{1}{2} r_y \exp \left\{ -\frac{r_x^2 + r_y^2 - r_z^2}{2l^2} \right\}, $$

(2)

where $C = 2l^{-4}l_z^{-1} \pi^{-3/2}, l = \sqrt{\hbar/m\omega}, l_z = \sqrt{\hbar/m\omega_z}$, and $l_z < l$.

With these wavefunctions, the on-site interaction can be evaluated with the direct and exchange terms:

$$ -U = \int d^3\vec{r}_1 d^3\vec{r}_2 V(\vec{r}_1 - \vec{r}_2) \left\{ |\psi_{p_x}(\vec{r}_1)\psi_{p_x}(\vec{r}_2)|^2 - |\psi_{p_x}(\vec{r}_1)\psi_{p_y}(\vec{r}_2)|^2 \right\} $$

$$ = C^2 \int d^3\vec{r} d^3\vec{R} V(\vec{r}) \left( \frac{R_x r_x^2 + R_y r_y^2}{2} \right) $$

$$ \times F_1(\vec{r}) F_2(\vec{R}), $$

(3)

where we have introduced the relative coordinate $\vec{r} = \vec{r}_1 - \vec{r}_2$ and the center of mass coordinate $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$, and defined

$$ F_1(\vec{r}) = \exp \left\{ -\frac{r_x^2 + r_y^2 - r_z^2}{2l^2} \right\}, $$

$$ F_2(\vec{R}) = \exp \left\{ -\frac{2(R_x^2 + R_y^2)}{l^2} - \frac{2R_z^2}{l_z^2} \right\}. $$

(4)

We propose to use fermionic atoms with large magnetic dipole moments $\vec{m}$. By polarizing the magnetic moments with an external magnetic field, the anisotropic interaction reads

$$ V(\vec{r}) = \frac{\mu_0}{4\pi} \frac{m^2[1 - 3(\vec{m} \cdot \hat{r})]^2}{r^3} $$

(5)

where $\vec{m} = \vec{m}/m$ and $\hat{r} = r/r$, respectively. We assume the polarization angle between $\vec{m}$ and the $xy$-plane is $\theta$, and perform the Gaussian integrals in Eq. (3). The result is expressed analytically as

$$ -U = \frac{\mu_0}{4\pi} \frac{m^2}{2l^3} (1 - \frac{3}{2} \cos^2 \theta) F(y), $$

(6)

where

$$ F(y) = \sqrt{\frac{2}{\pi}} (1 + y)^{3/2} [(3y + 1) \tan^{-1}(\frac{1}{\sqrt{y}}) - 3\sqrt{y}], $$

(7)

and $y$ is a function of $l_z/l$ as $y(l_z/l) = l_z^2/(l^2 - l_z^2)$. $F(y(l_z/l))$ is a monotonic decreasing function of $l_z$ as shown in Fig. 5 which reflects that the wavefunctions with a larger $l_z$ have smaller overlaps with each other.

The largest attractive interaction can be achieved by polarizing the magnetic moments in the $xy$-plane. If we use the fermionic atom of $^{167}$Er with $m = 7\mu_B$ and the laser beam with the wavelength $\lambda \approx 600nm$ to construct the honeycomb optical lattice, the recoil energy $E_R = h^2/2m\lambda^2 = 157nK$ and $l \approx 93(\pi/\lambda)^{1/2}$nm. Compared to the realistic band structure calculation with $V_0/E_R = 30$ in Ref. 13, $t_{||}$ is fitted as $t_{||} \approx 0.2E_R \approx 31nK$ and $l \approx 40nm$. With the choice of $l_z/l = 0.2$, $U$ reaches reach 96nK, thus $U/t_{||} \approx 3$ employed in this paper is achieved.
