Abstract

Chiral $p$-wave superfluids are fascinating topological quantum states of matter that have been found in the liquid $^3$He-A phase and arguably in the electronic Sr$_2$RuO$_4$ superconductor. They are shown fundamentally related to the fractional $5/2$ quantum Hall state which supports fractional exotic excitations. A common understanding is that such states require spin-triplet pairing of fermions due to $p$-wave interaction. Here we report by controlled theoretical approximation that a center-of-mass Wannier $p$-wave chiral superfluid state can arise from spin-singlet pairing for an $s$-wave interacting atomic Fermi gas in an optical lattice. Despite a conceptually different origin, it shows topological properties similar to the conventional chiral $p$-wave state. These include a non-zero Chern number and the appearance of chiral fermionic zero modes bounded to domain walls. Several signature quantities are calculated for the cold atom experimental condition.

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**Introduction.**— Topological superconductors, like the type of $p_x + ip_y$-wave pairing studied in the liquid $^3$He [1] and strontium ruthenates [2], are among the most desirable unconventional many-body states in condensed matter physics [3]. In two dimensions, their topological properties are fundamentally linked to a class of fractional quantum Hall states of non-Abelian statistics [4]. Studies of vortices in such materials point to fascinating braiding statistics and applications in topological quantum computing. The fate of topological superconductivity in two-dimensional electronic matter remains however debatable. In the field of ultracold atoms, this phase was predicted to appear near the $p$-wave Feshbach Resonance in Fermi gases [5]. However, the life time of such systems is severely limited by the three-body collisions, and achieving superfluidity in the resonance regime was found experimentally challenging [6]. Other strategies like spin-orbit coupling or dipolar interaction also meet new difficulties such as heating or ultracold chemical reactions [7, 8]. There is a separate approach being proposed to get around—hybridizing materials of separate topological and superconducting properties, which also encounters some engineering difficulties [9]. After all, the search for the homogeneous chiral $p$-wave superconductivity in two dimensions has stood largely open for both electronic and atomic matter systems.

Here we report the discovery of a new mechanism to achieve chiral topological superfluidity. We shall demonstrate this with cold fermionic atoms in optical lattices with the model to be introduced below. The key concept dramatically departing from the conventional wisdom that relies on the $p$ or higher partial wave pairing in relative motion is to keep the fermion interaction within the usual $s$-wave channel by pairing fermions from different Wannier orbitals, and the center-of-mass orbital motion of condensed pairs is examined for possible nontrivial topology. Recently the research of higher orbital bands in optical lattices has evolved rapidly [10], where the orbital degrees of freedom are found to play a crucial role as in solid state materials. From the early experimental attempt [11] to the breakthrough observation [12] of long-lived $p$-band bosonic atoms in a checkerboard lattice, a growing evidence points to an exotic $p_x + ip_y$ orbital Bose-Einstein condensate [10]. For fermions with attractive interaction, superfluid states similar to the type of Fulde-Ferrell-Larkin-Ovchinnikov were found in the theoretical studies of pairing in the $p$-bands [13] and that between the $s$-band and a single $p$-band [14]. As we shall show with the model below, pairing fermions from the orbitals of different angular momenta can lead to other unexpected results.

Let us consider an attractive $s$-wave interacting Fermi gas composed of two hyperfine states, to be referred to as spin $\uparrow$ and $\downarrow$, loaded in a spin-dependent 2D optical lattice shown in Fig.1(a).
The spin dependence of the lattice is motivated by various theoretical designs [15, 16] and most importantly the recent experimental demonstration of it with bosons [17, 18]. Further let the gas be tuned with a population imbalance between the two spin species by the techniques developed in the recent experimental advances [19–21]. A key condition that we propose here is to tune the population imbalance (or equivalently the chemical potential difference) sufficiently large such that the spin \( \uparrow \) and \( \downarrow \) Fermi levels reside in the \( s \) and \( p \) orbital bands, respectively. The rotation symmetry (\( C_4 \)) of the lattice dictates that the two \( p \) orbital bands, \( p_x \) and \( p_y \), are degenerated at the high symmetry points in the momentum space. Later on we shall see that this symmetry and hence degeneracy are necessary for the \( p_x + ip_y \)-wave paired superfluidity. Technically speaking, the Bravais lattices for the spin up and down fermions are 45\(^\circ\) rotated from each other.

**Effective model.**— A system of fermionic atoms, say \( ^6 \)Li, loaded into an optical lattice (Fig. 1) in the tight binding regime is described by a multi-orbital Fermi Hubbard model

\[
H = H_0 + H_{\text{int}},
\]

where \( H_0 \) describes tunneling pictorially represented in Fig. 1(b) and (c) (the expression for \( H_0 \) is...
standard and is given in Supplementary Materials) and $H_{\text{int}}$ is the Hubbard interaction,

\[
H_{\text{int}} = -U \sum_{\mathbf{R}} \left[ C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) - \frac{1}{2} \right] C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) + C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) C^A_{\nu \nu}^{\mathbf{R}}(\mathbf{R}) - 1.
\]

(2)

Here $C^A_{\nu \nu}(\mathbf{R})$ and $C^B_{\nu \nu}(\mathbf{R})$ are fermionic annihilation operators for the localized $\nu$ ($s$, $p_x$ or $p_y$) orbitals on $A$ and $B$ sites, respectively. The interactions between $s$ and $p$ orbitals originate from interactions between two hyperfine states, which are tunable by the $s$-wave Feshbach Resonance in ultracold atomic gases. We focus on the case with attractive interaction where superconducting pairing is energetically favorable.

The system, as described by the Hamiltonian in Eq. (1) exhibits lattice rotation $C_4$ and reflection symmetries. For the reflection in the $x$ and $y$ direction, the fermionic operators transform as $\mathcal{R}_x \equiv \{ C^A_{px}^{\mathbf{R}}(\mathbf{R}) \rightarrow -C^A_{px}^{\mathbf{R}}(-R_y, -R_x), C^B_{py}^{\mathbf{R}}(\mathbf{R}) \rightarrow C^A_{py}^{\mathbf{R}}(-R_y, -R_x) \}$ and $\mathcal{R}_y \equiv \{ C^A_{px}^{\mathbf{R}}(\mathbf{R}) \rightarrow C^A_{px}^{\mathbf{R}}(R_y, R_x), C^A_{py}^{\mathbf{R}}(\mathbf{R}) \rightarrow -C^A_{py}^{\mathbf{R}}(R_y, R_x) \}$, respectively. Under the lattice rotation, $C^A_{px}^{\mathbf{R}}(\mathbf{R}) \rightarrow C^A_{py}^{\mathbf{R}}(-R_y, R_x), C^A_{py}^{\mathbf{R}}(\mathbf{R}) \rightarrow C^A_{px}^{\mathbf{R}}(-R_y, R_x)$. These symmetries, reflection symmetries in particular, play an essential role in the following theory.

**Two-Flavor Ginzburg-Landau theory.**— From the analysis of Cooper’s problem (see Supplementary Materials), we conclude that condensation of Cooper pairs at $\mathbf{Q} = (\pi/a, \pi/a)$ is energetically favorable for the ground state, where $a$ is the lattice constant. Then, it is convenient to introduce two slowly varying bosonic fields $\Delta_x(\mathbf{x})$ and $\Delta_y(\mathbf{x})$, which represent Cooper pairs $(-1)^{R_x+R_y} U \langle C^A_{px}^{\mathbf{R}}(\mathbf{R}) C^A_{px}^{\mathbf{R}}(\mathbf{R}) \rangle$ and $(-1)^{R_x+R_y} U \langle C^A_{py}^{\mathbf{R}}(\mathbf{R}) C^A_{py}^{\mathbf{R}}(\mathbf{R}) \rangle$, respectively. That gives a two-flavor Ginzburg-Landau free energy respecting all the symmetries of the microscopic model as follows

\[
F[\Delta_x, \Delta_y] = \int d^2x \left[ f_{\text{Mean}}(\mathbf{x}) + f_{\text{Gaussian}}(\mathbf{x}) \right],
\]

(3)

with $f_{\text{Mean}} = r(|\Delta_x|^2 + |\Delta_y|^2) + g_1(|\Delta_x|^4 + |\Delta_y|^4) + g_2 |\Delta_x|^2|\Delta_y|^2 + g_3 (\Delta_x^* \Delta_y^* \Delta_x \Delta_y + h.c.)$, and $f_{\text{Gaussian}} = K (\partial_x |\Delta_x|^2 + \partial_y |\Delta_y|^2 + |\partial_x \Delta_x|^2 + |\partial_y \Delta_y|^2)$.

This free energy generalizes the theory of two-gap superconductivity as proposed in the context of transition metals [22]. We have neglected temporal fluctuations of Cooper pair fields and such a treatment is valid at finite temperature away from quantum critical regime. In this theory, we want to emphasize two key points due to the reflection symmetries: first, $\Delta_x$ and $\Delta_y$ are decoupled at quadratic level; second, linear derivatives such as $\Delta_x^* \partial_x \Delta_x + \Delta_y^* \partial_y \Delta_x$ are prohibited. The absence of linear derivatives makes the fluctuations of $\Delta_x \Delta_y$ suppressed, and condensation of Cooper pairs
FIG. 2: Zero-temperature phase diagram—The solid line illustrates the phase transition from normal gas (NG) to superfluid state. When $U/t_0 < 7$, the critical value of $t_3/t_0$ as shown by the dash line, beyond this threshold a phase transition from $p_x \pm p_y$ to $p_x \pm ip_y$ superfluid state occurs. When $U/t_0 \geq 7$, $p_x \pm ip_y$ superfluid state is the ground state with non-zero $t_3$. The thick solid line stands for a two-component superfluid state.

at $(\pi/a, \pi/a)$ is expected to be stable at least when $t_3$ is infinitesimal. For finite $t_3$ the stability (i.e., $K > 0$ in Eq. 3) is confirmed in our numerics (see Supplementary Materials).

With $r$ and $g_3$ obtained from integrating out fermions, we find a phase diagram shown in Fig. 2. With moderate attraction $U < 7t_0$, a first order phase transition from the $p_x \pm p_y$ to $p_x \pm ip_y$ phase occurs when $t_3$ is above some critical value. Surprisingly, when the attraction is strong enough $U > 7t_0$, we find that even infinitesimal $t_3$ makes the $p_x \pm ip_y$ favorable, opening a wide window for this non-trivial state. When $t_3 = 0$, the system has $U(1) \times U(1)$ symmetry, which means no phase coherence between the two components $\Delta_x$ and $\Delta_y$. We also study the finite temperature phase transitions (see Supplementary Materials) and find that the Kosterlitz-Thouless transition temperature can reach about 109nk, being accessible in the current experiments.[23, 24], when the lattice strengths are $V_s/E_R = 3$ and $V_p/2E_R = 5$ for $s$ and $p$ orbitals, respectively.

Gapless chiral fermions.— We now show that the $p_x \pm ip_y$ superfluid state possesses important measurable signatures due to the broken time reversal $Z_2$ symmetry which belongs to the Ising universality class. Following the standard procedure, our calculation finds that the state is topologically nontrivial by a non-zero Chern number, which is 1 and $-1$ for the $p_x + ip_y$ and $p_x - ip_y$ state, respectively. The topological properties are manifested in the existence of gapless chiral fermions, emergent on a domain wall connecting topologically distinct regions. In experiments, Ising domains of $p_x + ip_y$ and $p_x - ip_y$ are expected to spontaneously form as have been observed in the
recent cold atom experiment studying ferromagnetic transitions \cite{25}. In the following, we show that a domain wall defect carrying gapless fermions as bounded surface states is experimentally accessible.

Considering a lattice geometry in the presence of a domain wall decorated superconducting background as in Fig. 3(a), the mean-field Hamiltonian is given by

\[
H_M = H_0 - U \sum_{\mathbf{R}} [C_{s}^A(\mathbf{R})C_{p_x}^A(\mathbf{R}) < C_{s}^A(\mathbf{R})C_{p_x}^A(\mathbf{R}) > + < C_{s}^A(\mathbf{R})C_{p_x}^A(\mathbf{R}) > C_{p_x}^A(\mathbf{R})C_{s}^A(\mathbf{R})]
\]

\[
+ C_{s}^A(\mathbf{R})C_{p_y}^A(\mathbf{R}) < C_{s}^A(\mathbf{R})C_{p_y}^A(\mathbf{R}) > + < C_{s}^A(\mathbf{R})C_{p_y}^A(\mathbf{R}) > C_{p_y}^A(\mathbf{R})C_{s}^A(\mathbf{R})]
\]

\[
+ U \sum_{\mathbf{R}} \left\{ C_{s}^A(\mathbf{R})C_{s}^A(\mathbf{R}) + \frac{1}{2} [C_{p_x}^A(\mathbf{R})C_{p_x}^A(\mathbf{R}) + C_{p_y}^A(\mathbf{R})C_{p_y}^A(\mathbf{R})] \right\}.
\] (4)

The energy spectrum of fermionic excitations is obtained by diagonalizing Eq. (4). With the periodical boundary condition chosen in the $x$ direction (Fig. 3(a)), the momentum $k_x$ is a good quantum number and the energy spectra in Fig. 3(b) is thus labeled by $k_x$. For the same reason as in quantum Hall insulators, the number of gapless chiral modes moving along the interface is topologically determined by the difference of the Chern numbers in regions on either side of the interface \cite{26}; in this case $|\Delta C| = 2$. This conclusion is confirmed in our numerics. As shown in Fig. 3(b), we find four gapless chiral modes, with two localized on the domain wall (purple color) and the other two on the outer edges of the lattice (red color). From their spectra $\varepsilon_n(k_x)$, the two chiral modes on the domain wall have positive group velocities, which lead to anomalous mass flow along the domain wall. To characterize the localization of chiral fermions, we calculate the local density of states (LDOS) $\rho(y, E) = 1/2 \sum_{n,\nu} \int d k_x [ |u_n^\nu|^2 \delta(E - \varepsilon_n) + |v_n^\nu|^2 \delta(E + \varepsilon_n)]$, where $(u_n^\nu, v_n^\nu)^T$ is the eigenvector corresponding to the eigenenergy $\varepsilon_n$ of Hamiltonian Eq. (4) and $\nu$ runs over all the Wannier orbitals ($s$, $p_x$ or $p_y$) on $A$ and $B$ sites. The peak of LDOS located at the position of the domain wall, as shown in Fig. 3(c), (d) and (e), illustrates the existence of localized gapless surface states, reminiscent of the quantum Hall edge states. Taking a laser wavelength of $\lambda = 1024$nm typical for the current optical lattices, the width of the LDOS peak is estimated about $2\mu m$. This is greater than the reported spatial resolution (about $1.4\mu m$) in the radio frequency spectroscopy measurement \cite{27}, which makes the detection of this signal experimentally accessible.

In summary, when studying a spin imbalanced atomic Fermi gas with an $s$-wave interaction, we find surprisingly a topological $p$-wave superfluid state whose pairing symmetry and topological origin differ from the previous known superconducting or superfluid phases. To emphasize a
FIG. 3: (a) Schematic picture of a lattice system in the presence of a domain wall. (b) Energy spectrum of the system with a domain wall defect, when $t_1/t_0 = 8$, $t_2/t_0 = 2$, $t_3/t_0 = 0.1$ and $U/t_0 = 9$. The purple and red branches correspond to the modes at the domain wall and the edge of the lattice, respectively. (c), (d), and (e) show the local density of states (LDOS) defined in the main text. The peak of LDOS located at domain wall is shown by red color in (c) and further shown with $E/t_0 = 0$ and $y/a = 49$ in (d) and (e), respectively. The LDOS is in units of $1/\alpha t_0$.

remarkable difference, this phase does not require an interaction beyond the usual attractive $s$-wave component. Hence a short-ranged contact interaction as has been widely realized in cold gases should satisfy well. A key concept is the fermionic Cooper pairing between the orbitals of different angular momenta in an optical lattice. For the example presented here, they are the parity even $s$ and odd $p$ orbitals. The $p$-wave symmetry refers to the center-of-mass motion, not to the relative motion of each fermion pair as in the well-known $^3$He superfluid. For free or repulsively interacting systems, previous studies found that mixing orbitals of opposite parities leads to topological semimetal and insulator phases [28, 29]. Whether or how the two phenomena from either sign of the interaction are topologically related is an intriguing question for the future research.
Experimentally, one may consider the existing proposals for realizing spin-dependent optical lattices [15, 16]. Alternatively, the recent progress in group-II (alkaline-earth-metal) atoms points to the possibility of having even greater spin-dependence tunability if to load two-species fermionic atoms from the ground $^1S_0$ level and the long-lived metastable levels like $^3P_0$ and to take the advantage of the atomic orbit dependent AC Stark effect. This should in principle be able to make the lattices for different components being completely independent (so maximally spin-dependent lattice) by selection of the appropriate wavelengths [16]. The appearance of chiral fermionic zero modes bounded to domain walls associated with the orbital Ising order is predicted to be a fascinating and concrete experimental signature for this novel state. Both zero and finite temperature phase diagram are also established, providing the estimates for potential experiments.

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Supplementary Materials

S-1. HOPPING TERM

The hopping term $H_0$ in Eq. (1) can be written as

$$H_0 = \sum_{\mathbf{R}} [C^{\dagger}(\mathbf{R})T_0 C(\mathbf{R}) + C^{\dagger}(\mathbf{R})T_{1x} C(\mathbf{R} + \mathbf{e}_x) + C^{\dagger}(\mathbf{R})T_{1y} C(\mathbf{R} + \mathbf{e}_y) + C^{\dagger}(\mathbf{R})T_{1y} C(\mathbf{R} - \mathbf{e}_y) + C^{\dagger}(\mathbf{R})T_2 C(\mathbf{R} - \mathbf{e}_x + \mathbf{e}_y)]$$

(S1)

where the matrices $T$ and $T'$ are given as

$$T_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -t_2 & 0 \\ 0 & 0 & 0 & t_1 & 0 \\ 0 & -t_2 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & 0 \end{pmatrix}, \quad T_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -t_2 & 0 & 0 \\ 0 & 0 & 0 & t_1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad T_{1x} = \begin{pmatrix} -t_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t_3 & t_1 & 0 \\ 0 & t_3 & 0 & 0 & -t_2 \\ 0 & 0 & 0 & t_3 & 0 \\ 0 & 0 & t_3 & 0 & 0 \end{pmatrix},$$

$$T_2' = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -t_2 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & 0 \end{pmatrix}, \quad T_{1y}' = \begin{pmatrix} -t_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -t_3 & t_1 & 0 \\ 0 & t_3 & 0 & 0 & -t_2 \\ 0 & 0 & 0 & -t_3 & 0 \\ 0 & 0 & 0 & t_3 & 0 \end{pmatrix},$$

$$T_{1y} = \begin{pmatrix} -t_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -t_3 & 0 & 0 \\ 0 & -t_3 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & -t_3 \\ 0 & 0 & -t_2 & -t_3 & 0 \end{pmatrix}, \quad T_{1y}' = \begin{pmatrix} -t_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t_3 & 0 & 0 \\ 0 & t_3 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & t_3 \\ 0 & 0 & -t_2 & t_3 & 0 \end{pmatrix}.$$
between \( p_x \) and \( p_y \) orbitals and \( C(\mathbf{R}) = \begin{pmatrix} C_s^A(\mathbf{R}) \\ C_p^A(\mathbf{R}) \\ C_p^A(\mathbf{R}) \\ C_p^B(\mathbf{R}) \\ C_p^B(\mathbf{R}) \end{pmatrix} \) is the fermion annihilation operator located at \( \mathbf{R} = (x, y) \).

S-2. COOPER’S PROBLEM

From hopping term \( H_0 \) in Eq. (1), we find that there are five Bloch bands. The corresponding operators \( \alpha_s^\dagger(k) \) and \( \alpha_{pn}(k) \) for \( s \) and \( p \) bands are introduced, respectively. Because the width of \( p \) band is much larger than that of \( s \) band, intuitively we know that the condensation of Cooper pairs between these two bands at center-of-mass momentum \( \mathbf{Q} = (\pi/a, \pi/a) \), which is the energy minimal of \( p \) band, will be energetically favorable. Besides this intuitive picture, systematically, this conclusion is borne out by solving energy spectra of Cooper’s bound states, which are defined as \( |\Phi\rangle = \sum_{k, k', n} \phi_n(k, k') \alpha_{pn}^\dagger(k) \alpha_s^\dagger(k') |\Omega\rangle \), where \( |\Omega\rangle \) is the vacuum state and \( \phi_n(k, k') \) is the two-particle wavefunction. The summation \( \sum' \) here is over modes above the fermi level. Due to translational symmetry, the center-of-mass momentum \( \mathbf{Q} = k + k' \) is a good quantum number, which is used to label the energy spectra obtained from the eigenvalue problem, \( H|\Phi(\mathbf{Q})\rangle = E(\mathbf{Q})|\Phi(\mathbf{Q})\rangle \). Resulting from lattice rotation symmetry \( C_4 \), there are two branches of Cooper’s bound states, which are related to each other by rotation. These two branches are most clear in the limit of \( t_3 \to 0 \), i.e., without coupling between \( p_x \) and \( p_y \) orbitals. In this case, particle numbers of \( p_x \) and \( p_y \) orbitals are separately conserved. One type of bound state is formed by \( p_x \) and \( s \) orbital fermions leading to an energy dispersion \( E_x(\mathbf{Q}) \); while the other formed by \( p_y \) and \( s \) orbitals leads to a dispersion \( E_y(\mathbf{Q}) \).

As shown in Fig. [S1], we find that the bound state energy \( E_x(\mathbf{Q}) \) varies as a function of center-of-mass momentum \( \mathbf{Q} \) and the energy minimal is located at \( \mathbf{Q} = (\pi/a, \pi/a) \). Due to \( C_4 \) symmetry, the energy minimal of \( E_y(\mathbf{Q}) \) also locates at \( (\pi/a, \pi/a) \). Condensation of Cooper pairs at \( \mathbf{Q} = (\pi/a, \pi/a) \) is energetically favorable. The effect of finite coupling \( t_3 \) between \( p_x \) and \( p_y \) orbitals has been discussed in the frame work of effective field theory.
FIG. S1: Bound state energy $E_x(Q)/t_0$ varies as a function of center-of-mass momentum $Q$, when $t_1/t_0 = 8$, $t_2/t_0 = 2$, $t_3/t_0 = 0$ and $U/t_0 = 10$.

S-3. PATH INTEGRAL APPROACH

To calculate free energy from the path integral method, we introduce the Grassman fields $\bar{\Psi}(R, \tau)$ and $\Psi(R, \tau)$ and express the grand partition function of the system as

$$Z = \int D\bar{\Psi} D\Psi \exp(-S[\bar{\Psi}, \Psi]) \quad (S2)$$

with $\Psi(R, \tau) = \begin{pmatrix} \psi^A_s(R, \tau) \\ \bar{\psi}^A_s(R, \tau) \\ \psi^A_{px}(R, \tau) \\ \bar{\psi}^A_{px}(R, \tau) \\ \psi^A_{py}(R, \tau) \\ \bar{\psi}^A_{py}(R, \tau) \end{pmatrix}$. The quartic term in the interaction term of action $S$ can be decoupled with the Hubbard-Stranovich transformations,

$$\tilde{\Delta}_x(R, \tau) = U\psi^A_{px}(R, \tau)\psi^A_s(R, \tau),$$

$$\tilde{\Delta}_y(R, \tau) = U\psi^A_{py}(R, \tau)\psi^A_s(R, \tau). \quad (S3)$$

Then the partition function can be written as

$$Z = \int D\tilde{\Delta}_x D\tilde{\Delta}_x^* D\tilde{\Delta}_y D\tilde{\Delta}_y^* D\bar{\Psi} D\Psi \exp(-S[\bar{\Psi}, \Psi, \tilde{\Delta}_x, \tilde{\Delta}_x^*, \tilde{\Delta}_y, \tilde{\Delta}_y^*]). \quad (S4)$$
FIG. S2: (a) The coefficient \( r \) vs. interaction strength \( U/t_0 \); (b) and (d) The coefficient \( g_3 \) as a function of \( t_3/t_0 \); (c) The coefficient \( K \) vs. \( t_3/t_0 \).

The action in Eq. (S4) is

\[
S[\bar{\Psi}, \Psi, \bar{\Delta}_x, \bar{\Delta}_x^*, \bar{\Delta}_y, \bar{\Delta}_y^*] = \int d\tau dR \left\{ \left( \frac{|\bar{\Delta}_x(R, \tau)|^2}{U} + \frac{|\bar{\Delta}_y(R, \tau)|^2}{U} \right) - \int d\tau' dR' \bar{\Psi}(R, \tau) G^{-1}(R, \tau; R', \tau') \Psi(R', \tau') \right\},
\]

(S5)

where \( \int dR = \sum_R \). After doing an unitary transformation of fermionic fields, we replace \( \bar{\Delta}_x \) and \( \bar{\Delta}_y \) in Eq. (S5) by two slowly varying and time-independent bosonic fields \( \Delta_x(x) \) and \( \Delta_y(x) \), respectively. Integrating the fermionic fields, we get an effective action

\[
S_{eff}[\Delta_x, \Delta_y] = \int d\tau d^2x \left( \frac{|\Delta_x|^2}{U} + \frac{|\Delta_y|^2}{U} - \ln \det G^{-1}[\Delta_x, \Delta_x^*, \Delta_y, \Delta_y^*] \right)
\]

(S6)

where \( G^{-1} \) is the inverse Green’s function and \( \int d^2x = \sum_R \). By calculating free energy from Eq. (S6), we obtain coefficients \( r, g_1, g_2 \) and \( g_3 \) in Eq. (3). As shown in Fig. S2(a), since the low temperature limit is much smaller than the Fermi energy, the coefficient \( r \) changes sign from positive to negative with increasing \( U/t_0 \), which implies a second order phase transition from normal to a superfluid state with \( \Delta_x \neq 0 \) at mean field level (Fig. 2). Our numerics also find that \( 0 < g_1 < g_2/2 \) and \( |g_3| \ll g_1 \). Minimizing the free energy gives a field configuration with \( |\Delta_x| = |\Delta_y| \). The relative phase between \( \Delta_x \) and \( \Delta_y \) is fixed by \( g_3 \) as shown in Fig. S2(b) and (d). The coupling \( g_3 > 0 \) makes the relative phase locked at \( \pm \frac{\pi}{2} \) and leads to a \( p_x \pm ip_y \) superfluid state where the ‘\( \pm \)’ sign is spontaneously chosen; while \( g_3 < 0 \) favors a \( p_x \pm p_y \) state (Fig. 2).
S-4. FINITE TEMPERATURE PHASE TRANSITION

It is well known that in 2D the transition from the normal to superfluid state is of the Kosterlitz-Thouless type. To obtain the KT transition temperature, we should rewrite the complex order parameters \( \Delta_x(x) = \Delta_0 e^{i \theta_x(x)} \) and \( \Delta_y(x) = \Delta_0 e^{i \theta_y(x)} \) with the phase fluctuations \( \theta_x \) and \( \theta_y \). Introducing new variables \( \theta = \frac{1}{2} (\theta_x + \theta_y) \) and \( \Delta \theta = \theta_x - \theta_y \), from the Gaussian fluctuation part of free energy in Eq.(3), we derive the well-known XY model in terms of \( \theta \) as

\[
\Delta F[\Delta_x, \Delta_y] = \int d^2 x \tilde{K}(T) \left[ (\partial_x \theta)^2 + (\partial_y \theta)^2 \right].
\]

Here, the relative phase \( \Delta \theta \) is determined by the sign of \( g_3 \) in Eq. (3) at finite temperature. Specifically, \( \Delta \theta \) is locked at \( \pm \frac{\pi}{2} \) [or 0] for \( (p_x \pm ip_y) \) [or \( (p_x \pm p_y) \)]. The KT transition temperature is determined by the formula

\[
k_B T_{KT} = \frac{\pi a^2}{\tilde{K}(T = T_{KT})}.
\]

Solving this equation self-consistently, we get the KT transition temperature and plot it in Fig. S3.

We find that in the weak-coupling regime \( T_{KT} \) approaches the mean-field transition temperature \( T_{Mean} \) as determined by \( r = 0 \) in Eq. (3) at finite temperature. With stronger interaction, there is a large derivation of the two as expected [30], for the reason that mean field analysis underestimates fluctuation effects. Our numerics also find that \( k_B T_{KT} \) can reach 3.21\( t_0 \) accompanying with increasing of interaction strength when the lattice strengths are \( V_s/E_R = 5 \) and \( V_p/2E_R = 5 \) for \( s \) and \( p \) orbitals, respectively. As shown in the inset plot of Fig. S3 we also find that decreasing of lattice strength will increase \( T_{KT} \).

S-5. ANISOTROPIC SUPERCONDUCTING GAP

In this section, we discuss the superconducting gap for fermions resulting from this unconventional paring. The superconducting gap is calculated by solving the Mean field Hamiltonian (Eq. 4) without a domain wall defect. The anisotropy of the gap which is a remarkable property being absent in the conventional s-wave superconductors is characterized by the structure functions

\[
S_x(k) = U/N < C^A_{p_x}(-k + \mathbf{Q}) C^A_{s}(k) > \quad \text{and} \quad S_y(k) = U/N < C^A_{p_y}(-k + \mathbf{Q}) C^A_{s}(k) >,
\]

where \( N \) is the total site.

We find \( S_{x/y}(k) \) near the Fermi surface is highly anisotropic, that is it strongly depends on the polar angle of \( k \), \( \theta_{k_F} \), as shown in Fig. S4. In Fig. S4(a), when \( t_2 = 0 \) and \( t_3 = 0 \), the Fermi surface of \( p \) and \( s \) orbital bands fermions are matched very well when \( 0 \leq \theta_{k_F} \leq \pi/4 \), so the gap are almost at the same maximum value when \( \theta_{k_F} \) in that region. However, when \( \pi/4 < \theta_{k_F} < \pi/2 \), the gap decreases by increasing \( \theta_{k_F} \) due to the mismatch of Fermi surface. The situation is different
FIG. S3: Finite-temperature phase diagram–The solid line illustrates the KT transition temperature. The mean-field transition temperature is shown by the dot line. The regions for $p_x \pm ip_y$ and $p_x \pm py$ superfluid state are separated by the dash line. Here, the lattice strengths are $V_s/E_R = 5$ and $V_p/2E_R = 5$ with recoil energy $E_R = \frac{\hbar^2}{2m(2a)^2}$ and $a_s$ is the s-wave scattering length. The inset plot shows that increasing of lattice strength will decrease superfluid transition temperature.

for $t_2 \neq 0$ and $t_3 \neq 0$, where the Fermi surfaces are mismatched. The gap is non-monotonic when $\theta_{k_F}$ varies from 0 to $\pi/2$, and it is maximal at $\theta = \pi/4$ (Fig. S4(b)). This peculiar non-monotonic behavior is related to van-Hove singularities which lead to large density of states nearby.
FIG. S4: Structure function $S_x(\theta_{k_F})$ of superconducting gap near Fermi surfaces. (a) $U/t_0 = 7$, $t_1/t_0 = 8$, $t_2/t_0 = 0$ and $t_3/t_0 = 0$; (b) $U/t_0 = 7$, $t_1/t_0 = 8$, $t_2/t_0 = 2$ and $t_3/t_0 = 0.1$; (c) $\theta_{k_F}$ on the Fermi surface of s orbital band. Due to $C_4$ symmetry, the structure of $S_y$ is readily given by a $\pi/2$ rotation.