Palmer-Chalker Instability in an Orbital Superfluid

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We consider a bosonic s and p orbital system in a face-centered cubic optical lattice, and predict a fluctuation-induced instability towards the orbital analogy of Palmer-Chalker state, which is originally proposed in an electronic spin system. The single-particle spectrum has four degenerate band minima with their crystal momenta forming a tetrahedron in Brillouin zone. The Bosons condense at these degenerate minima, leading to a massive degeneracy. Within Gross-Pitaevskii approximation, the classical many-body ground states partially lift the degeneracy with the spontaneously generated p-orbital angular momenta living on a series of continuous manifolds. The fluctuations on top of the classical ground states are further taken into account. We show that the Palmer-Chalker ordering of p-orbital angular momenta is selected as the ground state by quantum and thermal fluctuations through order-by-disorder mechanism. These findings raise the exciting possibility of realizing the Palmer-Chalker state in ultracold atomic gases.

The Palmer-Chalker (PC) state proposed in a geometrically frustrated antiferromagnet refers to an exotic ordering that the spins on a four-sublattice tetrahedron are coplanar and are tangent to the sphere circumscribing a tetrahedron [1]. Over the past decades, intensive experimental efforts are denoted to search for this state in pyrochlore oxides [2, 3]. To date, the inelastic neutron scattering measurements show the evidence of PC state in several powder samples including Gd$_2$Sn$_2$O$_7$, Er$_2$Sn$_2$O$_7$ and Er$_2$Pt$_2$O$_7$ [4–7]. Yet, high-quality single crystal samples beyond the powder form are still highly desired to unambiguously pin down the magnetic structure. Ultracold atomic gases, on the other hand, have natural advantages in the quantum simulation of artificial solids in optical lattices with perfect lattice periodicity [8, 9]. In particular, the recent experiments have successfully observed the orbital superfluidity in two-dimensional bipartite optical lattices with the sublattices accommodating s and p orbitals [10–14]. It is crucial that the coherence between p orbitals established by the tunnelling process via s orbitals leads to an unexpected long lifetime of atoms in high Bloch bands. Theoretically, the two-dimensional bipartite optical lattices have also inspired numerous theoretical proposals to simulate the interacting orbital physics in optical lattices [15–22].

It is usually believed that the PC state in electronic spin systems is stabilized by dipolar interactions in strong coupling limit [1–3]. In contrast, here we show that the PC instability in a bosonic orbital system can be induced by the fluctuations from local Hubbard interactions in weak coupling limit, providing a compelling protocol towards its realization. To this end, we generalize the sp orbital system from a two-dimensional bipartite lattice to a three-dimensional face-centered cubic (FCC) lattice by retaining the essential bipartite ingredient. The single-particle spectrum has four degenerate band minima, which leads to a massive degeneracy for an ideal Bose-Einstein condensate. The multi-orbital Hubbard interaction partially lifts the degeneracy with a spontaneous four-sublattice ordering of p-orbital angular momenta, which lives on a series of continuous manifolds and prevents the system from choosing a unique ground state. Finally, we show that the PC ordering in superfluid phase possesses three Nambu-Goldstone (NG) modes [23, 24] with one arising from the broken global U(1) gauge field and the other two degenerate modes being protected by point group symmetries, and is finally favoured by quantum and thermal fluctuations via order-by-disorder mechanism [25–28].

We start with the optical potential for the face-
centered cubic lattice \([29, 30]\)

\[
V(r) = V \sum_{i=1}^{3} \cos [b_i \cdot r] + \Delta V \sum_{i=0}^{3} \cos [b_i \cdot r]
\]  

where \(b_1 = \pi (-\hat{x} + \hat{y} + \hat{z})/d, b_2 = \pi (\hat{x} - \hat{y} + \hat{z})/d,\) and \(b_3 = \pi (\hat{x} + \hat{y} - \hat{z})/d\) with \(d\) being the lattice spacing are the reciprocal lattice vectors, \(b_1 = -3\sum_{i=1}^{3} b_i\) and \(b_2 = b_1 + b_3\). The optical potential in Eq. (1) produces a three-dimensional bipartite lattice structure with \(\Delta V\) dictating the staggered potential difference between \(A\) and \(B\) sublattices shown in Fig. 1(a) and 1(b). Without loss of generality, we will restrict our discussion below in the case that \(V < 0\) and \(\Delta V < 0\). As depicted in Fig. 1(b), we consider the case when the \(B\) sublattice is much deeper than the \(A\) sublattice such that the former hosts \(p = (p_x, p_y, p_z)\) orbitals, while the latter hosts \(s\) orbitals. The low-lying \(s\) orbitals in sublattice \(B\) are well separated from the \(p\) orbitals in energy and are thus neglected. The local minima of the optical potential in Eq. (1) underlies a face-centered cubic Bravais lattice depicted in Fig. 1(a). The band structure is firstly solved by the plane-wave expansions. See Supplemental Material [31] for details. As shown in Fig. 1(d), the calculated band structure has degenerate band minima at four distinct momenta \(L_{\pm1} = (0,1,2,3)\) in the first Brillouin zone. To facilitate our understanding, the tight-binding model is desired to capture the band dispersion from plane-wave expansions. The minimal tight-binding model consists of the \(s\) bondings \(t_{ss\sigma}\) between \(s\) and \(p\) orbitals. The \(p\) bonding \(t_{pp\sigma}\) lies in the nodal plane of the \(p\) orbitals and is typically much weaker than the \(s\) bonding \(t_{pp\sigma}\). Thus, for practical consideration, we neglect the \(p\) bonding in the tight-binding approximation. We next address the on-site energies of the \(s\) and \(p\) orbitals from symmetry aspects [35]. Switching to spherical coordinates, the optical potential in Eq.(1) around \(A\) (–) and \(B\) (+) sublattices can be expressed as

\[
V(r) = \sum_{\ell \text{ even}} \sum_{m=-\ell}^{\ell} 4\pi \ell^2 \psi_{\ell m}^+ (r) Y_{\ell m}^* (\hat{r}),
\]

where \(j_\ell (z)\) is the spherical Bessel function of the first kind and \(Y_{\ell m} (\hat{r})\) is the spherical harmonic function. The \(s\) orbitals have zero angular momentum and only receives nonzero correction from the isotropic channel \(\ell = 0\), which is predicted by the section rule on the orbital angular momentum [35]. In contrast, the \(p\) orbitals form an \(\ell = 1\) angular momentum and thus receive corrections from both \(\ell = 0, 2\) channels. Direct evaluations show that \(\psi_{\ell=2, m}^+ (r)\) in Eq. (2) vanishes. Therefore, the \(p\) orbitals receive nonzero corrections only from the isotropic channel \(\ell = 0\) and therefore remain degenerate. With these in mind, we denote the on-site energies of \(s\) and \(p\) orbitals as \(\epsilon_s\) and \(\epsilon_p\), respectively. Introducing a spinor representation of the Bloch field operator \(\psi_k = (\psi_{ks}, \psi_{kp})^T\), the tight-binding model in momentum space is given by

\[
H_{\text{TB}} = \sum_k \psi_k^T \mathcal{H}_k \psi_k
\]

where

\[
\mathcal{H}_k = \begin{pmatrix}
\epsilon_s & 2t_{sp\sigma} s_x & 2t_{sp\sigma} s_y & 2t_{sp\sigma} s_z \\
-2t_{sp\sigma} s_x & -\epsilon_s & -2t_{pp\sigma} s_y & -2t_{pp\sigma} s_z \\
-2t_{sp\sigma} s_y & -2t_{pp\sigma} s_x & -\epsilon_s & -2t_{pp\sigma} s_z \\
-2t_{sp\sigma} s_z & -2t_{pp\sigma} s_x & -2t_{pp\sigma} s_y & -\epsilon_s
\end{pmatrix}
\]

with \(s_{\mu} \equiv \sin k_{\mu}\), \(\xi_s \equiv \sum_{\mu \neq \nu} t_{ss\sigma} \cos k_{\mu} \cos k_{\nu} + \epsilon_s\), and \(\xi_p \equiv \sum_{\nu \neq \mu} t_{pp\sigma} \cos k_{\mu} \cos k_{\nu} + \epsilon_p\). It is worth noticing that the relative difference, \(\epsilon_s - \epsilon_p\), between the on-site energies of \(s\) and \(p\) orbitals can be continuously tuned through the optical potential \(\Delta V\) in Eq. (1). In the band fitting procedure, the optical potentials in units of recoil energy \(E_R = \hbar^2 k^2 / 2m d^2\) are chosen as \(\{V, \Delta V\} = \{-5 E_R, -0.9023 E_R\}\) such that the on-site energies of \(s\) and \(p\) orbitals are degenerate \(\epsilon_s = \epsilon_p \equiv \epsilon\), which greatly simplifies our analysis below. As shown in Fig. 1(d), the tight-binding model with fitting parameters \(\{t_{sp\sigma}, t_{pp\sigma}, t_{pp\sigma}, \epsilon\} = \{0.073 E_R, -0.0006 E_R, 0.002 E_R, -3.529 E_R\}\) well reproduces the overall band dispersion from the plane-wave expansions, and faithfully captures the low-energy behavior around the band minima. With the constructed tight-binding model, the quasiparticles of the degenerate band minima have energy \(\epsilon_L = -2\sqrt{3t_{sp\sigma}^2 + t_{pp\sigma}^2} - 2t_{pp\sigma} + \epsilon\), and are given by

\[
\psi_L^i = \cos \Phi \psi_L^0 + i \sin \Phi \psi_L^1, \quad i = \{0, 1, 2, 3\};
\]

where \(\Phi = \arctan Y\) with the auxiliary function \(Y \equiv \sqrt{t_{pp\sigma}^2 + \sqrt{3} t_{sp\sigma}^2}/t_{sp\sigma}\). Based on these quasiparticles, a set of degenerate single-particle states that equally minimize the kinetic energy can be constructed by linear superposition of the band minima \(\psi_L^i = \sum_{j=0}^{3} \phi_j \psi_{Lj}^i\). Its manifold lives on the surface \(S^7\) in \(\mathbb{R}^8\), \(|\Phi| = 1\) with \(\Phi \equiv (\phi_0, \phi_1, \phi_2, \phi_3)\).

Having established the single-particle physics, we are then in a position to study how the many-body interaction lifts the infinite degeneracy of single-particle states. The on-site Hubbard interactions can be experimentally realized through the s-wave Feshbach resonance [30], and has the form

\[
H_1 = \frac{U_s}{2} \sum_r \tilde{n}_{sr} (\tilde{n}_{sr} - 1) + \frac{U_p}{2} \sum_r \left[ \tilde{n}_{pr}^2 - \tilde{n}_{pr} + \frac{J_p^2}{3} \right]
\]

where \(\tilde{n}_{sr} = s_{r}^+ s_r\) and \(\tilde{n}_{pr} = \sum_{\mu} p_{r\mu}^+ p_{r\mu}\) are the density operators for \(s\) and \(p\) orbitals respectively, the \(\mu\)-component orbital angular momentum operator \(J_p^\mu = \)
FIG. 2. (a) Illustrative the ground-state configurations of \( \phi = (\phi_0, \phi_1, \phi_2, \phi_3) \) obtained by the imaginary time evolution. Different types of points denote different initial configurations in the numerical simulations. (b) The inner blue cube denotes the magnetic Brillouin zone of \( p \)-orbital angular momenta in (c) due to the interference of condensates at momenta \( L_{(0,1,2,3)} \). (c) Trajectories of spontaneous \( p \)-orbital angular momenta with the color of arrows encoding the angle \( \theta \) in Eq. (7). The black solid points denote the results from numerical simulations.

\[-i \sum_{\lambda} \epsilon_{\mu \lambda} p^\dagger_{e \nu \lambda} p_{p \tau} \] and \( \epsilon_{\mu \lambda} \) is the Levi-Civita symbol. The interactions can be estimated as \( U_s = \frac{i}{4} [1 - 2U_V / (V + \Delta V)]^{3/2} U_p \equiv U \) from the harmonic approximation [37, 38]. The last term in Eq. (5) enjoys SU(2) rotational symmetry and favors the spontaneous orbital angular momentum to lower the energy, which is analogous to the Hund’s coupling for electrons in an atom. According to the orbital Hund’s rule, the bosons are not subject to the Pauli exclusion principle and tend to condensate in a single orbital to maximize the orbital angular momentum. We next turn to the many-particle wave function of the condensates. It is worth to mention that the fragmented condensate violates the orbital Hund’s rule and does not optimize the orbital Hund’s coupling due to the exchange correlations [39]. Below, we shall consider the coherent condensate \( |\Psi\rangle = \frac{1}{\sqrt{N_0}} \left( \sum_{i=0}^{3} \phi_i \psi^\dagger_{i L_i} \right)^{N_0} |0\rangle \) , where \( |0\rangle \) denotes the vacuum state and \( N_0 \) is the number of condensed bosons. Using the coherent state, the time-dependent Gross-Pitaevskii equation can be readily derived through the Euler-Lagrange equation [32]

\[
\frac{\partial \mathcal{L}}{\partial \phi^*_i} - \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{\phi}^*_i} \right) = 0, i = \{0, 1, 2, 3\},
\]

where the Lagrangian \( \mathcal{L} \equiv \sum_{i=0}^{3} i \hbar \left( \phi^*_i \dot{\phi}_i - \phi_i \dot{\phi}^*_i \right) - \mathcal{E}(\phi, \dot{\phi}) \) with \( \mathcal{E}(\phi^*, \phi) \equiv \langle \Psi | \mathcal{H}_{\text{TB}} + \mathcal{H}_1 | \Psi \rangle / N_0 \), the energy functional and \( N_0 \) the number of lattice sites. See Supplemental Material [31] for the derivation. Here let us briefly discuss the symmetry. As shown in Fig. 2(b), \( L_{0,1,2,3} \) connect the center of a tetrahedron to its vertices. The Lagrangian \( \mathcal{L} \) naturally inherits the \( T_d \) point group symmetry of the tetrahedron through the single-particle states in Eq. (4). The Gross-Pitaevskii equation is numerically solved with the imaginary time evolution by propagating an initial trial state [40]. With different initial states, a series of degenerate ground states are obtained. We illustrate the ground-state configuration \( \phi \) by several sets of numerical solutions depicted in Fig. 2(a).

The configuration \( \phi \) splits into two pairs each with identical complex modulus. The complex phases of \( \phi \) also have internal structures: two \( \phi \)'s have identical phase and the others are \( \pi/2 \) ahead and behind. With these insights, the numerical solutions can be described by the following analytic expression (up to a global \( U(1) \) phase)

\[
\phi = \frac{1}{\sqrt{2}} \left( i \cos \theta, \cos \theta, -i \sin \theta, \sin \theta \right), 0 \leq \theta \leq \pi
\]

or its counterparts with permutations, which is a manifestation of \( T_d \) point group symmetry [41]. Moreover, we have also verified that the ground-state energy density in numerical simulations is consistent with the analytic result \( \varepsilon_0 = \mathcal{E}_L N_0 + (\cos^4 \Phi U_s + 19 \sin^4 \Phi U_p / 27) N_0^3 / 2 \) where the condensation density \( n_0 = N_0 / N_L \). The ground states spontaneously break the time-reversal symmetry and support \( p \)-orbital angular momenta due to the aforementioned orbital Hund’s coupling. The \( p \)-orbital angular momenta involve the interference between the band minima at \( L_{0,1,2,3} \), resulting in a reduced Brillouin zone in Fig. 2(b). With the analytic configuration in Eq. (7), the trajectories of \( p \)-orbital angular momenta \( J_{\tau} \) in an enlarged unit cell with four sublattice forming a tetrahedron are plotted in Fig. 2(c) and show excellent agreement with the numerical simulations. The classical solution of the Gross-Pitaevskii equation partially lifts the single-particle degeneracy on surface \( S^2 \) and still enjoys the infinite degeneracy arising from the global \( U(1) \) phase and the continuous symmetry characterized by \( \theta \) in Eq. (7).

The ground states of Gross-Pitaevskii equation can evolve in the continuous-symmetry space without energy cost, e.g. the trajectories in Fig. 2(c), which makes the system particularly susceptible to fluctuations. We therefore proceed to examine the effects of fluctuations on the degenerate ground states. Following the standard Bogoliubov approximation [42, 43], the bosonic field \( \psi_{L_i + k} \) around the band minima \( L_i \) is separated into the classical condensation \( \phi_i \) and the fluctuating field \( \phi_{i k} \).

In the weak coupling limit, we project both the kinetic and interaction terms into four lowest branches at band minima, which captures the essential low-energy physics in the long-wavelength limit. Within the formalism of functional integral, the partition function is given by

\[
\mathcal{Z} = \int \mathcal{D}[\bar{\phi}, \phi] e^{-S_{\text{eff}}[\bar{\phi}, \phi]},
\]
FIG. 3. Schematic plot of the ordering pattern of \( p \)-orbital angular momenta on a single tetrahedron for (a) collinear antiferromagnetic ordering at \( \theta = 0, \pi/2 \) and (b) Palmer-Chalker ordering at \( \theta = \pi/4, 3\pi/4 \) (The \( p \)-orbital angular momenta are in the same color with the parallel edges of tetrahedron). (c) The thermodynamic potential from the zero-point fluctuation \( \Omega_{ZP} \) (solid blue line) and the sound velocities of Nambu-Goldstone modes (dash red line) in the long-wavelength limit with \( \{\beta, \beta', U, n\} = \{t_{spG}/\sqrt{3}, 0, t_{spG}/10, 1\} \). The solid squares and circles denote the analytical results. (d) Numerical evaluation on the solid-angle averaged sound velocities of Nambu-Goldstone modes for the collinear antiferromagnetic (open red squares) and Palmer-Chalker (open red circles) states with \( \{\beta, U, n\} = \{t_{spG}/\sqrt{3}, t_{spG}/10, 1\} \).

where the effective action reads

\[
S_{\text{eff}}[\tilde{\phi}, \tilde{\phi}] = \frac{1}{2} \sum_k (\tilde{\phi}_k \cdot \Phi_{-k} - \tilde{\Phi}_{-k} \cdot \Phi_k) \cdot \left( G_k^{-1} \right) \cdot \sum_k (\tilde{\Phi}_{-k} \cdot \Phi_k),
\]

with gamma matrices \( \gamma^{0,1,2,3,5} \) in the Pauli-Dirac representation, \( \sigma^{\mu
u} = \frac{i}{2} [\gamma^\mu, \gamma^\nu] \) the effective interaction parameters \( \{U_s, U_p\} = \{U_{sp} n \cos^4 \Phi, U_{pp} n \sin^4 \Phi/27\} \) and the total density of bosons \( n \). The band dispersions \( \epsilon_k = \text{diag}(\epsilon_{0k}, \epsilon_{1k}, \epsilon_{2k}, \epsilon_{3k}) \) are expanded in small \( k \) around the band minima, and are given by

\[
\epsilon_{ik} = \beta |k|^2 + \beta' (k_y k_z, k_z k_x, k_x k_y) \cdot \vec{L} \cdot \vec{d} + \mathcal{O}(|k|^4),
\]

with \( \{\beta, \beta'\} = \{t_{spG}/\sqrt{3} + t_{ppG}, -2(t_{ppG}/\sqrt{3} + \sqrt{3}t_{spG})\} \). The \( \sigma \) bondings \( t_{s\sigma s/p\sigma} \) between second nearest neighbors are relatively weak. In deriving Eq. (9), we keep up to the linear order in \( t_{s\sigma s/p\sigma} \). The distinguishing feature of the second term in Eq. (9) is the anisotropy, which will be discussed later. Below, we shall first focus on the isotropic case \( \beta' = 0 \). The excitation spectrum \( \omega_{ik} \) is determined by the poles of Green function

\( \det G_k^{-1} = 0 \) with an inverse Wick rotation \( i\omega_n \rightarrow \omega_k \). In the long-wavelength limit, the excitation spectrum for \( \theta \neq \pi/4 \) features two linearly dispersing NG modes, arising from the breaking of aforementioned continuous symmetries. In contrast, the collinear antiferromagnetic (PC) ordering of \( p \)-orbital angular momenta at \( \theta = 0, \pi/2 \) (\( \theta = \pi/4, 3\pi/4 \) shown in Fig. 3(a)(3(b)) preserves the \( \sigma_d \) (\( S_4 \)) symmetry of \( T_d \) point group and has an additional NG mode as a consequence of breaking the continuous symmetry of the \( \sigma_d \) (\( S_4 \)) counterpart in Fig. 3(c). This result is also supported by our analytical calculations at \( \theta = \pi/4 \). The collinear antiferromagnetic and PC states share an identical spectrum, two degenerate gapless modes with sound velocity \( v = \sqrt{2t_{spG}(U_s + 3U_p)/\sqrt{3}} \) and the other one with velocity \( v = \sqrt{2t_{spG}(U_s + 19U_p)/\sqrt{3}} \). For arbitrary \( \theta \), the numerical evaluation on the sound velocities of NG modes is shown in Fig. 3(c), indicating that the velocities are \( \theta \) independent within numerical resolutions. We next turn to discuss the thermodynamic potential \( \Omega = -T \ln Z = \Omega_{ZP} + \Omega_T \), originating from the zero-point fluctuation \( \Omega_{ZP} = \sum_k (\sum_\beta \omega_\beta - \text{Tr} G_{k,0})/4 \) and the thermal fluctuation \( \Omega_T = T \sum_k \ln(1 - \exp[-\beta \omega_\beta]) \). Since the effective action is only valid in the long-wavelength limit, the zero-point fluctuation in this limit is shown in Fig. 3(c), and favours both the collinear antiferromagnetic and PC states, which further confirms our previous analysis of NG modes from symmetry. At low temperatures, the thermodynamic potential is dominated by NG modes \( \omega_\beta = v |k| \) with the contributions following a power law behavior \( \Omega_T \propto -T^4/v^5 \). Finally, we discuss the anisotropy induced by the intraband-\( \sigma \) bondings \( t_{s\sigma s/p\sigma} \) in Eq. (9). The anisotropy \( \beta' \) with the present fitting parameters is weak and can, however, be enhanced through tuning the staggered potential \( \Delta V \) in Eq. (1). Hence we release \( \beta' \) as a free parameter. The anisotropic sound velocities are numerically evaluated by averaging over the solid angle of \( k \) and are found to be independent on the sign of \( \beta' \). As shown in Fig. 3(d), the averaged sound velocity of the degenerate NG modes in PC state is split into two branches with the low-lying one well below those in the collinear antiferromagnetic state. Therefore, the PC state will be selected as the ground state.
that our protocol will stimulate the immediate experimental search along this direction.

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SUPPLEMENTAL MATERIAL FOR "PALMER-CHALKER INSTABILITY IN AN ORBITAL SUPERFLUID"

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This Supplemental Material includes the following sections: (I) band structure calculation with plane-wave expansions, (II) derivation of the time-dependent Gross-Pitaevskii equation, and (III) derivation of the effective action.

(I) BAND STRUCTURE CALCULATION WITH PLANE-WAVE EXPANSIONS

In this section, we solve the band structure of the following Hamiltonian

$$\hat{H}_{OL} = \int d^3r \hat{\Psi}^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \hat{\Psi}(r)$$

with plane-wave expansions [1]. For the face-centered cubic optical lattice, the optical potential $V(r + R) = V(r)$ is invariant under discrete translation vectors $R = N_1 a_1 + N_2 a_2 + N_3 a_3$ with integer multiples of three primitive vectors

$$a_1 = d(\hat{y} + \hat{z}), \quad a_2 = d(\hat{z} + \hat{x}), \quad a_3 = d(\hat{x} + \hat{y})$$

where $d$ is the lattice spacing. Making use of Bloch’s theorem, the field operator in Eq. (S1) is represented as

$$\hat{\Psi}(r) = \sum_{n,k} \psi_{nk}(r) \hat{\Psi}_{nk}$$

where the quantum number $n$ is the band index and the crystal momentum $k$ can be composed from the reciprocal lattice vectors with fractional coefficients

$$k = k_1 b_1 + k_2 b_2 + k_3 b_3,$$

and the reciprocal lattice vectors

$$b_1 = \frac{\pi}{d} (-\hat{x} + \hat{y} + \hat{z}), \quad b_2 = \frac{\pi}{d} (\hat{x} - \hat{y} + \hat{z}), \quad b_3 = \frac{\pi}{d} (\hat{x} + \hat{y} - \hat{z}).$$

The Bloch orbitals $\phi_{nk}(r)$ in Eq. (S3) inherit the periodicity of the lattice potential, i.e. $\phi_{nk}(r + R) = \phi_{nk}(r)$. Therefore the Bloch wave function can be further rewritten as a linear combination of plane waves

$$\psi_{nk}(r) = \sum_G \exp[i(k + G) \cdot r] \phi_{nk}^G$$

with plane-wave vectors $G = G_1 b_1 + G_2 b_2 + G_3 b_3$. Taking the orthogonality of Bloch wave functions, the eigenstates of the Hamiltonian in Eq. (S1) can be recast to a coupled set of matrix eigenvalue equations

$$4E_R (k + G)^2 \phi_{nk}^G + \sum_{G'} V(G - G') \phi_{nk}^{G'} = \epsilon_{nk} \phi_{nk}^G$$

where the recoil energy $E_R = \pi^2 \hbar^2 / 2md^2$. The Fourier transform of lattice potential is given by

$$V(G) = \frac{1}{V_{uc}} \int_{\text{unit cell}} d^3r V(r) \exp[-iG \cdot r]$$

where $V_{uc} = |a_1 \cdot (a_2 \times a_3)|$ is the volume of primitive unit cell.
(II) DERIVATION OF THE TIME-DEPENDENT GROSS-PITAEVSKII EQUATION

The time-dependent Gross-Pitaevskii equation is obtained by neglecting the quantum fluctuations of the operators and replacing them by $c$ numbers, which are usually the averages of operators in the ground state. We consider the coherent condensed wave function of an ideal Bose gas

$$|\Psi\rangle = \frac{1}{\sqrt{N_0!}} \left( \sum_{i=0}^{N_0} \phi_i \psi^\dagger_{L_i} \right) |0\rangle,$$

(S9)

where $|0\rangle$ denotes the vacuum state and $N_0$ is the number of condensed bosons. The condensed boson density is therefore $n_0 = \frac{N_0}{N_L}$ with $N_L$ being the number of lattice sites. The thermodynamic limit is defined by taking the limit $N_0 \to \infty$ and $N_L \to \infty$ with fixed density $n_0$. In the Gross-Pitaevskii approximation, the operators $\psi_{L_i}$ are replaced by $c$ numbers

$$\psi_{L_i} \rightarrow \sqrt{N_0} \phi_i.$$  

(S10)

Accordingly, the operators $s_{L_i}$ and $p_{\mu L_i}$ are approximated as

$$s_{L_i} \rightarrow \sqrt{N_0} \phi_i \cos \Phi,$$

(S11)

$$p_{\mu L_i} \rightarrow i \sqrt{N_0} \phi_i \sin \Phi \hat{L}_\mu^\dagger.$$

(S12)

After a lengthy but straightforward algebra, the Lagrangian can be written as

$$\mathcal{L} \equiv \sum_i \frac{\hbar}{2} \left( \phi_i^* \dot{\phi}_i - \phi_i \dot{\phi}_i^* \right) - \mathcal{E} (\phi^*, \phi)$$

(S13)

where the energy functional

$$\mathcal{E} (\phi^*, \phi) \equiv \frac{1}{N_L} \left( \langle \Psi | H_{TB} | \Psi \rangle + \langle \Psi | H_I | \Psi \rangle \right),$$

(S14)

and

$$\langle \Psi | H_{TB} | \Psi \rangle = N_0 \left[ -2 \left( \sqrt{2t_{sp\sigma}^2 + t_{pp\sigma}^2} + t_{pp\sigma} \right) + \epsilon \right] \sum_i \phi_i^* \phi_i \equiv N_0 \epsilon_{L} \sum_i \phi_i^* \phi_i$$

(S15)

$$\langle \Psi | H_I | \Psi \rangle = \frac{n_0}{2} N_0 U_s \cos^4 \Phi \left( \sum_{ij} \phi_i^2 \phi_j^2 + 2 \sum_{i \neq j} \phi_i^* \phi_i \phi_j^* \phi_j + \sum_{(ijkl)} \phi_i^* \phi_j^* \phi_k \phi_l \right)$$

(S16)

$$+ \frac{n_0}{6} N_0 U_p \sin^4 \Phi \left( 3 \sum_i \phi_i^2 \phi_i^2 + \frac{11}{9} \sum_{i \neq j} \phi_i^2 \phi_j^2 \phi_i^* \phi_j + \frac{22}{9} \sum_{i \neq j} \phi_i^* \phi_i \phi_j^* \phi_j + \frac{1}{3} \sum_{(ijkl)} \phi_i^* \phi_j^* \phi_k \phi_l \right).$$

(S17)

Here $\epsilon_{L} \equiv -2 \sqrt{2t_{sp\sigma}^2 + t_{pp\sigma}^2} - 2t_{pp\sigma} + \epsilon$ and $(ijkl)$ denotes all possible permutations of $(0, 1, 2, 3)$. Plugging Eq. (S13) into the Euler-Lagrange equation,

$$\frac{\partial \mathcal{L}}{\partial \phi_i} - \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} \right) = 0, \ i = \{0, 1, 2, 3\},$$

(S18)

yields a set of coupled equations of motion [2]

$$i\hbar \dot{\phi}_i = \frac{\partial \mathcal{E} (\phi^*, \phi)}{\partial \phi_i^*}, \ i = \{0, 1, 2, 3\}.$$  

(S19)

The ground-state solution can be obtained by numerically evolving the imaginary-time equations of motion.
(III) DERIVATION OF THE EFFECTIVE ACTION

In this section, we will derive the low-energy effective action around the band minima at \( \mathbf{L}_{0,1,2,3} \), which describes the quadratic fluctuation on top of the classical solution of the Gross-Pitaevskii equation. Following the standard Bogoliubov approximation, the bosonic field \( \psi_{\mathbf{L}+\mathbf{k}} \) around the band minima \( \mathbf{L}_i \) is separated into the classical condensation \( \phi_i \) and the fluctuating field \( \phi_{ik} \) as \( \psi_{\mathbf{L}_i+\mathbf{k}} = \phi_i + \phi_{ik} \). The quadratic fluctuation includes the following three parts.

First, let us discuss the fluctuation arising from the energy functional of classical ground states. As illustrated in the main text, the configuration of the classical ground state is given by

\[
\phi = \frac{1}{\sqrt{2}} (i \cos \theta, \cos \theta, -i \sin \theta, \sin \theta).
\]  

Substituting Eq. (S20) into the energy functional in Eq. (S14), we have

\[
\mathcal{E} (\phi^*, \phi) = \epsilon_L n_0 + \frac{1}{2} \left( \cos^4 \Phi_u + \frac{19}{27} \sin^4 \Phi_u \right) n_0^2
\]  

where the condensation density \( n_0 = N_0/N_L \). The total bosons consist of condensed bosons in the band minima and excited bosons in the fluctuating fields. Therefore, the conservation of bosons is given by

\[
\mathcal{N} = N_0 + \sum_{ik} \phi_{ik}^\dagger \phi_{ik}.
\]

Substituting Eq. (S22) into the energy functional in Eq. (S21), the quadratic fluctuation is given by

\[
\mathcal{E}^{(2)} (\phi^*, \phi) = -\frac{1}{\mathcal{N}_L} \left[ \epsilon_L + \left( \cos^4 \Phi_u + \frac{19}{27} \sin^4 \Phi_u \right) n \right] \sum_{ik} \phi_{ik}^\dagger \phi_{ik}
\]

with \( n \) being total boson density.

Second, let us turn to the fluctuation from tight-binding model. The band structures of the tight-binding model have four degenerate minima \( \epsilon_L = -2 \sqrt{2} t_{s\sigma}^2 + t_{pp\sigma}^2 - 2 t_{pp\sigma} + \epsilon \) at momentum \( \mathbf{L}_{0,1,2,3} \). The eigenstates of the band minima at \( \mathbf{L}_i \) are given by

\[
\psi_i = \left[ \cos \Phi, i \sin \Phi \hat{L}_i^x, i \sin \Phi \hat{L}_i^y, i \sin \Phi \hat{L}_i^z \right]^T.
\]

The effective low-energy band dispersions around the band minima are obtained by projecting the tight-binding model onto the eigenstates in Eq. (S24), and have the form

\[
E_{ik} = \langle \psi_i | \mathcal{H}_{\mathbf{L}_i+\mathbf{k}} | \psi_i \rangle = \epsilon_L + \beta |k|^2 + \beta' (k_y k_x, k_z k_x, k_z k_y) \cdot \hat{\mathbf{L}}_i + \mathcal{O} (|k|^4)
\]

with \( \{ \beta, \beta' \} = \{ t_{s\sigma} / \sqrt{3} + t_{pp\sigma}, -2 (t_{pp\sigma} / \sqrt{3} + \sqrt{3} t_{ss\sigma}) \} \). In Eq. (S25) only the linear order in \( t_{ss\sigma/pps} \) is kept. It is worthy to mention that we have verified that the second-order virtual process in which the boson first hops from the lowest band to the upper bands and then hops back to the lowest band contributes in order \( |k|^4 \) and is thus neglected. Therefore, the quadratic fluctuation in tight-binding model is given by

\[
H^{(2)}_{\text{TB}} = E_{ik} \sum_{ik} \phi_{ik}^\dagger \phi_{ik}
\]

Finally, we shall discuss the fluctuation from the on-site Hubbard interaction. Let us illustrate the case for \( s \) orbitals first. The fluctuation for \( s \) orbitals takes the form

\[
H^{(2)}_{1,s} = \frac{U_s}{2} \cos^2 \Phi \sum_{\{i\} \mathbf{k}} \phi_{i1}^\dagger \phi_{i2} \phi_{i2}^\dagger \phi_{i1}^\dagger k \delta_{L_i} + L_{i2} - L_{i3} - L_{i4} G
\]

\[
+ \frac{U_s}{2} \cos^2 \Phi \sum_{\{i\} \mathbf{k}} \phi_{i1}^\dagger \phi_{i2} \phi_{i2}^\dagger \phi_{i1}^\dagger k \delta_{L_i} + L_{i2} - L_{i3} + L_{i4} G
\]

\[
+ \frac{U_s}{2} \cos^2 \Phi \sum_{\{i\} \mathbf{k}} \phi_{i1}^\dagger \phi_{i2} \phi_{i2}^\dagger \phi_{i1}^\dagger k \delta_{L_i} + L_{i2} - L_{i3} - L_{i4} G.
\]
Here we have replaced \( n_0 \) by \( n \), which is correct to the order we are calculating. After projecting onto the lowest band \( s_{L,-k} \approx \cos \Phi \phi_{ik} \) and summation over \( L_{\{ij\}} \), a lengthy but straightforward algebra leads to

\[
H_{1,s}^{(2)} = \frac{U_s}{2} n \cos^4 \Phi \sum_k \left[ \sum_{ij} \phi_i \phi_i^\dagger \phi_j^\dagger \phi_{j-k} + \sum_{i \neq j} 2 \phi_i \phi_j \phi_{ik} \phi_{j-k} + \sum_{ijkl} \phi_i \phi_j \phi_{ik} \phi_{l-k} \right]
\]

(S30)

\[
+ \frac{U_s}{2} n \cos^2 \Phi \sum_k \left[ \sum_i \phi_i^\dagger \phi_{ik} + \sum_{i \neq j} \left( \phi_i^\dagger \phi_j \phi_{ik} \phi_{j-k} + \phi_i^\dagger \phi_j \phi_{ik} \phi_{j-k} \right) + \sum_{ijkl} \phi_i^\dagger \phi_j \phi_{ik} \phi_{l-k} \right]
\]

(S31)

\[
+ \frac{U_s}{2} n \cos^2 \Phi \sum_k \left[ \sum_{ij} \phi_i^\dagger \phi_i^\dagger \phi_{j-k} + \sum_{i \neq j} 2 \phi_i^\dagger \phi_j^\dagger \phi_{ik} \phi_{l-k} + \sum_{ijkl} \phi_i^\dagger \phi_j^\dagger \phi_{ik} \phi_{l-k} \right]
\]

(S32)

where \((ijkl)\) denotes all possible permutations of \((0, 1, 2, 3)\). Similarly, the fluctuation for \( p \) orbitals is given by

\[
H_{1,p}^{(2)} = \frac{U_p}{6} n \sin^4 \Phi \sum_k \left[ \sum_i \left( \frac{16}{9} \phi_i^2 + \frac{11}{9} \sum_j \phi_j^2 \right) \phi_{ik} \phi_{i-k} + \sum_{i \neq j} \frac{22}{9} \phi_i \phi_j \phi_{ik} \phi_{j-k} + \sum_{ijkl} \frac{1}{3} \phi_i \phi_j \phi_{ik} \phi_{l-k} \right]
\]

(S33)

\[
+ \frac{2U_p}{3} n \sin^4 \Phi \sum_k \left[ \sum_i \left( \frac{16}{9} |\phi_i|^2 + \frac{11}{9} \phi_j^2 \right) \phi_{ik} \phi_{i-k} + \sum_{i \neq j} \frac{11}{9} \phi_i^\dagger \phi_j \phi_{ik} \phi_{j-k} + \sum_{ijkl} \frac{1}{3} \phi_i^\dagger \phi_j \phi_{ik} \phi_{l-k} \right]
\]

(S34)

\[
+ \frac{U_p}{6} n \sin^4 \Phi \sum_k \left[ \sum_i \left( \frac{16}{9} \phi_i^2 + \frac{11}{9} \sum_j \phi_j^2 \right) \phi_{ik} \phi_{i-k} + \sum_{i \neq j} \frac{22}{9} \phi_i^\dagger \phi_j^\dagger \phi_{ik} \phi_{j-k} + \sum_{ijkl} \frac{1}{3} \phi_i^\dagger \phi_j^\dagger \phi_{ik} \phi_{l-k} \right]
\]

(S35)

Collecting these fluctuations, the Hamiltonian for the quadratic fluctuation is given by

\[
H_Q^{(2)} = N_L \mathcal{E}^{(2)} (\phi^*, \phi) + H_{1,s}^{(2)} + H_{1,p}^{(2)}.
\]

(S36)

It is straightforward to construct the effective action by following Ref. [3].

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