Frustrated Bose-Einstein condensates with noncollinear orbital ordering

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We investigate the unconventional Bose-Einstein condensations with the orbital degree of freedom in the three-dimensional cubic optical lattice, which gives rise to various exotic features absent in conventional scalar and spinor Bose-Einstein condensations. Orbital angular momentum moments are formed on lattice sites breaking time-reversal symmetry spontaneously. Furthermore, they exhibit orbital frustrations and develop a chiral ordering selected by the “order-from-disorder” mechanism.

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Bose-Einstein condensation (BEC) is a striking phenomenon of quantum many-body systems, characterized by a uniform phase that spontaneously breaks the $U(1)$ symmetry. By introducing extra degrees of freedom, quantum condensates with even more exotic symmetry breaking patterns and topological structures emerge. A familiar example is the superfluid $^3$He phase, which is a spin-triplet $p$-wave Cooper pairing condensate with both spin and orbital degrees of freedom.1,2 It exhibits a variety of rich structures that simultaneously incorporate the symmetries of liquid crystals, magnets, and scalar superfluids. Consequently, the superfluid $^3$He systems possess fundamental connections with particle physics, and exemplify fundamental concepts of modern theoretical physics.3

The rapid development of cold atom gases provides an opportunity other than $^3$He to explore exotic condensations with internal degrees of freedom. Spinor atomic gases, composed of atoms with hyperfine spins, simultaneously exhibit magnetism and superfluidity.4–6 Furthermore, orbital is a degree of freedom independent of spin and charge. It is originally investigated in condensed matter transition metal oxides, which play an important role in superconductivity, metal-insulator transition, and quantum magnetism.7,8 Introducing orbital into cold atom gases has been theoretically investigated, which leads to unconventional BECs with complex-valued condensed wave function of bosons and spontaneously breaking of time-reversal symmetry.9–16 Excitingly, the recent experimental progress has realized the metastable BECs in high-orbital bands exhibiting complex-valued condensate wave functions at nonzero wave vectors and orbital orderings.17–19

In this Rapid Communication, we investigate the properties of an orbital BEC in the $p$-orbital bands of a cubic optical lattice. Although orbital BECs share many properties with the ferromagnetic phase in spinor BECs, there are crucial differences between them. In spinor BECs, the internal degrees of freedom of hyperfine spin degree is not coupled to the lattice. However for orbital BECs, the ordering of the orbital angular momentum comes from the atom motion within each optical site, and thus is closely related to the motion of atoms in optical lattice. As we will show, the uniqueness of the orbital degree of freedom gives rise to a whole host of exotic phenomena, such as orbital frustration and concomitant noncollinear orbital orderings selected by the “order-from-disorder” mechanism. The selected ordering pattern exhibits an orbital angular momentum moment chirality.

The Hamiltonian of bosons pumped to the $p$-orbital bands of a cubic optical lattice is described by a multiorbital Bose-Hubbard model, $H = H_I + H_{\text{int}}$,

$$H_I = \sum_{\mu,\nu} [t_{\mu\nu} (1 - \delta_{\mu\nu})] \langle \hat{p}_{\mu}^\dagger \hat{p}_{\nu} + \text{H.c.} \rangle,$$

$$H_{\text{int}} = \frac{U}{2} \left( n_{\pi}^2 - \frac{1}{3} \sum_{\mu} L_{\mu}^2 \right),$$

where $\mu, \nu = x,y,z$ denote the orbital indices and $a$ is the lattice constant. $p_{\mu}^\dagger (p_{\mu})$ are annihilation (creation) operators for bosons at site $\vec{r}$. In orbital $\mu$, $n_{\mu}$ is the total particle number operator and $L_{\mu}$ represents the total orbital angular momentum on site $\vec{r}$, and $t_{\mu\nu}$ describe the nearest-neighbor hopping matrix elements along the longitudinal and transverse directions, respectively. Using the terminology of chemistry, they are denoted as $\sigma$ and $\pi$ bonding, respectively. Due to the odd parity of $p$ orbitals, $t_{\uparrow\uparrow}$ and $t_{\downarrow\downarrow}$ are positive. The strong anisotropy of the $p$-band Wannier wave function implies that $t_{\uparrow\uparrow} < t_{\downarrow\downarrow}$. The on-site interaction term $H_{\text{int}}$ reflects the Hund’s type physics generalized to bosons, i.e., bosons prefer to occupy complex-valued orbitals of the $p_{\mu\uparrow} + ip_{\mu\downarrow}$ type with $\vec{e}_1 \perp \vec{e}_2$. This complex-valued orbital has larger spatial extension than the real ones of $p_{\mu\sigma}$, and thus the repulsive interactions are reduced and simultaneously the on-site orbital angular momenta are maximized.9,13

We consider the orbital superfluid phase. A remarkable feature of the band structure is that the energy minima of $p_{\mu}$ orbitals are located at finite momenta $Q_{\mu}$ rather than at zero momentum, which are $Q_{x} = (\frac{\pi}{a}, 0, 0)$; $Q_{y} = (0, \frac{\pi}{a}, 0)$; $Q_{z} = (0, 0, \frac{\pi}{a})$ for the three $p$-orbital subbands, respectively. In the three-dimensional (3D) cubic lattice, we will show that the on-site orbital angular momenta are no longer collinear but exhibit orbital frustrations. The single-particle states $\psi_{Q_{\mu}} = e^{i\varphi_{\mu}}$ ($\mu = x,y,z$) are degenerate, thus any condensate wave function of a linear superposition of these states,

$$|\tilde{Q}\rangle = c_1|Q_x\rangle + c_2|Q_y\rangle + c_3|Q_z\rangle,$$

yields the same kinetic energy. The complex vector $\tilde{c} = (c_1, c_2, c_3)$ satisfies the normalization condition, $|\tilde{c}|^2 = 1$. Next we will consider the interaction effect to lift the degeneracy and select the condensate wave functions.
but the lattice. To illustrate this point, let us recall the previous
that simultaneously maximizes the energy of all the bonds in a
degeneracy is a consequence of orbital frustration, which
on-site orbital angular momentum. (b) Sketch of the noncollinear
orderings of orbital angular momenta in real space from Eq. (4).

The SO(3) degeneracy at the classical level. At the classical
level (neglecting quantum fluctuations so that the boson operator
can be replaced by its average value), the minimum if the coefficient vector \( \tilde{c} \) in Eq. (2) can be expressed as
\( \tilde{c} = \frac{1}{\sqrt{2}} (\tilde{m} + i\tilde{n}) \), where \( \tilde{m} \) and \( \tilde{n} \) are two mutual perpendicular
unit vectors. Transforming back into real space, for the lattice
site with integer-valued coordinates \( \tilde{r} = (r_x, r_y, r_z) \), its on-site orbital configuration is
\( \psi_{\tilde{r}} = \frac{1}{\sqrt{2}} (p_{\tilde{r}1} + ip_{\tilde{r}2}) \) with the relation
\( \hat{e}_1 = (P_x)^{p_{\tilde{r}1}}(P_y)^{p_{\tilde{r}2}}(P_z)^{-p_{\tilde{r}3}} \tilde{m}; \hat{e}_2 = (P_x)^{p_{\tilde{r}1}}(P_y)^{p_{\tilde{r}2}}(P_z)^{-p_{\tilde{r}3}} \tilde{n} \), (3)
where \( P_{x,y,z} \) are reflection operators with respect to the \( x, y, z \)
axes, respectively. \( \hat{e}_{1,2} \) remain orthogonal to each other, and the on-site orbital angular momentum \( \hat{L}^2 \parallel \hat{e}_1 \times \hat{e}_2 \), such that
\( \hat{L}^2 \) is maximized to minimize \( H_{\text{int}} \). This denotes that at
the classical level, the ground state manifold is just the configuration space of the 3D orthogonal triad \( \tilde{m}, \tilde{n}, \tilde{l} \), and \( \tilde{l} = \tilde{m} \times \tilde{n} \), which is just the SO(3) group space and can be expressed in terms of Euler angles \( (\phi, \theta, \gamma) \), as illustrated in Fig. 1(a). Note that the multiplication of an overall U(1) phase \( e^{-i\varphi} \) is equivalent to the rotation of the triad around \( \tilde{l} \) by the angle \( \varphi \). Therefore, the U(1) superfluid phase is absorbed into the SO(3) group configuration space. For a given triad configuration \( \tilde{m}_0, \tilde{n}_0, \) and \( \tilde{l}_0 \), the corresponding real space distribution of the orbital angular momentum (OAM) orientation \( \hat{L}(\tilde{r}) \) becomes
\[
\hat{L}_{\tilde{r}} = [(−1)^{p_{\tilde{r}_1}}r_x, (−1)^{p_{\tilde{r}_2}}r_y, (−1)^{p_{\tilde{r}_3}}r_z],
\]
(4)

which is noncollinear as shown in Fig. 1(b).

Similarly to the case of frustrated magnets, this classic level degeneracy is a consequence of orbital frustration, which means that it is impossible to find an orbital configuration that simultaneously minimizes the energy of all the bonds in the lattice. To illustrate this point, let us recall the previously studied two-dimensional (2D) case for a comparison. The staggered OAM configuration in Fig. 2(a) simultaneously minimizes both the parallel \( (t_1) \) and transverse \( (t_\perp) \) hopping energies at all bonds of the square lattice, and thus there is no frustration. However, in the 3D cubic lattice, this is no longer the case. For example, if we take a similar state \( |Q_{\perp}\rangle = \frac{1}{\sqrt{2}} (|Q_x\rangle + i|Q_y\rangle) \), as shown in Fig. 2(b), the hopping energy of all bonds along \( x \) and \( y \) directions can be minimized, but the \( \sigma \) bond along the \( z \) direction is broken. Since the

hopping Hamiltonian equation (1) does not preserve the SO(3) symmetry, this classic level degeneracy should be lifted by quantum fluctuations.

Order from disorder. In frustrated magnetism, the infinite degeneracy is usually lifted by quantum or thermal fluctuations, which is known as the “order-from-disorder” mechanism. Below we perform the same analysis to the 3D \( p \)-orbital BECs. If we take quantum fluctuations around the mean-field values into account, \( p_{\mu} = |p_{\mu}| + \delta p_{\mu} \), and calculate the fluctuation-corrected ground state energy, quantum fluctuations lift the SO(3) classical degeneracy. We consider two typical condensate configurations and compare their ground state energies (the reason to choose these two states is due to their high symmetry):

\[
|Q_{\text{diag}}\rangle = \frac{1}{\sqrt{3}}(|Q_x\rangle + e^{i(2\pi/3)}|Q_y\rangle + e^{-i(2\pi/3)}|Q_z\rangle),
\]

(5)

\[
|Q_z\rangle = \frac{1}{\sqrt{2}}(|Q_x\rangle + i|Q_y\rangle).
\]

(6)

In the state of \( |Q_{\text{diag}}\rangle \), OAMs are along the body-diagonal directions, while for the state of \( |Q_z\rangle \), OAMs are along the \( z \) direction. These two configurations are degenerate at the classic level.

Here we perform the standard Bogoliubov analysis to calculate the zero-point motion energy of quasiparticles for these two configurations. We use the state of \( |Q_{\text{diag}}\rangle \) as an example, and the calculation for \( |Q_z\rangle \) is rather similar. For each \( p \) component the order parameter is

\[
\langle p_x \rangle = (−1)^{p_x} \phi, \quad \langle p_y \rangle = (−1)^{p_y} e^{2i\pi/3} \phi, \quad \langle p_z \rangle = (−1)^{p_z} e^{-2i\pi/3} \phi.
\]

(7)

To calculate the Bogoliubov spectra, we consider quantum fluctuations around the mean-field values: \( p_{\mu} = |p_{\mu}| + \delta p_{\mu} \). Expanding to the quadratic level, we arrive at

\[
\frac{i\hbar}{\partial T} \psi(k) = M(k)\psi(k),
\]

(8)

where \( \psi(k) \) is a six-component vector that represents the fluctuations: \( \psi(k) = [\delta\psi(k), \delta\psi^*(-k)]^T \), \( \delta\psi(k) = [\delta p_x(k), \delta p_y(k + Q_{xy}), \delta p_z(k + Q_{xz}), Q_{xy} = (\tau, \pi, 0), \) and

FIG. 1. (Color online) (a) The SO(3) manifold of the 3D \( p \)-orbital BEC order parameter in terms of Euler angles, where \( \text{I} \) is the direction of the orbital angular momentum. (b) Sketch of the noncollinear orderings of orbital angular momenta in real space from Eq. (4).

FIG. 2. (Color online) (a) 2D orbital BEC in the square lattice without frustration. (b) A typical configuration of 3D orbital BEC in a cubic lattice with frustration. The thick blue bonds minimize both the transverse and parallel hopping energy, while the thin red bonds only minimize the transverse hopping energy.
the ground state energy can be written as

\[ \mathcal{M}(k) = \begin{bmatrix} \mathcal{H}(k) & \Delta(k) \\ -\Delta^*(k) & -\mathcal{H}(-k) \end{bmatrix}, \]

in which both \( \mathcal{H} \) and \( \Delta \) are 3 x 3 matrices:

\[
\mathcal{H}(k) = \begin{bmatrix} \epsilon^x + 2w & -w & -w \\
-w & \epsilon^y + \epsilon_{k+Q_x} + 2w \\
-w & -w & \epsilon^x + \epsilon_{k+Q_y} + 2w \end{bmatrix},
\]

\[
\Delta(k) = \begin{bmatrix} w & e^{i(2\pi/3)}w & e^{-i(2\pi/3)}w \\
e^{-i(2\pi/3)}w & w & w \cos((k+Q_{x,y})/\Delta_1) \\
e^{-i(2\pi/3)}w & w & w \end{bmatrix},
\]

where \( w = \frac{3}{2} \phi_{dg}^2; \) \( \epsilon^x = 2 \sum_i | \Omega_i \delta_{\mu \nu} - \Omega_{\mu} (1-\delta_{\mu \nu}) | \cos(k_i a) \) is the single-particle energy spectrum for the \( \mu \) band boson. The self-consistent equation to determine the value of \( \phi_{dg} \) is

\[
n = |\phi_{dg}|^2 - \frac{1}{2} + \frac{1}{2} \sum_k \frac{\bar{\epsilon}(k) + 2U|\phi_{dg}|^2}{\bar{\epsilon}(k)|\phi_{dg}|^2} = 0,
\]

where \( \bar{\epsilon}(k) = (\epsilon^x + \epsilon_{k+Q_x} + \epsilon_{k+Q_y})/3 \), and \( n \) is the filling factor. The contribution from the zero-point motion energy to the ground state energy can be written as

\[
E_{\text{diag}}^0 = -3Un_c^2 - Un_c + t + \frac{1}{2} \sum_k \frac{\bar{\epsilon}(k)|\phi_{dg}|^2}{\bar{\epsilon}(k)|\phi_{dg}|^2} = E_c - E_{\text{diag}},
\]

where \( n_c = |\phi_{dg}|^2, t = t_1 + 2t_\perp \). Performing the same process, we obtain the correction for \( |Q_z| \), and the difference \( \Delta E = E_c - E_{\text{diag}} \) is plotted in Fig. 3.

For fixed parameters \( U, t, t_\perp \) and boson density \( n \), the energy of \( |Q_{\text{diag}}| \) is always lower than that of \( |Q_0| \), i.e., \( \Delta E = E_c - E_{\text{diag}} > 0 \), which means that orbital BECs in a cubic lattice prefer to develop OAM moments along the body-diagonal directions. Such a configuration has a high symmetry, and all the bonding strengths are uniform in the lattice. In comparison, all the \( \sigma \) bonds along the \( z \) direction are broken in the state of \( |Q_z| \). This order-from-disorder phenomenon is another feature that distinguishes orbital BECs from spinor BECs.

**Spontaneous chiral orbital order.** In condensed matter physics, the presence of spin chirality plays important roles in frustrated...
The last term is the minimal coupling between the superfluid and orbital orders and the parameters $g, u, u'$ are positive in our case. For the orbital BEC in Eq. (5), $\mathbf{L}$ is along the body-diagonal direction and the free energy Eq. (13) can be simplified to

$$F = r_0 \phi^2 + u_0 \phi^4 + r'_0 l^2 + u'_0 l^4 - g_0 \phi^2 l + \cdots.$$  \hspace{1cm} (14)

The free energy $F$ describes both thermodynamic phase transitions which are driven by temperature and quantum phase transitions where the parameters are a function of $U/t$. By minimizing the free energy in Eq. (14), we find that for $r'_0 < 0$ and $r_0 < \sqrt{-\frac{2g_0}{u'_0}}$, both $\phi$ and $l$ are nonzero at the free energy minima, which corresponds to orbital BECs with both superfluidity and orbital order; for $r'_0 < 0$ and $r_0 > \sqrt{-\frac{2g_0}{u'_0}}$, both $\phi$ and $l$ are zero, which means that both the superfluidity and orbital order have been destroyed, corresponding to the high temperature normal phases or featureless Mott insulator at zero temperature.

**Experimental detection.** Next we discuss the experimental detection of orbital ordering and unconventional BEC characterized by the ordering parameters in Eq. (7). The condensate wave function in Eq. (11) is a superposition of $p_{x, y, z}$, both $\phi$ and $l$ are nonzero, which means that both the superfluidity and orbital order have been destroyed, corresponding to the high temperature normal phases or featureless Mott insulator at zero temperature.

At last, we will briefly discuss the orbital BECs in higher bands. Recently, an unconventional BEC in the $f$ band of a bipartite optical square lattice has been observed experimentally.\(^\dagger\) \(^\ast\) Surprisingly, $d$-band BECs have also been observed in a distinct field: the exciton-polariton condensate.\(^\ddagger\) Orbital BECs in the $p$ band of a 3D optical lattice have three components $(p_x, p_y, p_z)$, and the interactions favor a ferromagnetic orbital state with OAM $L = 1$, which makes it similar to the ferromagnetic phase of spinor BECs with $F = 1$. Analogously, orbital BECs in higher bands behave similarly to spinor BECs with higher spin.\(^\ddagger\) Apparently for orbital BECs in higher bands, the geometry and symmetry group of the order parameters is far more complex and may give rise to richer physics.

In conclusion, we investigate the frustrated orbital ordering of $p$-band unconventional BECs in the cubic lattice, and we find that the uniqueness of the orbital degree of freedom gives rise to a lot of interesting phenomena that are absent in the spinor BECs and superfluid $^3$He, such as orbital frustration and concomitant noncollinear orbital orderings selected by the order-from-disorder mechanism. The chiral symmetry breaking and the elementary excitations have also been discussed.

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FRUSTRATED BOSE-EINSTEIN CONDENSATES WITH...

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