Prediction of quantum stripe ordering in optical lattices

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We predict the robust existence of a novel quantum orbital stripe order in the \( p \)-band Bose-Hubbard model of two-dimensional triangular optical lattices with cold bosonic atoms. An orbital angular momentum moment is formed on each site exhibiting a stripe order both in the superfluid and Mott-insulating phases. The stripe order spontaneously breaks time-reversal, lattice translation and rotation symmetries. In addition, it induces staggered plaquette bond currents in the superfluid phase. Possible signatures of this stripe order in the time of flight experiment are discussed.

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Cold atomic systems with multiple components, such as large spin systems, exhibit much richer phase diagrams and properties than the usual spinless bosons and spin-\( \frac{1}{2} \) fermions. For example, various spinor condensations and spin dynamics have been investigated [1,2]. Similarly, large spin fermions also exhibit novel features, including hidden symmetries [3], quintet Cooper pairing states [4], and multiple-particle clustering instabilities [5]. Motivated by such considerations, but for orbital degeneracy, we investigate the \( p \)-band Bose-Hubbard (BH) model for cold atom optical lattices, finding a novel quantum orbital stripe phase in triangular \( p \)-band optical lattices.

In solid state physics, orbital dynamics plays important roles in transition metal oxides leading to interesting phenomena, such as orbital ordering and colossal magnetoresistance [6]. In optical lattices, pioneering experiments on orbital physics have been recently carried out by Browaeys et. al [7] by accelerating the lattice of \( p \)-band Bose-Hubbard (BH) model for cold atom optical lattices, finding a novel quantum orbital stripe phase in triangular \( p \)-band optical lattices.

We begin with the construction of the \( p \)-band BH model in a 2D \((x,y)\) triangular lattice. The optical potential on each site is approximated by a 3D anisotropic harmonic potential with frequencies \( \omega_x \gg \omega_y = \omega_{xy} \). Thus we can neglect the \( p_x \)-band, and only consider a two-band model of \( p_x \) and \( p_y \). We define three unit vectors \( \hat{e}_1 = \hat{e}_x, \hat{e}_{2,3} = -\frac{1}{2}\hat{e}_x \pm \frac{\sqrt{3}}{2}\hat{e}_y \), and the two primitive lattice vectors can be taken as \( a\hat{e}_{1,2} \) (a the lattice constant). The projection of the \( p_{xy} \) orbitals along the \( \hat{e}_{1,2,3} \) directions are \( p_1 = p_x, p_{2,3} = -\frac{1}{2}p_x \pm \frac{\sqrt{3}}{2}p_y \). Due to the anisotropic nature of the \( p \)-orbitals, the hopping terms are dominated by the “head to tail” type \( \sigma \)-bonding (the \( \pi \)-bonding \( t_\perp \) term can be neglected here) as

\[
H_0 = t_\parallel \sum_{\vec{r},i=1,2,3} \left\{ p_i^\dagger \sigma \hat{p}_{\vec{r}+\hat{e}_i} + h.c. \right\}, \quad (1)
\]

where \( t_\parallel \) is positive due to the odd parity of the \( p \)-orbitals. The on-site Hubbard repulsion \( H_{\text{int}} \) can be calculated
The Brillouin zone takes the shape of a regular hexagon, with the edge length 4√3, for energetic more favorable for the 6-band minima Ψn of ψn. This is because the axial states are spatially more extended than the polar states, and thus are energetically more favorable for g > 0.

We first consider the weak coupling limit, U/t → 0. The Brillouin zone takes the shape of a regular hexagon with the edge length 4√3/(3a). The energy spectrum of H0 is E(k) = l∥\{\overline{f}_k \mp \sqrt{\bar{f}_k^2 - 3g_k^2}\}, where 3\bar{f}_k = \sum_{i=1}^3 \cos(\mathbf{k} \cdot \mathbf{e}_i) and 3g_k = \sum_{i \neq j \geq 1} \cos(\mathbf{k} \cdot \mathbf{e}_i) \cos(\mathbf{k} \cdot \mathbf{e}_j). The spectrum contains three degenerate minima located at K1 = (0, 0, 0), K2,3 = (±2√3, ±2√3), The factor e^{i\mathbf{K}_1 \cdot \mathbf{r}} takes the value of ±1 uniformly in each horizontal row but alternating in adjacent rows. If the above pattern is rotated at angles of ±2\pi/3, then we arrive at the patterns of e^{i\mathbf{K}_{2,3} \cdot \mathbf{r}}. Each eigenvector is a 2-component superposition vector of pα and pβ. The eigenvectors at energy minima are ψK1 = e^{i\mathbf{K}_1 \cdot \mathbf{r}}|p_y\rangle, ψK2,3 can be obtained by rotating ψ1 at angles of ±2π/3 respectively.

The ground state condensate wavefunction Ψc can be constructed as follows. Any linear superposition of the three band minima Ψc(\mathbf{r}) = c1ψK1 + c2ψK2 + c3ψK3 with the constraint |c1|^2 + |c2|^2 + |c3|^2 = 1 equally minimizes the kinetic energy H0. However, an infinitesimal U/t removes the band degeneracy to further optimize the interaction energy Hint. After straightforward algebra, we find the optimal configurations occur at c1 = 0, c2 = c3 = 1/√2, and its symmetrically equivalent partners. Thus the mean field condensate can be expressed as |1\over\sqrt{N_o}\{\psi^\dagger_{K_1} + i\psi^\dagger_{K_2}\}|N_o |0\rangle with |0\rangle the vacuum state and N0 the particle number in the condensate. This state breaks the U(1) gauge symmetry, as well as TR and lattice rotation symmetries, thus the ground state manifold is U(1) ⊕ Z_3 ⊕ Z_3. This state also breaks lattice translation symmetry, which is, however, equivalent to suitable combinations of U(1) and lattice rotation operations.

For better insight, we transform the above momentum space condensate to the real space. The orbital configuration on each site reads}

\[
e^{i\phi_\alpha}(\cos \alpha |p_x\rangle + i\sigma_\alpha \sin \alpha |p_y\rangle)\]

with α = ±π/4 as U/t → 0. The general configuration of α is depicted in Fig. 1 for later convenience. The U(1) phase φ_α is specified at the right lobe of the p-orbital. The Ising variable σ_α = ±1 denotes the direction of the OAM, and is represented by the anti-clockwise (clockwise) arrow on each site. Each site exhibits a nonzero OAM moment and breaks TR symmetry. At U/t → 0, p_{x,y} are not equally populated, and the moment per particle is ±2\hbar. This does not fully optimize H_{int} which requires L_{z, \mathbf{r}} = ±\hbar. However, it fully optimizes H0 which dominates over H_{int} in the weak coupling limit. We check that the phase difference is zero along each bond, and thus no inter-site bond current exists. Interestingly, as depicted in Fig. 1 OAM moments form a stripe order along each horizontal row. The driving force for this stripe formation in the SF regime is the kinetic energy, i.e., the phase coherence between bosons in each site. By contrast, the stripe formation in high Tc cuprates is driven by the competition between long range repulsion and the short range attraction in the interaction terms.

Next we discuss the ordering at large large values of U/t. We first minimize H_{int} with n particles per site. For simplicity, we consider the large n case, then Hn’s rule coupling favors the onsite state |\psi\rangle = \prod_{i \in \mathbb{Z}_n} \left(\cos \frac{\pi}{4} |p_x\rangle + i\sigma_\alpha \sin \frac{\pi}{4} |p_y\rangle\right)^n |0\rangle. This corresponds to the case α = ±π/4 in Fig. 1. Because of the anisotropic orientation of the p-orbitals, the phase difference between two sites along each bond not only depends on the U(1) and the Ising variables, but also on the direction of the bond as in the p + ip Josephson junction arrays. This effect can be captured by a U(1) gauge field. The effective Hamiltonian then reads H_{eff} = -\frac{1}{\sqrt{n}}\mathbb{I} \sum_{r, r_1, r_2} \cos \{\phi_{r_1} - \phi_{r_2} - \phi_{r_1, r_2} (\sigma_{r_1} - \sigma_{r_2})\} + \frac{1}{4} U \sum_{r} n_{r}^2, where the gauge field A_{\phi_{r_1, r_2}} = \sigma_{r_1} \theta_{r_1, r_2} - \sigma_{r_2} \theta_{r_2, r_1}; \theta_{r_1, r_2} is the angle between the bond from r_1 to r_2 and the x-axis, and thus
for example, it will also appear in the triangular-lattice plaquette with the total vorticity +1. The stripe phase obtained here is quite general: the neighboring plaquette Φ = 4θ/π along each tilted bond. As a result, on each bond around the rhombic plaquette, the Josephson current is $j = \frac{n_{0\pi}}{2} \sin \Delta \theta$ where $n_{0\pi}/n$ is the condensate fraction, and the current direction is specified by arrows in Fig. 1.

The total phase winding around each rhombic plaquette is $4\Delta \theta = \frac{3}{2} \pi$, and thus agrees with the vorticity of $\frac{3}{2}$. We emphasize that the $p$-band square lattice case does not have this interesting physics [11].

Since the stripe order exists in both strong and weak coupling limits, it should also exist at intermediate coupling strength. We have confirmed this conjecture using the Gutzwiller mean field (GMF) theory in a $30 \times 30$ lattice for three systems (marked as points 1, 2, and 3 in Fig. 2). We further apply the GMF theory to the $2 \times 2$ unit cell (Fig. 1), and obtain the phase diagram of the stripe ordered SF and MI phases (Fig. 2A). To understand the GMF numerical results, we write the trial condensate with the $p$-orbital configuration on each site as $e^{i\phi(r)}(\cos \alpha|p_x + i\sigma_y \sin \alpha|p_y|)$. It turns out that the pattern for the $U(1)$ phase does not depend on $\alpha$, and remains the same for all the coupling strength. The phase mismatch $\Delta \theta$ over the tilted bonds reads $\Delta \theta = 2\gamma - \pi/2$ with $\gamma = \sqrt{3} \tan \alpha$, and the corresponding Josephson current is $j = n_{0\pi} \sin \Delta \theta$. The value of $\alpha$ is determined by the minimization of the energy per particle of the trial condensate as

$$E(\alpha) = -t(1 + 2 \sin(2\alpha + \frac{\pi}{6})) - nU \sin^2 2\alpha + \frac{nU}{3}.$$  

In the strong (weak) coupling limit, the energy minimum is located at $\alpha = \frac{\pi}{6}$ ($\frac{\pi}{4}$), and thus the flux in each rhombic plaquette $\Phi = 4\Delta \theta/2\pi = 0$ ($\frac{1}{4}$), which agrees with the previous analyses. For the intermediate interaction, we present both results of $\Phi$ at $n = 3$ based on the GMF theory and Eq. 4 in Fig. 2B. They agree with each other very well, and confirm the validity of the trial condensate. Moreover, in the momentum space, the trial condensate for a general $\alpha$ can be expressed as $\sum_{\mathbf{k}} \left\{ \frac{1}{\sqrt{2}} (\psi_1^\dagger \psi_2 - i\psi_3^\dagger \psi_4) \right\} N_0 \langle 0 \rangle$, where $\psi_1^\dagger(r^\prime) = e^{iK_{2,3}r^\prime} \phi_{2,3}(\alpha)$ with $\phi_{2,3}(\alpha) = -\cos \alpha|p_x + \sin \alpha|p_y|$ respectively.

The OAM is of the Ising type, thus the stripe ordering is robust against small perturbations such as a small...
value of the $\pi$-type bonding $t_\perp \ll t_\parallel$. Further, we also check that the phase pattern in Fig. 1 remains unchanged from minimizing the ground state energy. In particular, in the weak-coupling limit, the band minima and corresponding eigenvectors do not change at all in the presence of a small $t_\perp$, which renders the above conclusion obvious.

The formation of the on-site orbital moment does not depend on the inter-site phase coherence, and thus the Ising variables can be ordered even in the MI state. We performed a ring exchange analysis showing the existence of the stripe-ordering at $n \geq 2$ provided the screening length of the interaction among vortices is larger compared to the size of the four-site plaquette. Due to loss of the inter-site phase coherence, bond currents disappear in the MI phase.

Our predicted stripe phase should manifest itself in the time of flight (TOF) signal as depicted in Fig. 3. In the SF state, we assume the stripe ordering wavevector $K_1$, and the corresponding condensation wavevectors at $K_{2,3}$. As a result, the TOF density peak position after a flight time of $t$ is shifted from the reciprocal lattice vectors $\vec{G}$ as follows

$$
\langle n(\vec{r}) \rangle_t \propto \sum_{\vec{G}} \left\{ |\phi_2(\alpha, \vec{k})|^2 \delta^2(\vec{k} - \vec{K}_2 - \vec{G}) + |\phi_3(\alpha, \vec{k})|^2 \delta^2(\vec{k} - \vec{K}_3 - \vec{G}) \right\},
$$

where $\vec{k} = m\vec{r}/(\hbar t)$; $\phi_{2,3}(\alpha, \vec{k})$ is the Fourier transform of the Wannier $p$-orbital wavefunction $|\phi_{2,3}(\alpha)|$, and $\vec{G} = \frac{2\pi}{a}[m, (-m + 2n)/\sqrt{3}]$ with $m, n$ integers. Thus Bragg peaks should occur at $\frac{2\pi}{a}[m \pm 1, \frac{1}{\sqrt{3}}(-m + 2n + \frac{1}{2})]$. Due to the form factors of the $p$-wave Wannier orbit wavefunction $|\phi_{2,3}(\alpha, \vec{k})|^2$, the locations of the highest peaks is not located at the origin but around $|k| \approx 1/l_{x,y}$. Due to the breaking of lattice rotation symmetry, the pattern of Bragg peaks can be rotated at angles of $\pm \frac{\pi}{2}$. In the MI phase, Bragg peaks disappear due to the loss of phase coherence. Instead, the stripe order appears in the absence of the screening function $\langle n(\vec{r})n(\vec{r}') \rangle$, which exhibit not only the usual peaks at $\vec{G}$, but also peaks located at $\vec{K}_1 + \vec{G}$.

In summary, optical lattices provide a promising direction to study new phases of orbital physics. We focus on the p-band bosons in the frustrated triangular lattice which exhibits novel stripe orbital ordering of the on-site OAM due to the geometric frustration effect to the phase coherence. In the SF phase, the staggered plaquette bond currents are also induced, reminiscent of the $d$-density wave proposal for the pseudogap phase in high $T_c$ cuprates[21] but with completely different microscopic origin. The stripe order persists in the MI phase even with the loss of superfluidity. The pattern of the stripe order can be observed in the TOF experiment. The orbital physics of cold atoms opens up intriguing problems yet to be explored, for example, the p-orbital ordering in other frustrated lattices such as the Kagome.

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