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Time reversal symmetry breaking of p -orbital bosons in a one-dimensional optical lattice

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We study bosons loaded in a one-dimensional optical lattice of two-fold p -orbital degeneracy at each site. Our numerical simulations find an anti-ferro-orbital $p_x + ip_y$, a homogeneous p_x Mott insulator phase and two kinds of superfluid phases distinguished by the orbital order (anti-ferro-orbital and para-orbital). The anti-ferro-orbital order breaks time reversal symmetry. Experimentally observable evidence is predicted for the phase transition between the two different superfluid phases. We also discover that the quantum noise measurement is able to provide a concrete evidence of time reversal symmetry breaking in the first Mott phase.

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The last decade has witnessed rapid experimental developments in the studies of ultracold quantum gases in optical lattices [1–3]. Ultracold bosons and fermions in optical lattices provide robust and controllable systems to study correlated quantum condensed matter physics beyond the scope of conventional many-body systems. For example, quantum phases and quantum phase transitions of bosons in optical lattices were studied in recent years [2–7].

Besides exploring quantum phases of bosons in the lowest band, the possibilities of observing exotic phases of higher orbital band bosons were also put forward [8, 9]. In more recent experiments, a superfluid phase with a complex order in a two dimensional p -orbital band boson system [10–12] has been reported, and evidences of exotic f -band superfluid phases have also been observed [13]. Theoretically exotic phases predicted for both fermions [14–18] and bosons [19–26] with orbital degrees of freedom are attracting considerable attention. A phase-sensitive scheme of detecting the complex order of the $p_x + ip_y$ superfluid (SF) was proposed very recently [27].

In this article, we study bosons loaded in p_x and p_y orbits of a one dimensional (1D) optical lattice at zero temperature with both the numerical simulations and field-theoretical methods. We find two SF phases distinguished by an orbital order—an anti-ferro-orbital (AFO) SF and a para-orbital (PO) SF, and two Mott insulating phases—an AFO Mott and a p_x Mott phase (FIG. 1). The AFO order is a staggered orbital current ($p_x \pm ip_y$) order [19, 20]. In the AFO SF phase, the inter-band phase difference is locked at $\pm \frac{\pi}{2}$ and the spontaneous AFO ($p_x \pm ip_y$) order in this phase breaks the time reversal symmetry (TRS), whereas the fluctuations of the relative phase restore the TRS in the PO SF phase. Based on our results, we propose an experimental method to distinguish different phases by measuring momentum distribution (FIG. 2), instead of directly measuring the local current flow resulting from TRS breaking. In this way the PO to AFO quantum phase transition, associated with

TRS breaking, can be observed in experiments. The finite momentum peaks in the momentum distribution of the AFO SF phase make it distinguishable from the conventional 1D SF phases [28, 29]. In the AFO Mott phase the quantum noise measurement will be able to provide a concrete evidence of spontaneous TRS breaking.

Experimental proposal.— The system we shall propose is a 1D lattice elongated along the x direction, and each lattice site has a rotation symmetry in the x - y plane (FIG. 1). In other words, the p_x and p_y orbits are locally degenerate, but the hopping differs significantly. Such a 1D system can be realized from a 2D optical lattice. Suppose the 2D optical lattice is formed by different laser beams in the x and y directions and the lattice potential reads $V = V_x \sin^2(k_x x) + V_y \sin^2(k_y y)$, where V_x and k_x (V_y and k_y) are the strength and wave numbers of the laser beams in the x (y) direction. In tight binding approximation, we can use the harmonic wavefunctions to approximate the Wannier functions. In the harmonic approximation, the local isotropy (rotation symmetry of each site in the x - y plane) requires $V_x k_x^2 = V_y k_y^2$. This relation, which guarantees the (approximate) two-fold orbital degeneracy at each lattice site, can be somewhat surprisingly well held in the 1D limit by taking the lattice potential depth $V_y \gg V_x$ and simultaneously the lattice constants $a_y (= \frac{\pi}{k_y}) > a_x (= \frac{\pi}{k_x})$. As a result, the local isotropy is maintained, but the system has stronger potential and larger lattice spacing in the y direction than x , which makes the hopping in the y direction much smaller than that in the x direction. As an example, we take $V_x/E_{R,x} = 6$, $V_y/E_{R,y} = 24$ and $a_y/a_x = \sqrt{2}$, where $E_{R,\alpha} \equiv \hbar^2 k_\alpha^2 / 2m$ is the recoil energy in the α direction. Such a system is locally isotropic, while the hopping of p_y orbital in the y direction is smaller than one percent of the hopping of p_x orbital in the x direction, and the system is dynamically 1D. With the technique in Ref. [11], bosons can be loaded in the p -orbits of optical lattices.

The life time and the phase coherence of p -orbital bosons could be enhanced by applying double wells as

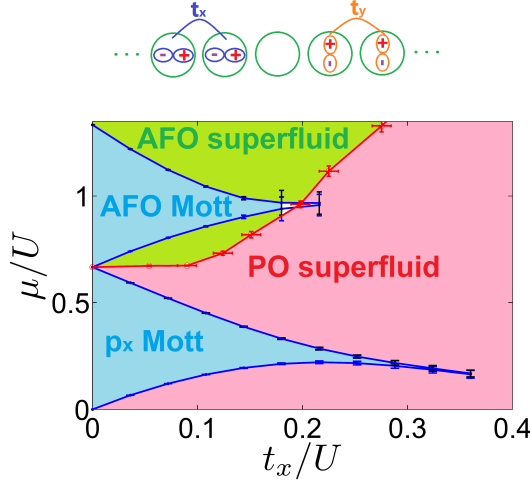


FIG. 1. (Color online). Phase diagram of a one dimensional lattice Bose gas with p_x and p_y orbital degrees of freedom. The upper panel shows the sketch of experimental setup we proposed. The green circles are used to denote the requirement of the approximate local isotropy of the lattice potential at each site. The lowest Mott lobe (with filling $\nu = 1$) is dominated by p_x bosons. The Mott state (with $\nu > 1$) has an AFO order (see text). We do not claim another phase for the tiny tip of the second Mott lobe beyond the red line because of numerical errors. For sufficiently large hopping t_x or for low filling, the Bose gas has a crossover from PO SF to a p_x SF phase, which will not be discussed in this work.

in the experiment [11]. The double well lattice gives unequal band gaps (between the p and the lower and higher orbital bands), suppressing the decay of p -band bosons. Here, for the sake of illustrating the salient features of the 1D degenerate p -orbitals, we employ a simple single-well lattice to simplify analysis. Given the consistency of the experiment [11] with the theory on a simple square lattice [19, 20], we do not expect the complexity induced by double wells would alter the basic properties and the understanding of the reported quantum phases.

In the 1D limit, the Hamiltonian describing bosons loaded in these p_x and p_y orbits reads [20]

$$H = \sum_{\langle jj' \rangle} -t_x \hat{a}_x^\dagger(j) \hat{a}_x(j') - t_y \hat{a}_y^\dagger(j) \hat{a}_y(j') + \sum_j \frac{U}{2} \left[\hat{n}(j)(\hat{n}(j) - \frac{2}{3}) - \frac{1}{3} \hat{L}_z^2(j) - \mu \hat{n}(j) \right]. \quad (1)$$

Here $\hat{a}_x(j)$ ($\hat{a}_y(j)$) is the annihilation operator for p_x (p_y) orbital at site j . The discrete variable j labels the sites of the 1D chain, with the lattice constant a_x . The local particle number operator $\hat{n}(j)$ is defined as $\sum_{\alpha=x,y} \hat{a}_\alpha^\dagger(j) \hat{a}_\alpha(j)$, and the local angular momentum operator $\hat{L}_z(j)$ is defined as $\sum_{\alpha,\beta} \epsilon_{\alpha\beta} (-i \hat{a}_\alpha^\dagger(j) \hat{a}_\beta(j))$, where the superscripts α and β run over x and y . U (> 0) is the repulsive Hubbard interaction. The average number of bosons per site is fixed by chemical potential μ . t_x (< 0) is the longitudinal hopping of p_x bosons, and t_y (> 0) is the transverse hopping of p_y bosons (FIG. 1). Due to

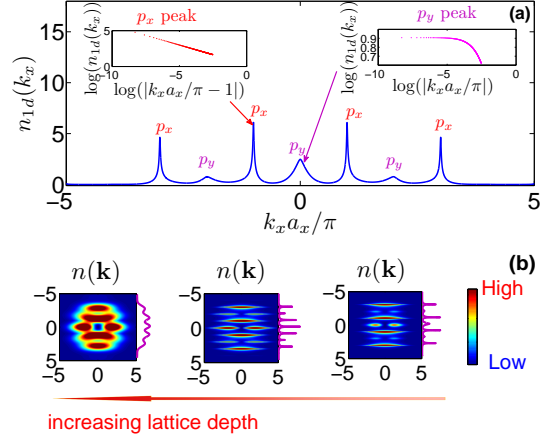


FIG. 2. (Color online). Momentum distributions $\tilde{n}(\mathbf{k})$. (a) shows the 1D momentum distribution $\tilde{n}_{1d}(k_x)$ in a geometrically 2D experimental setting (see paragraph “*Experimental proposal*”) for PO SF phase. p_x peaks at $k_x a_x = (2j+1)\pi$ (j is some integer) are sharp, and p_y peaks at $k_x a_x = 2j\pi$ are broad. The insets show that the double logarithmic plot of $\tilde{n}_{1d}(k_x)$ near the sharp (broad) peaks is linear (non-linear). (b) shows the sketch of 2D momentum distributions ($\tilde{n}(\mathbf{k})$) in different phases (PO SF, AFO SF and AFO Mott from right to left). In three subgraphs the horizontal (vertical) axis is $k_y a_y / \pi$ ($k_x a_x / \pi$). The purple wiggles along each subgraph shows $\tilde{n}_{1d}(k_x)$. In the AFO SF phase, the p_y peaks which are broad in PO SF, are replaced by sharp peaks. In the AFO Mott phase, there are no sharp peaks.

anisotropy of the p -orbitals, the longitudinal hopping (“ σ bond”) is typically much larger than the transverse hopping (“ π bond”) [19–21]. In this paper the ratio $|t_x/t_y|$ is taken as 9, which corresponds to $V_x \approx 6E_{R,x}$ (based on the estimation $|t_x/t_y| \approx \frac{1}{2}(\pi^2 \sqrt{\frac{V_x}{E_{R,x}}} - 6)$ under tight binding approximation).

The hopping term has a $U(1) \times U(1)$ symmetry, which is $\hat{a}_\alpha(j) \rightarrow [e^{i\sigma_0\theta} e^{i\sigma_z\phi}]_{\alpha\beta} \hat{a}_\beta(j)$, with $\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. It appears that the particle numbers of p_x and p_y components, $N_x = \sum_j n_x(j)$ and $N_y = \sum_j n_y(j)$ are separately conserved. However the pair hopping term $\hat{a}_y^\dagger \hat{a}_y^\dagger \hat{a}_x \hat{a}_x$ from \hat{L}_z^2 does not conserve N_x and N_y separately, and thus breaks the $U(1) \times U(1)$ symmetry. Only the total particle number $N = N_x + N_y$ is conserved. The $U(1) \times U(1)$ symmetry is reduced to $U(1) \times Z_2$ defined as $\hat{a}_\alpha(j) \rightarrow [e^{i\sigma_0\theta} e^{i\sigma_z\frac{\pi}{2}}]_{\alpha\beta} \hat{a}_\beta(j)$.

Numerical Methods.— We use a matrix product state to represent the ground state. The ground state is obtained by iterative optimization [30]. White’s correction is implemented to avoid potential trapping in the iteration procedure [31]. An open boundary condition is adopted in this work. The good quantum number we used in our numerical calculation is the total particle

number N . The chemical potential is calculated as the energy it takes to add a particle (hole) to the many-body state [32, 33]. The Mott gaps are determined by extrapolating to the thermodynamic limit. The largest system studied has 120 sites, which is large enough to compare with the experiments on 1D quantum gases. With the numerical method the ground state phase diagram of Hamiltonian in Eq. (1) is mapped out and shown in FIG. 1. The phase boundary of the Mott insulating phase is determined by the vanishing of Mott gap. The phase boundary between the AFO and PO SF phases is determined by the vanishing of the Z_2 order parameter, defined as $\tilde{L}_z \equiv \frac{1}{L} \sum_j \langle e^{iQj} \hat{L}_z(j) \rangle$, with $Q = \pi$. We use a system of 40 sites to determine this phase boundary. The existence of the AFO and PO SF phases is verified for a system with up to 100 sites. The central focus of this paper is the finding of unexpected quantum orbital phases in a 1D optical lattice. A more accurate calculation of phase boundaries is left for future study.

Mott phases.— For the Mott phases (FIG. 1), the filling factor $\nu = \langle \hat{n}(j) \rangle$ at each site is commensurate. The occupation number for each orbit, both $\langle \hat{a}_x^\dagger \hat{a}_x \rangle$ and $\langle \hat{a}_y^\dagger \hat{a}_y \rangle$ are incommensurate. For filling ν greater than 1, the Mott phase features a complex order $\langle \hat{a}_x^\dagger(j) \hat{a}_y(j) \rangle \sim e^{iQj} e^{i\zeta \frac{\pi}{2}}$ with $\zeta = \pm$ spontaneously chosen, which breaks the $U(1) \times Z_2$ symmetry down to $U(1)$. Equivalently this Mott state has a staggered angular momentum order $\langle \hat{L}_z(j) \rangle \sim e^{iQj}$. The order parameter \tilde{L}_z is finite. Without loss of generality, we have assumed \tilde{L}_z is positive. This Z_2 order also breaks the TRS, because finite \tilde{L}_z means a finite local vortex-like current flow. For filling ν equal to 1, the Z_2 order does not exist for $|t_y| \ll |t_x|$. We call it p_x Mott since p_x boson dominates this Mott phase, i.e., $\langle \hat{a}_x^\dagger \hat{a}_x \rangle \gg \langle \hat{a}_y^\dagger \hat{a}_y \rangle$ for $|t_x| \gg |t_y|$.

AFO superfluid phase.— By increasing the hopping the system goes into the SF phase when the Mott gap closes. The system has a phase transition from the AFO Mott phase to the AFO SF phase (FIG. 1). Since the Z_2 symmetry is broken in this SF phase, it behaves like a single component SF phase far from the Z_2 critical point. This AFO SF phase is thus characterized by an algebraic correlation $\langle \hat{a}_\uparrow^\dagger(j') \hat{a}_\uparrow(j) \rangle \sim |j - j'|^{-K/2}$, where $\hat{a}_\uparrow^\dagger(j) = e^{iQj} \hat{a}_x^\dagger(j) + i\xi \hat{a}_y^\dagger(j)$, with $\xi \in (0, 1]$. $\xi = 1$ in the limit of $t_x/U \rightarrow 0$. The phase correlations of original boson operators, defined as $G_{\alpha\beta}(j, j') = \langle \hat{a}_\alpha^\dagger(j) \hat{a}_\beta(j') \rangle$, are given by $G_{xx}(j, j') \sim e^{iQ(j-j')} |j - j'|^{-K/2}$, $G_{xy}(j, j') \sim i e^{iQj} |j - j'|^{-K/2}$ and $G_{yy}(j, j') \sim |j - j'|^{-K/2}$ in the AFO SF phase. We emphasize that the TRS is broken in this phase, because the off-diagonal correlation $G_{xy}(j, j')$ is complex. The key feature is that the power law decay ($|j - j'|^{-K/2}$) correlations (G_{xx} , G_{xy} and G_{yy}) exhibit the same power exponent $K/2$. In this phase, the relative phase (φ_-) between the p_x and p_y SF components is locked. The two components share the same $U(1)$ phase φ_+ at low energy. The Lagrangian describing phase fluc-

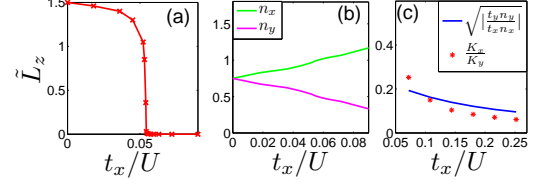


FIG. 3. (Color online). Properties of the AFO to PO phase transitions with total filling $\nu = 1.5$. (a) shows the Z_2 order parameter \tilde{L}_z . Our results indicate a continuous phase transition of the AFO order. (b) shows the filling of p_x and p_y bosons. The p_y component does not vanish across the phase transition. (c) shows the ratio K_x/K_y in the PO SF phase.

tuations is

$$\mathcal{L}[\varphi_+] = \frac{1}{2\pi K} [v_+^{-1} (\partial_\tau \varphi_+)^2 + v_+ (\partial_x \varphi_+)^2]. \quad (2)$$

The Bose liquid is completely characterized by the sound velocity v_+ and Luttinger parameter K . For $K < \frac{1}{2}$, the AFO SF phase is stable against the periodic lattice potential; for $K > \frac{1}{2}$ at commensurate filling, this phase is unstable and undergoes a localization transition towards the Mott phase [34, 35]. The AFO order is preserved across the localization transition in our system.

PO superfluid phase.— The AFO order disappears for larger hopping, and the AFO SF gives way to the PO SF. The behavior of the Z_2 order parameter \tilde{L}_z and occupation numbers of p_x and p_y bosons across the phase transition is shown in FIG. 3. The Z_2 order is destroyed by quantum fluctuations of φ_- and thus the TRS is restored in the PO SF phase. The phase correlations of the original bosons in this phase are given by $G_{xx}(j, j') \sim e^{iQ(j-j')} |j - j'|^{-K_x/2}$ and $G_{yy}(j, j') \sim |j - j'|^{-K_y/2}$. The phase coherence between p_x and p_y components— $G_{xy}(j, j')$ —vanishes in this phase. By numerical simulations, we find $K_x \ll K_y$. Following Haldane [36], an analytic expression estimating K_x/K_y is derived, $\frac{K_x}{K_y} \approx \sqrt{|t_y n_y / t_x n_x|}$, where n_x (n_y) is the filling of p_x (p_y) bosons. This is in qualitative agreement with the numerical results (FIG. 3(c)). The Lagrangian describing this PO SF phase is

$$\mathcal{L}[\varphi_x, \varphi_y] = \sum_{\alpha=x,y} \frac{1}{2\pi K_\alpha} [v_\alpha^{-1} (\partial_\tau \varphi_\alpha)^2 + v_\alpha (\partial_x \varphi_\alpha)^2] + \lambda (\partial_\tau \varphi_x) (\partial_\tau \varphi_y), \quad (3)$$

where φ_x (φ_y) is the phase of p_x (p_y) SF component. The mixing term (λ) is much smaller than the kinetic term ($\frac{1}{2\pi K_\alpha v_\alpha}$) in our system.

Quantum phase transition from AFO to PO in the superfluid phases.— The phase transition from the AFO SF to the PO SF is described by a sine-Gordon model of the relative phase φ_- . The Lagrangian is

$$\mathcal{L}[\varphi_-] = \frac{1}{2\pi K_-} [v_-^{-1} (\partial_\tau \varphi_-)^2 + v_- (\partial_x \varphi_-)^2] + m \cos(2\varphi_-), \quad (4)$$

where m is estimated as $m \approx \frac{1}{3}Un_xn_y$. When m is greater than some critical $m_c(K_-)$, the sine-Gordon theory is in a gapped phase [37], and therefore φ_- field is locked at one minimum of $m \cos(2\varphi_-)$. Such an orbital gapped phase is the AFO SF phase. When $m < m_c(K_-)$, the sine-Gordon term $m \cos(2\varphi_-)$ is irrelevant in the sense of renormalization group, and the theory is in a gapless phase for which φ_- is unlocked. This orbital gapless phase is the PO SF phase. We emphasize here the sine-Gordon term is not perturbative in our model.

Experimental signatures.— Since the quantum phases we have found are characterized by distinct phase correlations, measuring the momentum distributions by time-of-flight (TOF) will distinguish different phases. Assuming the interaction of atoms in TOF is negligible, the density obtained in TOF experiment (n_{tof}) measures the momentum distribution given as $\tilde{n}(\mathbf{k}) \propto \sum_{\alpha=x,y} \sum_n \tilde{G}_{\alpha\alpha}(k_x a_x + 2n\pi) \tilde{\phi}_\alpha^*(\mathbf{k}) \tilde{\phi}_\alpha(\mathbf{k})$ in our system (shown in FIG. 2), with $\tilde{G}_{\alpha\alpha}(k_x a_x)$ the Fourier transform of $G_{\alpha\alpha}(j, j')$ and $\tilde{\phi}_\alpha(\mathbf{k})$ the momentum-space form of p -orbital Wannier functions. The 1D momentum distribution is defined as $\tilde{n}_{1d}(k_x) = \int dk_y \tilde{n}(\mathbf{k})$. The strong peaks of momentum distribution at finite momenta $k_x = \pi/a_x \bmod 2\pi/a_x$ will distinguish the AFO SF phases from conventional 1D SF phases [28, 29]. The Luttinger parameter can be estimated by measuring momentum distribution since it behaves as $\log(\tilde{n}_{1d}(k_x)) \sim (\frac{K}{2} - 1) \log(|k_x \pm \pi/a_x|)$ for k_x near peaks $\pm\pi/a_x$. Including the effect of Wannier functions $\phi_\alpha(\mathbf{k})$, which are smooth slowly varying functions, does not alter appreciably the form of $\tilde{n}_{1d}(k_x)$ near $\pm\pi/a_x$. The effects of the harmonic trapping potential [38] and the interactions in TOF, which cause difficulties of extracting the Luttinger parameter, are left for future studies.

The AFO order in the Mott phase will have experimental signatures in the quantum noise measurement. The quantum noise is defined as $C(\mathbf{d}) = \int d^2\mathbf{R} g(\mathbf{R}, \mathbf{d})$, with $g(\mathbf{R}, \mathbf{d}) = \langle n_{\text{tof}}(\mathbf{R} + \frac{1}{2}\mathbf{d}) n_{\text{tof}}(\mathbf{R} - \frac{1}{2}\mathbf{d}) \rangle - \langle n_{\text{tof}}(\mathbf{R} + \frac{1}{2}\mathbf{d}) \rangle \langle n_{\text{tof}}(\mathbf{R} - \frac{1}{2}\mathbf{d}) \rangle$, and $\mathbf{R} = (R_x, R_y)$, $\mathbf{d} = (d_x, d_y)$. The brackets $\langle \rangle$ denote statistical averages of independently acquired TOF images in experiments [39]. For the Mott phases in our proposed 2D optical lattice, $g(\mathbf{R}, \mathbf{d})$ is given by

$$g(\mathbf{R}, \mathbf{d}) = L \left\{ \sum_{\mathbf{K}} \delta^{(2)}\left(\frac{m}{\hbar t}\mathbf{d} - \mathbf{K}\right) (\zeta_{xx}n_x + \zeta_{yy}n_y)^2 + \sum_{\mathbf{K}} \delta^{(2)}\left(\frac{m}{\hbar t}\mathbf{d} - \mathbf{K} + \mathbf{Q}_x + \mathbf{Q}_y\right) \times |\zeta_{xy}\mathcal{G}_{xy} + \zeta_{yx}\mathcal{G}_{xy}^*|^2 \right\}, \quad (5)$$

where t is the time of flight and L is the number of lattice sites. Here, $\mathcal{G}_{xy} = G_{xy}(0, 0)$, $\zeta_{\alpha\beta} \sim (R_\alpha + \frac{1}{2}d_\alpha)(R_\beta - \frac{1}{2}d_\beta)$, $\mathbf{Q}_x = (\frac{\pi}{a_x}, 0)$, $\mathbf{Q}_y = (0, \frac{\pi}{a_y})$ and $\mathbf{K} = 2j_1\mathbf{Q}_x + 2j_2\mathbf{Q}_y$ (j_1 and j_2 are integers). In Eq. (5) the smooth Gaussian part of Wannier functions $\tilde{\phi}_\alpha(\mathbf{k})$ is approximated by a constant function, which is typical in quantum noise measurement [39]. The center of the

trapped cold gas is taken as the origin of coordinates here. The sharp peaks of $C(\mathbf{d})$ at $\mathbf{d} = \mathbf{d}_0 \equiv \frac{\hbar t}{m}(\mathbf{K} - \mathbf{Q}_x - \mathbf{Q}_y)$ signify that the off-diagonal term \mathcal{G}_{xy} is finite, which distinguishes the AFO Mott state from the p_x Mott. The experimental signature of an imaginary \mathcal{G}_{xy} is predicted to be that $g(\mathbf{R}, \mathbf{d})$ exhibits nodal lines at $\mathbf{R} \parallel \mathbf{d}_0$. \mathcal{G}_{xy} being imaginary tells a local vortex-like current flow, which is a concrete evidence for the TRS breaking.

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