Atomic matter of nonzero-momentum Bose-Einstein condensation and orbital current order

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The paradigm of Bose-Einstein condensation has been associated with zero momentum to which a macroscopic fraction of bosons condense. Here we propose a new quantum state where bosonic alkali-metal atoms condense at nonzero momenta, defying the paradigm. This becomes possible when the atoms are confined in the *p*-orbital Bloch band of an optical lattice rather than the usual *s*-orbital band. The new condensate simultaneously forms an order of transversely staggered orbital currents, reminiscent of orbital antiferromagnetism or *d*-density wave in correlated electronic systems but different in fundamental ways. We discuss several approaches of preparing atoms to the *p*-orbital band and propose an "energy blocking" mechanism by Feshbach resonance to protect them from decaying to the lowest *s*-orbital band. Such a model system seems very unique and novel to atomic gases. It suggests a new concept of quantum collective phenomena of no prior example from solid state materials.

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I. INTRODUCTION

Confining bosonic atoms in an optical lattice can bring out different and new physics beyond the standard Bose-Einstein condensation (BEC) observed in a single trap [1,2]. The superfluid–Mott-insulator experiment on an optical lattice [3], based on an early theoretical idea [4,5], demonstrated one such example with bosons. Proposals of exploring various lattice atomic systems, many concerning spin, have further extended the scope of interest into different directions, experimentally [6–12] and theoretically (see Refs. [13–19] and references therein).

Atomic optical lattices not only can realize many standard solid-state problems but also may bring new and unique aspects specific to the atomic gas. One possible direction is orbital physics [20]. This is a new direction that has not yet received as much attention as spin. The pioneering experiments of Browaeys et al. [9] and Köhl et al. [10], which demonstrated the occupation of bosonic and fermionic atoms, respectively, in the higher orbital bands, further justify and motivate theoretical interest in the orbital degrees of freedom of cold atoms beyond the conventional s-orbital band, such as the next three p orbitals. In electronic solids such as manganese oxides and other transition-metal oxides, the orbital physics is believed to be essential for understanding their metal-insulator transitions, superconductivity, and colossal magnetoresistance. The solids are of periodic arrays of ions. The quantum-mechanical wave function of an electron takes various shapes when bound to an atomic nucleus by the Coulomb force. For those oxides, the relevant orbitals of the electron are the five d-wave orbitals (usually split into two groups of e_g and t_{2g} due to the crystal field). The orbital degree of freedom, having intrinsic anisotropy due to various orbital orientations, interplaying with the spin and charge, gives rise to an arena of interesting new phenomena in the field of strongly correlated electrons [21,22]. We will focus on the orbital degree of freedom of cold atoms below.

In this paper, we point out that the current experimental condition makes it possible to study a whole new class of lattice system—the dilute *p*-orbital Bose gas—beyond the conventional *s*-orbital Bose-Hubbard model. We show that the system reveals in the superfluid limit a new state of matter in which atoms undergo Bose-Einstein condensation at *nonzero momenta* and form a staggered orbital current order simultaneously. These features distinguish the *p*-orbital atomic gases from the *d*-orbital electronic oxide compounds. The unique signature of the state is predicted for the time-of-flight experiment.

II. ATOMS IN THE p-ORBITAL STATE

Let us study an optical lattice of bosonic atoms in a single internal (hyperfine spin) state. To gain a qualitative understanding, we approximate the lattice potential well by a harmonic potential around minimum. The characteristic "harmonic oscillator" frequency is $\omega_b = \sqrt{4V_0^b E_R^b}$ where V_0^b is the three-dimensional (3D) lattice potential depth and E_R^b the recoil energy for the bosonic atoms. The recoil energy is determined by the laser wavelength and atom mass. In the presence of periodic lattice potentials, the boson state can be expanded in the basis of Wannier functions, to be denoted as $\phi_{\mathbf{n}}^{b}(\mathbf{x})$, with **n** the Bloch-band index. The lowest Bloch band is s-wave symmetric with $\mathbf{n} = (000)$. The next band is a p-wave band with threefold degeneracy, p_{μ} with $\mu = x, y, z$, corresponding to $\mathbf{n} = (100), (010), (001)$. The energy splitting between s and p is $\hbar \omega_b$. (Note that the three degenerate p-wave energy subbands disperse anisotropically when hopping process included.) The fact that the next band starts at the p orbital instead of the s tells an important difference between the optical lattice potential and the (Coulomb) ionic lattice potential in electronic solids.

In a dilute weakly interacting atomic boson gas confined in optical lattices, bosons intend to aggregate into the lowest s band in the low-temperature limit, with an exponentially small fraction in the higher Bloch bands, suppressed by the factor $e^{-\hbar\omega_b/k_BT}$. A single-band approximation is then adequate, which was proven successful, both theoretically and experimentally [3,5].

Several approaches are available for transferring cold atoms to the first excited p-orbital band. In the study of a related but different model, Isacsson and Girvin [20] suggested (A) to use an appropriate vibrational π pulse with frequency on resonance with the s-p state transition and (B) to apply the method demonstrated in the experiment of Browaeys $et\ al.$ [9] by accelerating atoms in a lattice. We may also add a third possible approach—that is, (C) to sweep atoms adiabatically across a Feshbach resonance. Köhl $et\ al.$ [10] pioneered this method experimentally by showing fermionic atoms transferred to higher bands; the phenomenon was subsequently explained in theory [23]. Whether bosonic atoms can be transferred this way remains to be seen.

Now suppose that a metastable p-orbital Bose gas has been prepared on the optical lattice. The remaining challenge is that the system is not in the ground state, and thus genuinely has a finite lifetime. The interactions between two (bosonic) atoms, although weak, can cause atoms in the p-orbital states to decay. An elastic decaying process (which conserves total energy) is that two atoms initially in the p-orbital band scatter into the final state of one atom in the n=0 (1s) band and another in the n=2 orbital (2s, 1d) band, where n represents the principle (energy level) quantum number and the states of the harmonic oscillator are labeled in the Landau-Lifshitz notation [24]. For a related model, Isacsson and Girvin [20] have studied the decaying rate and estimated that the lifetime is about 10–100 times longer than the time scale of tunneling in an optical lattice. However, such a lifetime can be still short to achieve condensation and perform experimental detection. In the following, we propose a new mechanism that should suppress the above decaying process and thus extend the lifetime.

III. ENERGY BLOCKING OF THE p-ORBITAL DECAY

We propose a deep fermion optical lattice on top of a relatively shallow optical lattice for bosons, such that the characteristic lattice well frequencies are very different (ω_h $\ll \omega_f$). Consider loading a fermion density around $n^f \approx 1$ (that is, one fermion per site). Now one tunes a Feshbach resonance between the boson and fermion [25,26] to set the interspecies interaction strength in energy scale between $\hbar \omega_b$ and $\hbar\omega_f$. In this case, the fermions fill up the s band completely, so essentially behaving as an band insulator whose dynamical effect on bosons becomes exponentially suppressed by the band energy gap. The lowest-s-orbital wave function is approximately a Gaussian peaked at the center of the lattice well. The role of fermions then can be thought as providing a repulsive central potential barrier, in addition to the optical lattice potential, for bosons on the same lattice site. As a result, all energy bands are shifted up significantly (including s and p of course) by the Feshbach interaction with the s-orbital fermion. Because the overlap integrals are different as shown in Fig. 1, the energy shifts are different in magnitude for different orbital states (Fig. 2).

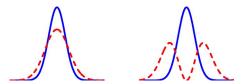


FIG. 1. (Color online) The overlap between s and p density clouds (wave functions squared) is smaller than between two s clouds.

The lowest orbit for a single particle in a single site must be nodeless; it is actually not possible to increase the s-state energy higher than the p-state energy. However, the gap Δ_{sp} between (n=0) s and (n=1) p can be significantly reduced to very small by a sufficiently strong interspecies Feshbach resonance, as illustrated in Fig. 2. In Appendix A 2, we give an estimate of the interaction strength needed. On the other hand, the splittings between the 1p state and states in the n=2 level (2s and 1d) should not change much because the wave functions of the latter all are spatially more extended than the 1s state. In summary, the lowest two Bloch bands (s-p) are close in energy while all other Bloch bands $(n \ge 2)$ have energy far above the first excited p-orbital band (in the energy scale of Δ_{sp}). The low-energy quantum theory of the system effectively reduces to a two-band problem.

The lattice gas under study is also assumed to be in the tight-binding limit such that the tunneling amplitude is smaller than Δ_{sp} , so much smaller than the band-level splitting between the p and all other higher bands (i.e., $t_{\parallel} \ll \Delta_{sp} \ll \hbar \omega_b$). Any elastic scattering process that scatters atoms out of the p-orbital band must conserve the total energy. Under the proper condition described above, the decay rate of the p-orbital Bose gas must be suppressed by the energy conservation law: any two atoms initially in the (n=1) p-orbital band cannot scatter out of the band by the two-body scattering process. (Of course, the scattering within the three subbands of p orbits are allowed.) This idea is one of our main results (see Appendix A for technical detail).

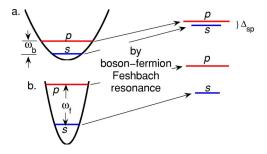
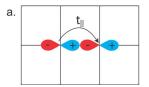


FIG. 2. (Color online) Energy-band shift due to Feshbach resonance between bosons and fermions. (a) The bosonic 1s band is moved close to the 1p band while the 2s and 1d bands (not shown) are both pushed higher. (b) The fermions fill up their own lowest s band as an band insulator. The relative shift of the fermionic band energy is less significant than that of the bosonic case, for ω_f can be made far larger than both ω_b and the (Feshbach tunable) energy shift.



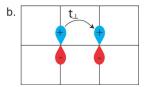


FIG. 3. (Color online) Anisotropic hopping matrix elements of p-orbital bosons on a cubic lattice. The longitudinal t_{\parallel} is in general far greater than t_{\perp} because the overlap integral for the latter is exponentially suppressed. The " \pm " symbols indicate the sign of two lobes of p-orbital wave function.

IV. LATTICE GAS OF p-ORBITAL BOSONS

The quantum theory of bosonic atoms prepared in the p-orbital state is effectively described by a p-band Bose-Hubbard model. A standard derivation (see Appendix B) gives the Hamiltonian

$$H = \sum_{\mathbf{r}\mu\nu} \left[t_{\parallel} \delta_{\mu\nu} - t_{\perp} (1 - \delta_{\mu\nu}) \right] (b_{\mu,\mathbf{r}+a\mathbf{e}_{\nu}}^{\dagger} b_{\mu\mathbf{r}} + \text{H.c.})$$
$$+ \frac{1}{2} U \sum_{\mathbf{r}} \left[n_{\mathbf{r}}^{2} - \frac{1}{3} \mathbf{L}_{\mathbf{r}}^{2} \right], \tag{1}$$

where a is lattice constant. Here, $b_{\mu \mathbf{r}}$, $b_{\mu \mathbf{r}}^{\dagger}$ are annihilation and creation operators for bosons in lattice site \mathbf{r} and orbital state p_{μ} (index label $\mu \nu = x, y, z$); n and \mathbf{L} are the boson density and angular momentum operators $n_{\mathbf{r}} = \Sigma_{\mu} b_{\mu \mathbf{r}}^{\dagger} b_{\mu \mathbf{r}}$ and $L_{\mu \mathbf{r}} = -i \Sigma_{\nu \lambda} \epsilon_{\mu \nu \lambda} b_{\nu \mathbf{r}}^{\dagger} b_{\lambda \mathbf{r}}$. This model is invariant under U(1) phase transformation, cubic lattice rotations, and time-reversal transformation.

The model is determined by the following parameters: t_{\parallel} and t_{\perp} are the nearest-neighbor hopping matrix elements in longitudinal and transverse directions, respectively, with respect to p-orbital orientation, and U is the on-site (repulsive) interaction due to the intrinsic (nonresonant) s-wave scattering between two bosons. In quantum chemistry, $t_{\parallel,\perp}$ are named the $\sigma(\pi)$ bond, respectively. Their precise definition is given in the Appendixes. By definition of the Hamiltonian, both t_{\parallel} and t_{\perp} are positive; note that $t_{\parallel} \gg t_{\perp}$ for the tunneling overlap is sensitive to orientation (Fig. 3).

The quantum physics of p-orbital bosons seems to have never been studied before except very recently by Isacsson and Girvin [20] in a different, interesting limit in which the transverse tunneling t_{\perp} is completely suppressed. Different from ours in symmetry and ordering, their model had infinite and subextensive (local) gauge symmetries and columnar orderings. Another difference is that it is not obvious whether their on-site interaction were SO(3) invariant.

The interaction in the lattice Hamiltonian (1) is *ferro-orbital* (U>0), suggesting that the bosons at the same site prefer to occupy the same orbital-polarized state carrying maximal angular momentum. This is analogous to the Hund's rule for electrons to fill in a degenerate atomic energy shell which favors a spin-polarized configuration. Next, we shall show that the ferro-orbital interaction, together with the p-band hopping, gives rise to an orbital ordered BEC.

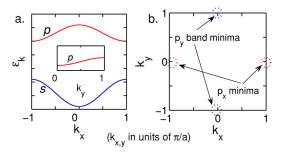


FIG. 4. (Color online) Illustration of p-band dispersions. (a) The energy dispersion of the p_x orbital band (as an example) on the k_x axis in the first Brillouin zone, in comparison with the s band. Inset: its dispersion along the line $\left(\frac{\pi}{a}, -\frac{\pi}{a}, 0\right) - \left(\frac{\pi}{a}, \frac{\pi}{a}, 0\right)$; the energy zero line is shifted arbitrarily for display. Note that the s and p bands have different locations for minimum energy. The band gap between the two levels is tuned small by the Feshbach resonance. (b) The p-band minima in the $k_x - k_y$ plane (the p_z 's minima are not shown but can be obtained by rotating 90° out of the plane). Orbital BEC should occur at a subset of the minima, spontaneously breaking the lattice translational and (orbital) rotational symmetry, in addition to the U(1).

V. ORBITAL BOSE-EINSTEIN CONDENSATION

A weakly interacting Bose gas is expected to undergo BEC, becoming superfluid at low temperatures. In the optical lattice, such a state has been firmly established, both experimentally and theoretically, for bosonic atoms occupying the s band (the widely studied Bose-Hubbard model). In our p-band model when the interaction is weak and repulsive $(0 < U \le t_{\parallel})$, the noninteracting term of the Hamiltonian dominates. The p-band bosons have the energy dispersion $\epsilon_{\mu \mathbf{k}} = 2 \Sigma_{\nu} [t_{\parallel} \delta_{\mu \nu} - t_{\perp} (1 - \delta_{\mu \nu})] \cos(k_{\nu} a)$, where μ , ν label the three subbands and a is the lattice constant.

There are two new aspects of the p-orbital bosons. The first is that BEC takes place at nonzero momenta. While the paradigm of BEC should occur at zero momentum, there is no real reason that has to be so. Only the lowest-energy state matters. The p-band energy dispersion shows an *exceptional* and remarkable case in which the lowest-energy state of boson happens to be at finite momenta \mathbf{Q}_{μ} , defined as

$$\mathbf{Q}_x = \left(\frac{\pi}{a}, 0, 0\right), \quad \mathbf{Q}_y = \left(0, \frac{\pi}{a}, 0\right), \quad \mathbf{Q}_z = \left(0, 0, \frac{\pi}{a}\right), \quad (2)$$

for the respective p-orbital states (Fig. 4). Note that $\pm \mathbf{Q}_{\mu}$ are identified by a reciprocal lattice vector, $2\mathbf{Q}_{\mu} = 0 \pmod{2\pi/a}$. The condensate at momentum $+\mathbf{Q}_{\mu}$ is essentially equivalent to that at $-\mathbf{Q}_{\mu}$ on the lattice. Therefore, the sum of atoms over all modes does not show any net current flow in any direction. This feature is important for a possible experimental test of the state that we shall elaborate below.

The second aspect is that the orbital degeneracy of p-band bosons opens possibilities of novel orbital physics. Orbital ordering, typically involving d-orbital (fermionic) electrons that are argued to be essential to understanding a class of strongly correlated transition-metal oxides, has become a topical subject in condensed-matter physics [21]. In our p-band model, condensing into any of these momenta Q_{μ} or their linear superpositions equally minimizes the total kinetic

energy. It thus provides a first bosonic version of such kind from atomic physics. Being ferro-orbital, the interaction in the Hamiltonian will be shown later to favor a condensate of angular momentum ordering, to have $\langle \mathbf{L}_{\mathbf{r}}^2 \rangle \neq 0$.

Keeping the above aspects in mind, we seek a condensate described by the following order parameter of total six real variables:

$$\begin{pmatrix} \langle b_{x\mathbf{k}=\mathbf{Q}_{x}} \rangle \\ \langle b_{y\mathbf{k}=\mathbf{Q}_{y}} \rangle \\ \langle b_{z\mathbf{k}=\mathbf{Q}_{z}} \rangle \end{pmatrix} = \rho e^{i\varphi - i\mathbf{T} \cdot \theta} \begin{pmatrix} \cos \chi \\ i \sin \chi \\ 0 \end{pmatrix}, \tag{3}$$

with $\mathbf{T} = (T_x, T_y, T_z)$ the generators of SO (3) orbital rotation in the following matrix representation (an adjoint 3 for the group theory experts) defined by its elements: $[T_\mu]_{\nu\lambda} = -i\epsilon_{\mu\nu\lambda}$, $\mu, \nu, \lambda = x, y, z$. Such a parametrization manifests symmetry: φ is the overall phase of the U(1) symmetry; the three angle variables $\boldsymbol{\theta} = (\theta_x, \theta_y, \theta_z)$ are the orbital rotation of SO(3) and χ changes sign under time reversal; ρ is the modulus field, fixed by the total boson density in the condensate n_0^b through $\rho = \sqrt{\nu} n_0^b$ where ν is the 3D lattice volume in the units of a^3 (so ν dimensionless).

We now proceed to calculate the mean field interaction energy. While the full Hamiltonian only has cubic lattice symmetry, the interaction term, being on site, enjoys, however, a continuous SO(3) rotation invariance. Therefore, the symmetry dictates that the mean value of the interaction term be independent of φ and θ . [The former is due to the exact U(1).] This argument reduces our calculation essentially to a problem for a single-variable order parameter: namely, χ . Then, a straightforward evaluation of the mean value of the interaction energy determines

$$\langle H_{U \text{ term}} \rangle = \frac{1}{2} \mathcal{V} U n_0^{b^2} \left[1 - \frac{1}{3} \sin^2(2\chi) \right].$$

The interaction energy is minimized at $\chi = \chi_{\pm} \equiv \pm \frac{\pi}{4}$.

The two minima $\chi = \chi_{\pm}$ are degenerate and discrete, reflecting the time-reversal symmetry. Of course, shifting the value of χ_{\pm} by π gives other minima of the same energy, but the π shift can be absorbed away by an overall U(1) phase adjustment or an orbital rotation. The order parameter points to one of the two discrete minima, spontaneously breaking the time-reversal symmetry. The resultant quantum state is an axial superfluid having a macroscopic angular momentum ordering. The order parameter is then found to be (say for $\chi = \chi_{+} = +\frac{\pi}{4}$)

$$\begin{pmatrix} \langle b_{x\mathbf{k}=\mathbf{Q}_x} \rangle \\ \langle b_{y\mathbf{k}=\mathbf{Q}_y} \rangle \\ \langle b_{z\mathbf{k}=\mathbf{Q}_z} \rangle \end{pmatrix} = \sqrt{\frac{\mathcal{V}n_0^b}{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \tag{4}$$

with a degenerate manifold characterized by phase φ and rotational angles θ . This is our *p*-orbital BEC (*p*-OBEC). It breaks the U(1) phase, lattice translation, orbital SO(3) rotation and time-reversal symmetries. Quantum or thermal fluctuations, which will be studied in the future, are expected to break the SO(3) rotational symmetry and align the orbital condensate to specific lattice directions.

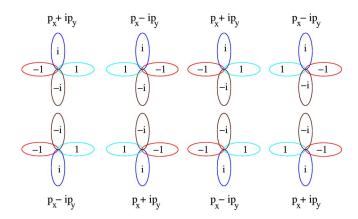


FIG. 5. (Color online) The real-space configuration of the TSOC state, which exhibits a staggered and uniform orbital current pattern in the *xy* plane and along the *z* axis, respectively.

VI. STAGGERED ORBITAL CURRENT

The p-OBEC contains one novel feature that is absent in the conventional BEC. To illustrate this, we assume that the lattice has a small anisotropy such that the state is pinned to the xy plane—i.e., the $p_x \pm ip_y$ order (see the phase diagram in Appendix C). The novel feature is contained in the structure factor of the boson number and angular momentum operators. Taking, for example, the state of $\chi = \chi_+ = \frac{\pi}{4}$, we found $\langle \mathbf{L_q} \rangle = (0, 0, n_0^b \delta_{\mathbf{q}, \mathbf{Q}_v + \mathbf{Q}_v})$. The momentum dependence of the angular momentum operator reveals that the p-OBEC is also an orbital current wave, in analogy with a commensurate spin-density-wave order in antiferromagnets. In real space, the order has the staggering pattern: $\langle L_{xr} \rangle = \langle L_{vr} \rangle = 0$, $\langle L_{zr} \rangle$ $=n_0^b(-)^{(x+y)/a}$. We shall call it transversely staggered orbital current (TSOC) for the direction of L_z alternates only in the x,y directions. The reader should bear in mind that at the mean-field level the direction of orbital ordering is arbitrary for a fully SO(3)-invariant interaction. In real experiments, the presence of a symmetry-breaking perturbation, such as a weak anisotropy in lattice potentials we assumed or the effect of quantum fluctuations is expected to pin down the direction.

We next provide an explanation for the appearance of TSOC in real space (Fig. 5). The interaction favors a maximum angular momentum at each site. So the orbit configuration on each site is $p_x \pm ip_y$, corresponding to angular momentum quanta $\pm\hbar$ per atom. On the other hand, the longitudinal and transverse hopping amplitudes are of opposite sign. In order to maximally facilitate the intersite hopping, the phases of $p_{x,y}$ orbits should be staggered in the longitudinal direction and uniform in the transverse directions. As a result, $\langle L_{zr} \rangle$ or the orbital current exhibits a staggered (uniform) pattern in the x-y (z) directions. This state bears some similarity to its fermionic counterpart of the orbital antiferromagnetism or d-density wave (DDW) [27] proposed for the high-temperature cuprates. A major difference is that the DDW current flows on bonds around each plaquette with staggered magnetic moments through lattice whereas the current here circulates inside each site.

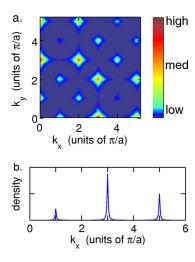


FIG. 6. (Color online) Prediction of density of atoms for timeof-flight experiment. (a) Density integrated over the z axis is shown in a quarter of $k_x - k_y$ momentum plane, with other quarters obtained by reflection symmetry. (b) Density shown along the k_x axis. Assuming a free expansion, the atom density at distance \mathbf{r} is $\langle n^b(\mathbf{r}) \rangle_{\tau} \propto |\phi_{p_u}^b(\mathbf{k})|^2 \delta^3(\mathbf{k} - \mathbf{G} - \mathbf{Q}_x) + |\phi_{p_u}^b(\mathbf{k})|^2 \delta^3(\mathbf{k} - \mathbf{G} - \mathbf{Q}_y)$ where \mathbf{k} $=m\mathbf{r}/\hbar\tau$, τ is the time of flight, and \mathbf{G} runs over all threedimensional reciprocal lattice vectors. The absence of peak at \mathbf{k} =0 distinguishes the p-OBEC from paradigmatic BEC. The highest peak is not necessarily the closest to zero-momentum origin, a unique feature of orbital BEC, depending on the size l_b of the bosonic Wannier function $\phi_u^b(\mathbf{r})$. Parameters are $l_b/a=0.1$; the δ function is replaced by a Lorentzian line for display.

VII. EXPERIMENTAL SIGNATURE

In a time-of-flight experiment which has been widely used to probe the momentum distribution of cold atoms, the p-OBEC will distinguish itself from a conventional s-BEC with unique structural factor. There are two new aspects (Fig. 6). The first is that the condensation peaks are not located at zero momentum, nor at any other momenta related to zero by a reciprocal lattice vector **G**. The second is that, unlike the s-wave case, the p-wave Wannier function superposes a nontrivial profile on the height of density peaks. As a result, the highest peaks are shifted from the origin—a standard for the s-wave peak—to the reciprocal lattice vectors whose magnitude is around $1/l_b$. In the following, we show the details of the calculations that led to the above predictions.

We consider the density distribution of the time-of-flight experiment, assuming ballistic expansion. In our p-orbital case, it can be written as

$$\langle n(\mathbf{r}) \rangle_{t} = \left(\frac{m}{\hbar t}\right)^{3} \sum_{\mu,\nu} \phi_{p_{\mu}}^{*}(\mathbf{k}) \phi_{p_{\nu}}(\mathbf{k}) \langle b_{\mu}^{\dagger}(\underline{\mathbf{k}}) b_{\nu}(\underline{\mathbf{k}}) \rangle, \tag{5}$$

where $\mu, \nu = x, y, z$; $\mathbf{k} = m\mathbf{r}/(\hbar t)$; $\phi_{p_{\mu}}(\mathbf{k})$ is the Fourier transform of the *p*-orbital band Wannier function $\phi_{p_{\mu}}(\mathbf{r})$; and $\underline{\mathbf{k}}$ =k mod (primitive reciprocal lattice vectors). Taking into account that bosons condense into the p_x+ip_y orbital state spontaneously [according to Eq. (4)], we arrive at

$$\langle n(\mathbf{r}) \rangle_t \propto \sum_{\mathbf{G}} \{ |\phi_{p_x}(\mathbf{k})|^2 \delta^3(\mathbf{k} - \mathbf{Q}_x - \mathbf{G}) + |\phi_{p_y}(\mathbf{k})|^2 \times \delta^3(\mathbf{k} - \mathbf{Q}_y - \mathbf{G}) \}.$$
(6)

That means that the Bragg peaks are at $(\frac{(2m+1)\pi}{a}, \frac{2n\pi}{a}, \frac{2l\pi}{a})$ and $(\frac{2m\pi}{a}, \frac{(2n+1)\pi}{a}, \frac{2l\pi}{a})$ where m, n, l are integer numbers. The Fourier transform of the p-wave Wannier orbits ex-

hibits the following nontrivial form factor:

$$|\phi_{p_x}(\mathbf{k})|^2 = |\phi_1(k_x)\phi_0(k_y)\phi_0(k_z)|^2,$$

$$|\phi_1(k)|^2 \propto (kl_b)^2 e^{-(kl_b)^2/2},$$

$$|\phi_0(k)|^2 \propto e^{-(kl_b)^2/2},$$
(7

where $\phi_{0,1}$ refer to the ground and first excited states of the one-dimensional harmonic oscillator, respectively, and l_b is the oscillator length of the boson optical lattice potential. As a result, unlike the conventional s-orbital case where the highest weight is located at the origin of the reciprocal lattice with a distribution width about $1/l_b$, the p-orbital case has the highest weight shifted from the origin to the reciprocal lattice vectors around $1/l_b$. In Fig. 6, where we used the parameter $1/l_b = \frac{10}{a} \approx \frac{3\pi}{a}$, the highest intensity thus appears at the second Bragg peak.

VIII. CONCLUSION AND DISCUSSION

In conclusion, we have proposed a new state of matter in which p-orbital bosonic atoms condense at separate nonzero momenta according to orbital orientations, defying the zeromomentum hallmark characteristic of all standard Bose-Einstein condensates. This new state is a prediction for a p-orbital Bose gas on lattice. We have shown how bosons, in Feshbach resonance with fermions, can be effectively blocked from occupying the s band by the energy conservation. Our idea may be generalizable to a mixture of two species of bosons. Realizing this new state (p-OBEC) will change the standard way of thinking BEC as normally attached to zero momentum.

The topic of ultracold atomic gases has been flourishing at the interface between atomic and condensed-matter physics. The latest progress in Feshbach resonance and optical lattice has further extended its scope of interest. One current focus in correlated quantum-condensed matter is the spontaneous time-reversal symmetry-breaking ground states-for example, the d-density wave state [27] proposed as a competing order for the pseudogap phase of the high- T_c superconductivity and the incommensurate staggered orbital current phase suggested as the mechanism for the hidden-order transition in the heavy-fermion system URu₂Si₂ [28]. Unfortunately, experimental observation of these states so far remains elusive and controversial. The p-OBEC state we proposed here is perhaps the first bosonic example of this kind from ultracold atomic gases. The extraordinary controllability of the atomic system, widely recognized by far, opens up the possibility of observing this kind of novel states for the first time.

Note added. Upon the completion of this manuscript, there appeared an independent work [29] that also proposes a *p*-orbital BEC based on a related but different mechanism.

ACKNOWLEDGMENT

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APPENDIX A: THE MICROSCOPIC MODEL FOR A BOSE-FERMI MIXTURE

Our model system is a gas of two species of atoms, one being bosonic and another fermionic, confined in two overlapping sublattices with separate potential heights. The Hamiltonian is

$$H = \int d^{3}\mathbf{x} \left\{ \sum_{\alpha=b,f} \psi_{\alpha}^{\dagger} \left[-\frac{\nabla^{2}}{2m_{\alpha}} + V_{\alpha}(\mathbf{x}) \right] \psi_{\alpha} + g_{\text{res}} \psi_{f}^{\dagger} \psi_{b}^{\dagger} \psi_{b} \psi_{f} \right.$$
$$\left. + g \psi_{b}^{\dagger} \psi_{b}^{\dagger} \psi_{b} \psi_{b} \right\}, \tag{A1}$$

where the indexes $\alpha = b$ and f label the boson and fermion species, respectively, $g_{\rm res}$ is the interspecies interaction tuned by a Feshbach resonance, and g is a weak repulsive interaction between bosons themselves. The (single-component) fermions do not interact between themselves at short range. $V_{b,f}(\mathbf{x})$ are the 3D optical lattice potentials constructed by counterpropagating laser beams. We assume

$$V_{\alpha}(\mathbf{x}) = V_{\alpha 0} \sum_{\mu=1}^{3} \sin^{2}(k_{L}x_{\mu}), \quad \alpha = b, f,$$
 (A2)

with k_L the wave vector of the light. The recoil energy for each species is $E_R^\alpha = \hbar^2 k_L^2 / (2m_\alpha)$, assumed different between boson and fermion for different masses. In the presence of such periodic potentials, the boson and fermion operators $\psi_\alpha(\mathbf{x})$ can be expanded on the basis of the Wannier functions $\phi_\mathbf{n}^\alpha(\mathbf{x})$, with \mathbf{n} the band index. Including the lowest- and first-excited Bloch bands (s-wave and p_μ -wave bands), we write

$$\psi_b(\mathbf{x}) = \sum_{\mathbf{r}} \left[b_{s\mathbf{r}} \phi_s^b(\mathbf{x} - \mathbf{r}) + \sum_{\mu} b_{\mu \mathbf{r}} \phi_{p_{\mu}}^b(\mathbf{x} - \mathbf{r}) \right], \quad (A3)$$

$$\psi_f(\mathbf{x}) = \sum_{\mathbf{r}} \left[f_{s\mathbf{r}} \phi_s^f(\mathbf{x} - \mathbf{r}) + \sum_{\mu} f_{\mu \mathbf{r}} \phi_{p_{\mu}}^f(\mathbf{x} - \mathbf{r}) \right], \quad (A4)$$

where $\mu=x,y,z$ label the three p-orbital bands. In the harmonic approximation, the s- and p-orbital states are directly given by the harmonic oscillator (HO) eigenfunctions $\phi_{\mathbf{n}}^{\alpha}(\mathbf{x}) = [\phi_{n_x}^{\alpha}(x)\phi_{n_y}^{\alpha}(y)\phi_{n_z}^{\alpha}(z)]_{\mathrm{HO}}$, with $\mathbf{n}=(000)$ for s-band and $\mathbf{n}=(100)$, (010) and (001) for p_x , p_y , and p_z , respectively, in Cartesian coordinates. The basis functions are kept separate between fermion and boson for they can have different lattice potential depths and atomic masses.

1. Hartree approximation of interspecies interaction

We examine possible configurations of the band occupation that may minimize energy. There are several: both fermions and bosons in the s band (ss), fermions in the s band and bosons in the p band (FsBp), and fermions in the p band and bosons in the s band (FpBs). The three configurations have different interspecies interaction energies per boson-fermion pair as follows:

$$I_{ss} = g_{\text{res}} \mathcal{I}_{(000);(000)}$$

$$= \frac{g_{\text{res}}}{[(l_b^2 + l_f^2)\pi]^{3/2}} \equiv W,$$
(A5)

$$I_{\text{FsBp}} = g_{\text{res}} \mathcal{I}_{(000);(100)} = \frac{W l_f^2}{l_b^2 + l_f^2} \equiv W_{\times},$$
 (A6)

$$I_{\text{FpBs}} = g_{\text{res}} \mathcal{I}_{(100);(000)} = \frac{W l_b^2}{l_b^2 + l_f^2} \equiv W_{\times}', \quad (A7)$$

where $\mathcal{I}_{\mathbf{n},\mathbf{n}'} \equiv \int d^3\mathbf{x} |\phi_{\mathbf{n}}^f(\mathbf{x})|^2 |\phi_{\mathbf{n}'}^b(\mathbf{x})|^2$ and $l_{b,f}$ are the harmonic oscillator lengths for boson and fermion, respectively, $l_{\alpha} \equiv \sqrt{\hbar/(m_{\alpha}\omega_{\alpha})}$.

2. Condition for band-gap closing

To further achieve a simpler effective model, let us examine the single-particle Hamiltonian at a single site—say, at \mathbf{r} —in turn for the boson and fermion. We shall show quantitatively how one species shifts the energy levels of another, through the Feshbach interaction. First, consider the effects of an s band of fermions on bosons. At Hartree approximation, the single-particle, on-site energy is shifted due to the interspecies (Feshbach) interaction with a term in the Hamiltonian

$$H_{\text{single site}}^{b} = \left(\frac{3}{2}\omega_{b} + Wn^{f}\right)b_{s\mathbf{r}}^{\dagger}b_{s\mathbf{r}} + \sum_{\mu} \left(\frac{5}{2}\omega_{b} + W_{\times}n^{f}\right)b_{\mu\mathbf{r}}^{\dagger}b_{\mu\mathbf{r}},$$
(A8)

where n^f is the number of fermions per site, assumed all in the s band. Likewise, an s band of bosons shift up both the s-and p-band energies of fermion, yielding a similar term in Hamiltonian

$$H_{\text{single site}}^f = H_{\text{single site}}^b [b \rightleftharpoons f; W_{\times} \to W_{\times}']$$
 (A9)

and n^b is the number of bosons per lattice site, all in the s. For $\omega_f \gg \omega_b$, the energy shift for the fermionic bands is small compared with the band energy spacing $\hbar \omega_f$; the s band remains lower than the p. The situation is opposite for boson in this Hartree treatment. The ordering of energies of the s and p bands, if one naively trusts the Hartree approximation, can be even reversed.

Here we provide a Hartree estimate for how strong the interspecies Feshbach resonance is needed to close the s-p-band gap for bosons. The condition for the effect can be met by requiring that the s-band Hartree energy be higher than that of the p,

$$\omega_b + W_{\times} n^f < W n^f, \tag{A10}$$

from Eq. (A8). This condition is satisfied when the Feshbach resonance scattering length $a_{\rm res}$, related to $g_{\rm res}$ by $g_{\rm res} = 2\pi a_{\rm res}(m_b + m_f)/(m_b m_f)$, is sufficient large such that

$$a_{\text{res}} > \frac{\sqrt{\pi}}{2} \frac{1}{n^f} \frac{m_f}{m_b + m_f} \left(\frac{l_b^2 + l_f^2}{l_b^2}\right)^{5/2} l_b \equiv a_{\text{res}}^{\text{min}}.$$
 (A11)

(The derivation implicitly assumed $n^f \leq 1$ to avoid higher band complication due to Pauli exclusion.) This condition can be achieved without tuning the scattering length $a_{\rm res}$ to very large via Feshbach resonance if the minimally required $a_{\rm res}$ is made sufficiently small. That can be done by tuning the depth of optical potentials to make an adequately small l_b and keep $l_f \leq l_b$ in the same time. As we will discuss next, our condition for band-gap closing can, in principle, avoid the three-body loss problem in the experiments by means of operating the system adequately far from the resonance point.

In the experiment of resonant atomic gases, there is always the issue of a finite lifetime. Near the Feshbach resonance, a weakly bound dimer relaxes into deep bound states after colliding with a third atom. The released binding energy transformed into the kinetic energy of atoms in the outgoing scattering channel that will escape from the trap. Such a process of three-body collisions determines the lifetime of the trapped gas. The relaxation rate is believed to be highest in the boson-boson resonance and lowest in the fermionfermion resonance, with the rate for the boson-fermion resonance in between 30 —though there is no explicit calculation for the boson-fermion resonance yet to the best of our knowledge. More relevantly, two recent experiments have observed the boson-fermion interspecies Feshbach resonances in the systems of ⁶Li-²³Na atoms [25] and ⁴⁰K-⁸⁷Rb atoms [26], respectively, which seem to be very stable. This is part of the reason that we are proposing a Bose-Fermi mixture as opposed to a generally less-stable single-statistics Bose gas. (Another important reason is, of course, that the fermion component of the mixture can be made be a band insulator with virtually no dynamical effects on bosons other than providing a central potential barrier; see the main text.)

On general grounds, we expect that the larger the detuning from the resonance is, the smaller the three-body loss rate should be, obeying some power-law suppression. In our model, the estimated scattering length between fermions and bosons is of the order of $l_b m_f / (m_b + m_f)$ (see above) to enable the effect of s-p-band-gap closing for bosons. It can be made sufficient small. For example, this can be as small as 50 bohr radius for a 23 Na- 6 Li mixture, taking lattice constant $a \approx 400$ nm and the 23 Na oscillator length $l_b \approx 0.1a$. That means that the system does not have to be operated close to resonance. This makes the relaxation lifetime practically infinitely long, so the three-body loss problem is experimentally avoidable.

Finally, in contact with the discussion of the energy blocking of the *p*-orbital decay in the main text, we do not require that the *s-p*-band gap Δ_{sp} be vanishing but just small compared with that between the *p* and higher bands. Therefore, the above quantitative evaluation of the resonance in-

teraction strength is but an estimate for the scale.

3. Is an equilibrium nodal Bose-Einstein condensate possible?

The mean-field Hartree argument would imply that when the boson-fermion interaction is tuned strong enough $(a_{\rm res} > a_{\rm res}^{\rm min})$, the p-orbital state has lower energy than the s (see Fig. 2). However, if all the effect of fermions on boson is replaced by a single-particle central potential barrier at every lattice site as in the Hartree approximation, the lowest orbit of the single-boson state must be nodeless (which is s-wave but likely extended) from simple quantum mechanics. The single-particle Hartree argument must be wrong in predicting the p orbital be a ground state. For a bosonic many-body system (such as 4 He liquid), a similar conclusion is expected, due to Feynman, who drew an analogy between a single particle and a many-body system and argued that the 4 He ground-state wave function be nodeless.

Can the p-orbital Bose-Einstein condensate be a true equilibrium (ground) state instead of a metastable state as we described so far? We believe the possibility is not completely ruled out by Feynman's argument. Let us explain it. Feynman did not specify the requirement of the form of the twobody interaction but a careful examination of his argument would show that the whole argument implicitly assumes a short-range interaction compared with the average interparticle distance. For a finite or long-range interaction, smoothing out the wave function will definitely lower the kinetic energy per each particle coordinate but at the same time will necessarily increase the interaction potential of all neighbor particles within the scope of the interaction range. In other words, the energy cost or saving is about the completion of one-particle kinetic energy versus many-particle interaction energy. When the interaction range is long enough, we conjecture that the many-body effect becomes dominant. Another way to think of our argument is that a long-range interaction has a strong momentum dependence after Fourier transformation. We can always think of a potential that is expandable about zero or some characteristic momentum. That corresponds to derivative terms of the real-space interaction potential. Once the two-body interaction potential explicitly involves derivative terms, Feynman's argument seems to fail.

A long-range interaction is not exotic for cold atoms. For atoms in a *narrow* Feshbach resonance, it is known that the effective interaction between two atoms can be longer than or comparable with the average interparticle distance [31]. Given the rapid advancement in the control of atomic gases, it seems not entirely impossible to realize an equilibrium, not just metastable, nodal Bose condensate in the future.

APPENDIX B: TIGHT-BINDING APPROXIMATION FOR THE p-BAND BOSE-HUBBARD MODEL

In this section, we use the tight-binding approximation to derive the general p-band Bose-Hubbard Hamiltonian where each lattice site is approximated as a three-dimensional anisotropic harmonic potential with frequencies $\omega_{b\mu}(\mu=x,y,z)$ in three directions, respectively.

The free boson Hamiltonian includes the hopping and onsite zero-point energies: i.e.,

$$H_0 = \sum_{\mathbf{r}\mu} t_{\mu;\nu} (b_{\mu,\mathbf{r}+a\mathbf{e}_{\nu}}^{\dagger} b_{\mu\mathbf{r}} + \text{H.c.}) + \sum_{\mathbf{r}\mu} \hbar \omega_{\mu} b_{\mu\mathbf{r}}^{\dagger} b_{\mu\mathbf{r}}, \quad (B1)$$

where the hopping amplitudes are determined by

$$t_{\mu;\nu} = \int d^3 \mathbf{x} \, \phi_{p_{\mu}}^b(\mathbf{x})^* \left[-\frac{\nabla^2}{2m_b} + V_b(\mathbf{x}) \right] \phi_{p_{\mu}}^b(\mathbf{x} + a\mathbf{e}_{\nu})$$
$$= t_{\parallel} \delta_{\mu\nu} - (1 - \delta_{\mu\nu}) t_{\perp}. \tag{B2}$$

In this definition, both t_{\parallel} and t_{\perp} are positive and $t_{\parallel} \gg t_{\perp}$ in general (Fig. 3). Here we have neglected the difference among the values of t_{\parallel} and t_{\perp} in the x,y,z directions because the major anisotropic effect comes from the on-site energy difference among $\omega_{x,y,z}$.

In momentum space, H_0 reads

$$H_{\text{hop}} = \sum_{\mathbf{k}\mu} \left(\epsilon_{\mu\mathbf{k}} + \hbar \omega_{\mu} \right) b_{\mu\mathbf{k}}^{\dagger} b_{\mu\mathbf{k}}, \tag{B3}$$

with the energy dispersion of boson $\epsilon_{\mu \mathbf{k}} = 2 \Sigma_{\nu} [t_{\parallel} \delta_{\mu \nu} - t_{\perp} (1 - \delta_{\mu \nu})] \cos(k_{\nu} a)$ (a is the lattice constant). The momentum representation of H_0 is useful in determining how the p-band bosons condense.

The short-range interaction between bosonic atoms in the original microscopic model gives rise to an on-site interaction energy between bosons in the p orbitals. It can be classified into three terms

$$H_{int1} = \frac{1}{2} \sum_{\mathbf{r},\mu} U_{\mu} n_{\mathbf{r}\mu} (n_{\mathbf{r}\mu} - 1),$$

$$H_{int2} = \sum_{\mathbf{r}, \mu \neq \nu} V_{\mu\nu} n_{\mathbf{r}\mu} n_{\mathbf{r}\nu},$$

$$H_{int3} = \frac{1}{2} \sum_{\mathbf{r}\mu \neq \nu} V_{\mu\nu} p_{\mathbf{r}\mu}^{\dagger} p_{\mathbf{r}\mu}^{\dagger} p_{\mathbf{r}\nu} p_{\mathbf{r}\nu}, \tag{B4}$$

with

$$U_{\mu} = g \int d^3 \mathbf{x} |\phi_{p_{\mu}}(\mathbf{x})|^4,$$

$$V_{\mu\nu} = g \int d^3 \mathbf{x} |\phi_{p_{\mu}}(\mathbf{x})|^2 |\phi_{p_{\nu}}(\mathbf{x})|^2.$$
 (B5)

By straightforward calculation, we obtain the following relations regardless of the anisotropy of the lattice potential:

$$U = U_x = U_y = U_z$$
, $V = V_{xy} = V_{yz} = V_{zx}$,

$$U = 3V = \frac{3g}{4(2\pi)^{3/2}l_x l_y l_z},$$
 (B6)

where $l_b = \sqrt{\frac{\hbar}{m\omega_b}}$ are the harmonic oscillator length.

As a result, the interaction part can still be reorganized as in Eq. (1) as

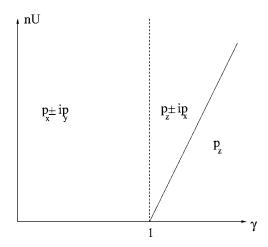


FIG. 7. Proposed phase diagram for a system of anisotropic lattice potentials, sketched as a function of the mean interaction energy nU and the anisotropic ratio $\gamma = \omega_{x,y}/\omega_z$.

$$H_{int} = \frac{U}{2} \sum_{\mathbf{r}} \left[n_{\mathbf{r}}^2 - \frac{1}{3} \mathbf{L}_{\mathbf{r}}^2 \right]. \tag{B7}$$

Note that H_{int} is surprisingly the same as that in the isotropic case of Eq. (1), even if the lattice potentials are anisotropic. After setting $\omega_{x,y,z} = \omega_b$, the general Hamiltonian in above reduces to Eq. (1) for the isotropic case.

APPENDIX C: THE CASE OF AN ANISOTROPIC LATTICE POTENTIAL

Let us consider the case of cylindrical symmetry—i.e., $\omega_x = \omega_y = \gamma \omega_z$. At $\gamma < 1$, particles condense into the $p_x(Q_x) \pm i p_y(Q_y)$ state to minimize both the kinetic and interaction energy as discussed in the main text. The $\gamma = 1$ point is subtle. Although the full Hamiltonian (because of the hopping term) does not possess the SO(3) symmetry, the condensation manifold recovers the SO(3) symmetry at the mean-field level. The quantum fluctuation effect is expected to break this SO(3) down to the cubic lattice symmetry.

At $\gamma > 1$, a quantum phase transition takes place from a time-reversal-invariant polar condensate to a time-reversal symmetry-broken TSOC state, as the boson density increases (see Fig. 7). Let us parametrize the condensate as

$$\begin{pmatrix} \langle b_{z\mathbf{k}=\mathbf{Q}_z} \rangle \\ \langle b_{y\mathbf{k}=\mathbf{Q}_z} \rangle \end{pmatrix} = \sqrt{n} \begin{pmatrix} \cos \chi \\ i \sin \chi \end{pmatrix}, \tag{C1}$$

where n is the boson density. Then the mean-field energy per unit volume is

$$E/\mathcal{V} = n(\omega_z \cos^2 \chi + \omega_x \sin^2 \chi) + \frac{Un^2}{2} \left(1 - \frac{1}{3} \sin^2 2\chi \right)$$
$$= n\bar{\omega} + \frac{U}{3}n^2 + \left\{ \frac{Un^2}{6} \cos^2 2\chi - \frac{n}{2}\Delta\omega \cos 2\chi \right\}, \quad (C2)$$

where $\bar{\omega} = \omega_z (1 + \gamma)/2$ and $\Delta \omega = (1 - \gamma)\omega_z$. Minimizing the energy, we find

$$\cos 2\chi = \begin{cases} \frac{3}{2} \frac{\Delta \omega}{nU} & \left(nU > \frac{3}{2} \Delta \omega \right), \\ 1 & \left(nU < \frac{3}{2} \Delta \omega \right). \end{cases}$$
 (C3)

When n is small, kinetic energy dominates over interaction. Therefore a polar condensate in $p_z(Q_z)$ is favorable. As n increases to become larger, the interaction part becomes more important, and thus the TSOC state appears. Again in the TSOC state, there is an SO(2) symmetry (of x-y-plane rotations) in the manifold of the mean-field ground state, $p_z\pm i(\cos\alpha p_x+\sin\alpha p_y)$, where α is an arbitrary azimuthal angle. Fluctuation effects are expected to break this symmetry down to the tetragonal symmetry.

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